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 included three scientific divisions and a large-scale guest program. The incorporation of a Seminar- and Workshop-Program within the guest 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 traditionally. 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. The scientific activities started on July 1st, 1993, in Stuttgart, lacking proper office space in Dresden, which was supplied by January 1994 thanks to the support of the TU Dresden. The TU Dresden, itself lacking office space, generously offered a temporary location for the institute in a barrack in the Bayreuther Straße, close to the university campus. 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 considerably broaden its research spectrum 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 began 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 took over the newly constructed main building, together with the three guest houses. The inauguration of the buildings was held during 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 professor position 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 bridging the field 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. Tolic-Norrelykke* (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 of a department head at the Physikalisch-Technische Bundesanstalt in Berlin in the fall of 2004.

2005-2006 • In 2005 *Dr. S. Kümmel* accepted a Professor position 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 Leibnitz 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 Professor positions at the University of Saarbrücken and the École normale Supérieure in Lyon.

2007-2008 • During that 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* has been 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. Laeuchli*. Recently *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.

The institute hosts approximately 50-100 long-term guest scientists at a given time, together with 1200-1500 short-term guests who annually participate in the workshop and seminar program. The new wing of the institute turned quickly into a new and vital focal point of meetings, poster sessions, discussions and collaborations.

The Board of Trustees has been supporting 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:

- The division *Condensed Matter* headed by *Prof. Moessner* studies the classical and quantum statistical mechanics of condensed matter.
- 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.

Furthermore, three research groups are broadening and strengthening the work of the corresponding divisions. Additional groups interpolate with their research between and add to the above listed research topics:

- 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 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 is operating 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. Tolic-Norrelykke is located at the MPI-CBG.

1.3 Workshop and Visitors Program

A central task of the institute is to conduct international *Workshops and Seminars* (p. 132), 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 advise to the (usually external) scientific coordinators on the various aspects of planning and conducting the corresponding event.
The *Visitors Program* (p. 123) offers research visits ranging from a few weeks to two years in duration. Guest scientists are using 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. 195).
Proposals for workshops and seminars, as well as applications for guest scientist positions, are evaluated by two different committees. Members of each committee include external scientists and scientists of the institute.
In order to further strengthen and structure the Visitors Program, mpi**pks** started in 2000 to annually award the *Martin Gutzwiller Fellowship* to an internationally recognized and experienced scientist. The awardees *Prof. M. S. Hussein* (Sao Paolo) 2007 and *Prof. J. M. R. Parrondo* (Madrid) 2008 have spent up to one academic year at mpi**pks** (p. 129).
The mpi**pks** also offers one *Distinguished PKS Postdoctoral fellowship* annually. It aims at excellent young researchers, shortly before accepting a tenure track position (p. 124).
In 2007 the institute launched *Advanced Study Groups* 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. The first *Advanced Study group* in 2007 on *Localizing Energy through Nonlinearity, Discreteness and Disorder* was headed by *Prof. S. Aubry*. In the following year 2008 we hosted already two *Advanced Study Groups*: one on *Time: Quantum and Statistical Mechanics Aspects* headed by *Prof. L. S. Schulman*, and a second one on *Quantum Aggregates* is reaching into the year 2009 under the leadership of *Prof. J. Briggs*.
The success of our workshop program 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 conduct workshops in Palma and Dresden, which focus on the theme of the joint program *Trends in Complex Systems*.

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. 177). 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. 181).

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 39 events during 2007-2008, 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 have been 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** is participating 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 were able to attract several young participants, who could join the scientific program of workshops while their children were nursed 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 work hours due to 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 and development 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 workshops for high school teachers, winter schools for high school students, and lectures at schools in order to spread the fascination of science as it happens.
Since 1999, mpi**pks** has been coordinating, together with the TU Dresden and the City of Dresden, the lecture series *Science in the City Hall*, aiming at a public interested in science. Well-known scientists are invited to give lectures for the broad public, which

are intended to popularize modern research (p. 180). 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 been participating in numerous activities, which are part of the full year 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. 181).

1.7 Research Networking

Local • The mpi**pks** finds itself in the midst of a rich research environment, formed by the TU Dresden and many other research institutes. An intensive scientific dialogue with the Physics Department of the TU Dresden is taking place, e.g., with regular joint seminars (*Quantum Dynamics* with Prof. Schmidt), 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 four Research Focus Programs of the DFG (p. 175). It is also participating in the SFB 463. 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* 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*.
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. 131).

1.8 Departments and Research Groups

Division: Condensed Matter
(Head: Prof. Dr. R. Moessner (since 10/07))

The collective behavior of condensed matter systems is the common theme of the research pursued by members of the division. Our research follows two closely interconnected tracks. Firstly, we seek to develop theories – as quantitative as possible – of phenomena observed in nature or in the laboratory, such as superconductivity or magnetism. Secondly, we aim to work towards a systematic understanding of the large variety of these phenomena.

The first category has included work on systems as varied as graphene, the new pnictide superconductors, frustrated magnets, cold atoms and micromagnets. An example of the latter is the study of phases of matter which are neither ordered nor disordered in the conventional sense of the framework based on local symmetry-breaking and order parameters. Current activities center on topological properties of such phases, as evidenced by entanglement entropies and captured by effective field theories. Indeed, the connection of effective low-energy descriptions of these phases with microscopic (lattice) models exhibiting them is one important aspect of our work.

A particular emphasis of the current research is the aim of making contact between fundamental questions – such as: what kinds of order are there – and experiment: how are new types of order manifested in the laboratory?

Research Topics

Magnetic monopoles in spin ice:
The low-temperature state of spin ice, a class of magnetic materials (including $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$) discovered in 1997, is highly unusual. It exhibits the 'residual entropy' predicted by Pauling for water ice, and its correlations are characteristic of a classical Coulomb spin liquid, a new type of magnetic phase with topological features. Perhaps the most remarkable manifestation of this new phase are its low-energy excitations: the magnetic dipoles of the spins fractionalise, which leads to the emergence of magnetic monopoles. Our publication establishing spin ice as the first fractionalised magnetic material in three dimensions, which has appeared on the cover of Nature, also provided a theory for the hitherto unexplained phase diagram of spin ice in a magnetic field in the crystallographic [111] direction, which turned out to be a field-drive liquid-gas transition of the Coulomb liquid formed by the magnetic monopoles.

A wavefunction-based theory of Bosonic lattice supersolids:
There has been sustained interest in using ultracold atoms confined in optical lattice potentials to realize strongly-correlated systems of interest to condensed matter physics. The recently discussed possibility that Helium has a supersolid phase has led, in this context, to a natural question: Can the lattice analog of this, namely a superfluid phase that simultaneously breaks lattice translation symmetry, be seen in such optical lattice experiments? Perhaps the best candidate for such a lattice supersolid persisting over a wide range of parameters is that observed numerically for strongly interacting bosons on the triangular lattice. We have developed a theory of a variational wavefunction which yields the behaviour of this supersolid state quantitatively. The trial wavefunction used is special in that (i) it implements the *hard* constraint imposed by the strong repulsive nearest-neighbour interactions without approximation and (ii) its properties can be evaluated exactly.

Graphene: relativistic Fermions in two dimensions
In 2005 experiments on graphene, a single layer of carbon atoms, were first reported. These exhibited exotic physical properties such as a universal minimum conductivity and an anomalous integer quantum Hall effect. These phenomena are due to the fact that the hexagonal lattice of graphene exhibits two Dirac points with a linear dispersion relation, which lead to a long-wavelength description in terms of massless Dirac Fermions. As part of an ongoing research effort, several aspects of the physics of

graphene have been studied by members of the group, including the effects of disorder, the response to external driving, and the transport properties of multilayer graphene.

Entanglement Skyrmions in multi-component quantum Hall systems:
Electrons moving in two dimensions, subject to a strong perpendicular magnetic field, exhibit a wide variety of unusual many-body phenomena. The most celebrated of these are the quantum Hall effects, after which the field of their study is named. These effects appear when the number of flux quanta is commensurate with the number of electrons in the system. Near commensurability, the elementary excitations can be non-trivial charged spin textures known as Skyrmions. We have studied the properties of Skyrmions in systems with several internal degrees of freedom (such as graphene or bilayer systems). We have found that, even in the presence of anisotropies, there are families of degenerate Skyrmions which differ in the degree to which the different internal degrees of freedom are entangled. We discovered that there exists a unique 'most entangled' topological excitation, which we call the 'entanglement Skyrmion'.

Perspectives

The division is currently taking shape, being built up since its inception in 2007. After the arrival in Dresden of Roderich Moessner from Oxford in December 2007, Andreas Läuchli followed from Lausanne as the first group leader in September 2008. In February 2009, Stefan Kirchner from Houston joins to lead a group attached to both mpi**pks** and the neighboring MPI for the Chemical Physics of Solids.

The field of new and unconventional forms of order is developing rapidly and offers a number of unchartered research direction. So far, most work has focused on static properties with little work on dynamical phenomena. For example, in the case of spin ice, one immediate question is how the presence of pointlike defects (magnetic monopoles) in a three-dimensional magnet shows up in dynamics, both in and out of equilibrium. In particular, how the presence of topological sectors slows down response times is a natural question to ask.

In a quantum setting, the best-studied experimental system exhibiting topological order is provided by the fractional quantum Hall states. More generally, quantum Hall systems are a good place to look for the physics of entanglement. One aim of future research is to carry out model calculations to find under what circumstances entanglement for multi-component quantum Hall systems will arise. Further, since connections between topological order and entanglement measures have emerged in the recent literature, we aim to understand and utilize these connections employing large-scale exact diagonalization of finite-size quantum Hall systems on torus geometries. These calculations seek to explore and exploit novel connections between entanglement measures and topological order, and to develop these connections into applicable techniques for investigating topological properties of quantum Hall states.

A promising, quite distinct, direction for future research lies in the field of quantum information theory. There has been recent key progress in particular in the study of adiabatic quantum computing, where computational problems are solved by following the evolution of the quantum ground state of a time-dependent Hamiltonian. Conceptual similarities to the field of quantum systems with competing interactions

provide a natural entry point to this field. Over the past 15 years, there has been a productive interchange ideas between statistical mechanics of glassy systems and combinatorial/computational problems. We plan to develop a similar programme for the quantum realm.

Cooperations

- Europe
  - Lyon, École Normale Supérieure: collaboration with group of Peter Holdsworth on topological phase transitions
  - Orsay, Université Paris VI (Jussieu) and Paris XI: collaboration with Benoit Douçot and Mark Goerbig on quantum Hall physics
  - Oxford, Oxford University: collaboration with group of John Chalker on disorder in topological phases
  - Toulouse, Université Paul Sabatier: collaboration with group of Didier Poilblanc on constrained lattice models
- Overseas
  - Baltimore, Johns Hopkins University: collaboration with group of Oleg Tchernyshyov on frustrated magnetism
  - Mumbai, Tata Institute for Fundamental Research: collaboration with group of Kedar Damle on supersolidity and frustrated magnetism
  - Princeton, Princeton University: collaboration with group of Shivaji Sondhi on novel phases in condensed matter
- Experimental groups
  - Regular exchanges with experimental groups such as that of Philippe Mendels, Orsay; Alan Tennant at Hahn-Meitner in Berlin; Santiago Grigera at St. Andrew's; Peter Schiffer at Penn State; and Steve Bramwell at the London Centre for Nanotechnology and University College London.

Research Group: New States of Quantum Matter
(Head: Dr. A. Läuchli (since 9/08))

The research group "New states of quantum matter" started its activity at the mpi**pks** in September 2008. Our goal 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 first months at mpi**pks** we worked particularly on:

Dynamical spin correlations of prototypical quantum magnets:

(a) The square lattice Heisenberg model is known to have an antiferromagnetically ordered ground state in the absence of a magnetic field, and the excitation spectrum consists of stable spin wave. Advanced theoretical and experimental work over the last 15 years has beautifully confirmed this semiclassical picture even for the quantum case of spin $S = 1/2$, and only subtle corrections to spin wave theory were revealed at specific wave vectors in the Brillouin zone. With the recent synthesis of new square lattice materials with small exchange constants J, these systems can also be studied in a uniform magnetic field up to the saturation field. In our numerical work we studied the static and dynamical properties in great detail and discovered an unanticipated strong field dependence of the excitation energies for wave vectors along the magnetic zone boundary. Furthermore we found numerical evidence for the decay of the elementary spin wave excitations at very high magnetic fields, confirming an earlier theoretical proposal.

(b) The kagome antiferromagnet is a prototypical model system among highly frustrated quantum magnets. Despite a long history of attempts the nature of the ground state of the system is still not resolved. There are however a number of materials available which are believed to realize a quantum antiferromagnet on the kagome lattice to some extent. Unbiased theoretical predictions for the dynamical response in inelastic neutron scattering and Raman scattering are basically absent. In our study we determined the dynamical response functions of the $S = 1/2$ system based on large-scale exact diagonalizations combined with a continued fraction technique. The dynamical spin structure factor has important spectral weight predominantly along the boundary of the extended Brillouin zone and energy scans reveal broad response extending over a range of $2 \sim 3J$ concomitant with pronounced intensity at lowest available energies. Dispersive features are largely absent. Dynamical singlet correlations – which are relevant for inelastic light probes – reveal a similar broad response, with a high intensity at low frequencies $\omega/J \lesssim 0.2J$. These low energy singlet excitations do however not seem to favor a specific valence bond crystal, but instead spread over many symmetry allowed eigenstates.

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.
  - Dortmund, TU Dortmund, collaboration with the group of K.P. Schmidt on magnetic systems close to the Mott transition.
  - Ithaca (USA), Cornell University: collaboration with C.L. Henley on correlation density matrices.
- Experimental groups
  - Collaborations with neutron scattering groups at the University College London (Ch. Rüegg) and the ILL Grenoble (M. Enderle) on the modelling and interpretation of inelastic neutron scattering experiments performed on low-dimensional quantum magnets.

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

The department *Finite Systems* studies the dynamics of finite microscopic systems coupled to different environments. One class of environment consists of similar systems as the atom or molecule under consideration (e.g., clusters, quantum aggregates, interaction between ultracold Rydberg atoms). Strong light pulses form another quite universal type of environment. Finally, we are interested in noise, which is a more abstract form of environment and plays a prominent role in research at mpi**pks** also outside the *Finite Systems* department.

With two group leaders (Profs. Andreas Becker and Buchleitner) having left, the department has won two new group leaders. The fundamental and formal mathematical aspects of finite systems coupled to an environment and in particular the phenomenon of decoherence will be investigated by *Klaus Hornberger* and his newly established research group. The effect of an ultracold environment on atoms is in the center 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). Although experimentally quite far apart, as a theory group we can view both kinds of pulses on the same footing which leads to synergetic effects.

Research topics

Basic coupling mechanisms of short XUV pulses to matter Almost simultaneous absorption of many photons by many bound electrons has not been considered so far since it was experimentally infeasible. This situation has changed with the new light sources. We explore non-equilibrium multi-electron dynamics triggered by intense subfemtosecond light absorption.

The progress in the use of attosecond pulses depends strongly on an understanding of their effect on bound and excited electron dynamics with a simplified quasi-analytical approach. Based on semi-classical approximations of these dynamics, we are working towards finding such a description.

Electron 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 ("photoelectrons"), 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.

We have found fast electron migration towards the formation of an extremely efficiently absorbing non-isotropic electron plasma as a consequence of irradiation with an intense 800nm pulse in composite clusters. There, the stronger absorbing material in the center serves as a seed for the plasma formation. A similar mechanism may also explain enhanced absorption by clusters "polluted" by a small percentage of different material.

Time-resolved electron transport Only very 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. Understanding the excitation and relaxation induced by external driving voltages will allow us to propose scenarios of controlled manipulation of the quantum dot states with implications for quantum computing.

Ultracold Rydberg dynamics With the experimental proof of the existence of long range ultracold molecules, consisting of a ground state atom and a Rydberg atom, a new regime for molecular binding has become reality. Several ground state atoms may undergo binding with a Rydberg atom to form a Rydberg oligomer. This kind of "Rydberg chemistry" has intricate features not known from standard molecular physics. We share the interest in ultracold Rydberg dynamics with *Dr. T. Pohl's* group.

Ultracold Rydberg atoms in a trap 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 could be achieved in the ultracold realization. Hence, we study the effect of excitonic excitation on the motion of ultracold atoms in a trap.

Quantum aggregates Self-organized aggregates of dye molecules have become remarkably versatile quantum systems with applications in photography, opto-electronics, solar cells, photo-biology and as supra-molecular fibers. In addition to these traditional aggregates in recent years new types of quantum aggregate have emerged: e.g. assemblies of ultra-cold Rydberg atoms, "molecules" and "crystals" composed of quantum dots or arrays of nano-size metallic particles. On electronic excitation, the (transition) dipole-dipole interaction between the individual monomers leads to migration of electronic excitation through the aggregate.

However, this coherent energy transfer is strongly influenced by coupling to nuclear degrees of freedom and interactions with the surrounding medium. To study the impact of a complex, structured environment we have developed a new approach, based on a non-Markovian stochastic Schrödinger equation, that allows to treat uniformly the transition from coherent to incoherent exciton motion. The approach is also well suited to simulate femtosecond two-dimensional electronic spectroscopy. This work was done in collaboration with Prof. Strunz (TU Dresden).

Noise in quantum systems Intense noise, generated by shaped laser pulses ("chaotic light") offers a new experimental way to couple a small system (atom/molecule) in a controlled way to an environment. We have explored the simplest atom and molecules in order to identify the fundamental mechanisms which govern this coupling see, p.66. Part of this work is done in close collaboration with Frank Großmann (TU Dresden).

Perspectives

In the context of ultrafast dynamics we will concentrate on transient and non-equilibrium behavior of dissipative, or more generally, incoherent processes of complex systems. Here, subfemtosecond laser pulses allow novel insight and help to pave the way towards a better understanding of non-equilibrium dynamics.

We will continue to develop an understanding of multi-electron dynamics under X-ray pulses and use it to propose suitable control of Coulomb explosion dynamics in order to make single-molecules feasible. In the long run we will need to improve our theoretical framework for cluster dynamics since the short wavelength of the light requires a better description of the bound state dynamics. One option we investigate is the concept of electron force fields (eFF).

Ultracold Rydberg physics is gaining momentum and spreads well beyond traditional atomic physics. In response to this development *Thomas Pohl* will contribute to this field with his research group in our department in the future. Work in the *Research group Finite Systems* will concentrate on the possibilities of Rydberg chemistry as discussed above and on mechanisms how to control the motion of atoms through excitons benefitting from expertise gained with quantum aggregates.

Cooperations

With experimental groups
We have been in close contact with the groups of Prof. Weidemüller (Heidelberg) regarding ultracold Rydberg atoms, with Prof. Killian (Rice, USA) regarding ultracold plasmas and with Prof. Stienkemeier (Freiburg) regarding molecular aggregates in helium nano-droplets.

New collaborations with Profs. Berrah (Kalamazou, USA) and Möller (Berlin) have emerged related to 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 classical dynamics of quantum systems with A. Emmanouilidou (Amherst, USA)
– 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. Engel (Würzburg, Germany) and V. Malyshev (Groningen, Netherlands)

Local cooperations
The interaction with Prof. Schmidt's group from the TU Dresden has continued. Common research activities include *quantum adiabatic molecular dynamics*. With Dr. Großmann from the TU Dresden we enjoy a productive collaboration on *semiclassical propagation techniques* and the *effect of external noise on quantum systems*. New attractive possibilities for interaction have opened up through Prof. Strunz and his group. Such local cooperations are facilitated through our International Max Planck Research School (see p.3.2) with its monthly seminar taking place at mpi**pks**.

Research Group: Nonlinear Processes in Strong Fields
(Head: Dr. Andreas Becker (until 8/08))

The group was founded in October 2002 and had a typical size of 1-2 PhD students and 2-3 Postdocs. Soon after the appointment of the group leader as an associate professor at the Department of Physics at the University of Colorado and as an associate fellow of JILA in Boulder, USA, in August 2008 the activities of the group came to an end. The research interests of the group were the theoretical analysis and computational simulation of ultrafast processes in atoms and molecules interacting with intense laser pulses. They include the correlated dynamics of two-electron systems (namely helium and hydrogen molecule), the control of electron dynamics in a molecule using attosecond (1 as = 10^{-18}s) laser pulses, imaging of molecular structure, as well as the generation of few-cycle pulses during the filamentation of powerful lasers in the air. We have used ab-initio numerical simulations, the intense-field many-body S-matrix theory, as well as analytical methods and models for our theoretical studies.

In the period 2007-08, we have in particular used a numerical two-electron model, previously proposed by us, to further investigate the dynamics during the so-called non-sequential double ionization of atoms and molecules in an intense laser pulse. We were able to gain new insights in the microscopic dynamics of the correlated emission of two electrons and to relate our findings to the well-known scattering dynamics in the field-free case. Next, we proposed a two-pulse control scheme to direct and locate an electron in a molecule. The unexpected high probabilities for localization of the electron in the dissociating hydrogen molecular ion at one of the two protons, obtained in our numerical calculations, might be considered as one of the first steps towards a control of electron dynamics on a sub-femtosecond time scale. Another major line of our research has been the ionization and high-harmonic generation of fullerenes in intense laser fields. Multi-slit interference effects, arising from the contributions of the different atomic centers in the complex molecule lead to a suppression of the ionization probability as compared to an atom. We could show that related interference minima in the high-harmonic spectra of the fullerenes can be used to obtain structural information, such as the radius, of the fullerene. Therefore, high-order harmonic generation may be a useful tool to identify structural changes in such complex molecules induced by intense laser light.

Cooperations

- with S.L. Chin (Quebec, Canada; experimental group) on the generation of tunable ultrashort laser pulses during the filamentation of a laser in the air,
- with P.B. Corkum (Ottawa, Canada; experimental group) and R. Dörner (Frankfurt am Main; experimental group) on nonsequential double ionization,
- with A. Jaroń-Becker (Dresden) on high-order harmonic generation in fullerenes,
- with L. Plaja (Salamanca, Spain; theoretical group) on the numerical simulation of hydrogen molecule in intense laser pulses (funded by the DAAD),
- with U. Thumm (Manhattan, Kansas, USA; theoretical group) on the laser-driven electron dynamics in small molecules.

Research Group: Nonlinear Dynamics in Quantum Systems
(Head: Dr. A. Buchleitner (until 9/07))

The group dealt with the complex dynamics of apparently simple quantum systems. "Complexity" can be of classical and/or quantum origin: strongly coupled degrees of freedom, disorder and stochastic activation, but also interference, decoherence and entanglement may limit the predictability of the specific physical systems at hand, and enforce a statistical treatment.

During the group's last months at mpi**pks**, our work focused on

- open system entanglement evolution (Markus Tiersch, Fernando de Melo, Florian Mintert, Simeon Sauer, Malena Osorio Hor-Meyll, Alejo Salles, Agung Budyiono);
- the dynamics of ultracold atoms in optical potentials (Alexey Ponomarev, Hannah Venzl, Alexej Schelle, Carlos Trallero Giner, Victor Lopez Richard, Ming-Chiang Chung);
- the spectral properties of the coherent backscattering signal of trapped cold atoms (Vyacheslav Shatokhin, Thomas Wellens);
- strongly driven helium (Celsus Bouri);

where the names in parentheses identify the main actors. All these theoretical endeavors are closely related to experimental activities, and combine various aspects of quantum transport theory, in a very well controlled – quantum optical – setting, with different and, as we believe, innovative perspectives on decoherence theory.

Besides the local pillars of the group's scientific performance, the visitors' program of mpi**pks** complemented by support of DAAD and VolkswagenStiftung allowed us to maintain close links to partner groups in Warsaw, Kraków, Paris, Bogotá, Havana, and Rio de Janeiro, with a continuous exchange of students and young postdocs.

Since October 2007, the group's coach and, to this coach's fortune, the largest part of the group, have moved to the Albert-Ludwigs-University of Freiburg, where they are now playing on their own turf, under the label "Quantum Optics and Statistics". Though, we still enjoy stable contacts to mpi**pks**, where we have spent eight highly productive, enjoyable, and inspiring years.

Research Group: Complex Dynamics in Cold Gases
(Head: Dr. T. Pohl (since 9/08))

The group was founded in September 2008, and currently hosts two PhD students and three postdoctoral guest scientists. Our main research interest is devoted to cold and ultracold many-body systems, and in particular to their dynamical behavior driven by strong long-range interactions.
Rapid progress in cooling and manipulating atoms and molecules continues to open up several new vistas to synthesize and study long-range interacting systems. Examples include quantum-degenerate gases of dipole-dipole interacting atoms and molecules, ultracold plasmas as well as cold Rydberg atom ensembles. Although originating from similar physical settings, understanding their dynamics often poses diverse questions, requiring different methods ranging from kinetic approaches and (semi)classical particle simulations to few- and many-body quantum calculations.

Ultracold plasmas as produced by photoionization of laser-cooled atoms are currently studied in several laboratories. With their low temperatures they stretch the traditional parameter regime of plasma physics. Fundamental interest, e.g., stems from the possibility of realizing so-called strongly coupled plasmas, in which the potential energy exceeds the thermal energy of the charges. Since ultracold plasmas are created far from equilibrium, they also provide an ideal platform to study non-equilibrium phenomena in strongly correlated plasmas on enlarged spatiotemporal scales.
We are developing a microscopic description of the plasma dynamics that will allow us to isolate and separately study relaxation under various conditions, extending from the well-understood ideal plasma limit to the liquid-like regime and the extreme case of crystalline plasma phases. On a longer term perspective this will enable us to explore the utility of external fields to control certain relaxation processes, to steer the non-equilibrium plasma dynamics and mitigate often undesired heating processes.
Cold Rydberg gases emerge in ultracold plasmas, but can also be created through coherent laser-excitation below the ionization threshold. The latter realizes a peculiar state with "frozen" motional degrees of freedom but highly energetic internal excitations. This results in interactions that can be more than ten orders magnitude larger than for ground-state atoms. Depending on the involved time and energy scales a number of different questions arise. Some specific problems are:
»*Short-time excitation dynamics.* Recently, we developed an efficient numerical procedure to describe the coherent dynamics of small atom clouds in collectively excited Rydberg states. Under certain conditions, the underlying Hamiltonian resembles that of quantum magnets, which we utilized to devise appropriate excitation schemes, that produce regular Rydberg crystals out of disordered atomic ensembles. In a separate work we showed that coupling of more than two Rydberg levels can induce higher order three-body interactions. Here, one of our future objectives will be to understand the (non)adiabatic excitation dynamics driven by such unusual interactions as well as the phase diagram of the corresponding spin Hamiltonians.
»*Long-time evolution.* The potential of cold Rydberg gases in providing a clean realization of long-range interacting, many-body systems is largely limited by the finite lifetime of the excited atomic states. As one possibility to overcome such limitations we will explore far off-resonant single-photon and Raman coupling schemes. If successful, this may provide a quantum gas, in which, e.g., isotropic long-range interactions, deep

potential wells or higher-order N-body interactions can be implemented and controlled to a high degree. Among the arising questions, we will address the stability of localized structures under the action of higher-order N-body nonlinearities.
»*Collective electronic excitations.* Dense ensembles of overlapping Rydberg atoms could provide an implementation of interacting fermion systems, whose realizability has, however, long been questioned due to their apparent fragility with respect to autoionization processes. Here, we are aiming at a better understanding of the electronic stability of multiple excitations in closely spaced few atom configurations. One of our objectives is to identify and isolate metastable collective bound-states and find pathways to minimize their continuum coupling, e.g., by optical fields.
»*Exotic molecules.* Systems of low Rydberg atom concentration are dominated by interactions between excited- and ground-state atoms, which directly probe the Rydberg-electron wavefunction on a mesoscopic scale. Our interest in the dynamics of such systems is twofold. On the one hand, we study the influence of such interactions on coherence properties of many-body Rabi-floppings − an essential prerequisite for proposed applications, e.g., in quantum information processing. On the other hand, we explore the utility of macroscopic coherence in Bose-Einstein condensates for an indirect mapping of the complex interaction potential onto macroscopic scales.
Ion-atom mixtures are currently discussed in the context of sympathetic cooling. On the other hand, a mixture of like species, is simultaneously driven by long-range polarization potentials as well as short range charge exchange reactions. The former was pointed out to form mesoscopically condensed clusters, while the latter is expected to induce coherent charge transport through the atom cloud. We would like to understand the complex interplay between these two effects. As a related problem, we are studying charge transport in atomic chains and its control through optical coupling, within a joint project with Alexander Eisfeld in the Finite Systems Division.
Generally, we share interest in the physics of cold Rydberg gases with the Finite Systems group and greatly benefit from interactions with several members of the mpi**pks**, working on related problems. Further, we have

Cooperations:

- Thomas C. Killian (Rice University, Houston, USA)
  on expansion dynamics and relaxation processes in ultracold plasmas,
- Georg Raithel (University of Michigan, Ann Arbor, USA)
  on excitation dynamics of ultracold Rydberg gases near Förster resonances,
- Matthias Weidemüller (University of Heidelberg)
  on excitation transport in structured systems,
- Mikhail D. Lukin (Harvard University, Cambridge, USA) and
  Eugene A. Demler (Harvard University, Cambridge, USA)
  on many-body correlations and controlled excitation of ultracold gases,
- Paul R. Berman (University of Michigan, Ann Arbor, USA)
  on interactions in few-level, few-body systems,
- Hossein R. Sadeghpour (ITAMP, Harvard-Smithsonian CfA, Cambridge, USA)
  on collisional recombination at low-temperatures,
- Igor Lesanovsky (University of Nottingham, Nottingham, UK)
  on coherent control of ion transport in ultracold atomic lattices.

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

The department Biological Physics studies active dynamic phenomena in cells and in tissues. From the point of view of physics, cellular systems are 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. They result from the collective behaviors of many subunits on smaller scales (e.g. molecules, molecular aggregates, cells) and are coordinated by regulation and 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.

In addition to the study of physical principles which play a key role in cellular systems, current problems of cell and developmental biology are studied theoretically in close cooperation with biologists. These projects focus on spatiotemporal aspects and 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. Since then, a close interdisciplinary cooperation with the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG) in Dresden was established. In a series of research projects, fundamental problems on cell dynamics, as well as the dynamic organization of tissues are studied in close interaction between theory and experiment. Our group is linked to the International Max-Planck Research School on Cell Biology, Bioengineering, and Biophysics, managed by the MPI-CBG. These interactions have been deepened further by the creation of a joint research program on the Physics of Biological Systems which includes three junior research groups that are affiliated jointly with both institutes. 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. Recent research projects include:

Physics of active fluids and gels. Cellular dynamics is an important example of behaviors of active matter. In collaboration with the Institut Curie in Paris, we have recently developed a hydrodynamic theory of active fluids and gels. Spatial anisotropies in incompressible active gels lead to rich phenomena such as novel hydrodynamic instabilities. Active gels represent a paradigm for the dynamics of the cell cytoskeleton. In this case, the multicomponent character of the system becomes important. Furthermore, in the framework of the hydrodynamic theory, the effects of fluctuations can be described by noise terms in the hydrodynamic equations.

Physics of cell division. The position and orientation of the mitotic spindle defines the axis and the plane of cell division. This permits cells to undergo asymmetric cell divisions or to control the orientation of the cell division axis. Molecular motors in the cell cortex exert pulling forces on microtubules of the spindle. The resulting forces and torques position and orient the spindle prior to division. Recently, it could be shown that the angular distribution of axis orientation can be predicted by a simple stochastic description of torque balances which quantitatively matches experimentally determined distributions.

Dynamic organization and patterning of two dimensional tissues. An important model system for the patterning of tissues during the development of organisms are epithelia, which are two dimensional tissues. They grow by repeated cell division starting from a small group of almost identical cells. The morphology of emerging cell packings and the topology of the network of cell bonds can be described by a vertex model.

Of particular interest is the role and maintenance of anisotropies in the system. Anisotropic cell division generates source terms as well as anisotropic stresses. The resulting anisotropic growth permits the system not only to control the size but also the shape of the tissue. While the molecular and structural basis of these anisotropies are not yet understood, there is strong evidence that morphogens influence the degree of anisotropy and also are involved in growth regulation. Morphogens are signaling molecules which are transported in the growing tissue and develop graded concentration profiles. They are involved in the patterning of the tissue. The kinetics of morphogen transport can be quantitatively described in comparison with experimental data.

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. Cell movements are regulated by cellular signaling systems and permit a cell to move to a target. An important model system is the chemotaxis of sperm. Sperm of many species including humans find the egg by following a chemoattractant. The principles of sperm chemotaxis are based on a general steering mechanism which controls a helical swimming path.

Physics of hearing: Nonlinear amplification by active cellular processes. 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. Recently, it could be shown that cooperativity of small groups of oscillating hair bundles gives rise to significant enhancement of amplification gain as compared to individual hair bundles. This suggests that hair bundle oscillations could account for an essential part of cochlear amplification.

Perspectives

Approaches and concepts from physics will in the future play an increasingly important role in the study of biological systems. The recent rise of "Systems Biology", the quantitative study of the behavior of functional modules in cells, demonstrates the growing role of theoretical approaches for the understanding of biological complexity. The use of quantitative and theoretical approaches in biology is however still in its infancy. The close interaction between physics and cell biology has in recent years stimulated many new research avenues.

Biological processes are organized hierarchically and occur on a large range of scales. Biology is quickly unraveling the key genes and molecules involved in many cellular processes. At the same time, there is only very limited understanding of the main organizing principles by which these components coordinate. Quantitative descriptions of biological processes are therefore still rare and new approaches are required to study biological complexity. Physics can provide key concepts to quantify biological processes and to theoretically analyze underlying mechanisms. An important goal of our research at the interface between physics and biology is to establish theory as a key component of biological research.

The Max Planck Institute for the physics of complex systems provides a unique environment for theoretical work in biological physics. Of particular importance is the strong and fruitful collaboration with the MPI-CBG. An important challenge for the future is the study of the dynamic organization of multicellular systems, in particular the patterning and morphogenesis in developing tissues. The question of how structures form reliably on large scales controlled by the expression of genes which interact in complex cellular networks remains a formidable challenge. Physical approaches can help trigger key advances.

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 Carl-Phillip Heisenberg on the study of cell movements and flows during the development of the zebrafish
  - Collaboration with Marino Zerial on the dynamics of the endosomal network in cells

- Institute 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
  - Collaboration with Michel Bornens on the physics of cell division
- AMOLF, Amsterdam
  - Collaboration with Marileen Dogterom on cytoskeletal dynamics
- Cavendish Laboratory, Cambridge, UK
  - Collaboration with Thomas Duke on the physics of hearing and active wave phenomena in the cochlea
- University of Geneva
  - Collaboration with Marcos González-Gaitán on the role of morphogens in tissue patterning and growth

Research Group: Biological Physics of Olfaction
(Head: Dr. M. Zapotocky (until 3/08))

The group operated until March 2008, when Martin Zapotocky took a permanent position at the Institute of Physiology, Academy of Sciences of the Czech Republic, Prague. Two postdoctoral researchers from the group are staying at mpi**pks** until May 2009 (supported from a VolkswagenStiftung grant).

The group has used techniques from statistical physics, nonlinear dynamics and soft condensed matter physics to study biological sensory systems, with emphasis on olfaction (the sense of smell) and mechanosensation. Our interests also extend more broadly into developmental biology and biochemical network theory. Research in the group has recently concentrated on three specific areas:

1. Collective effects in axon guidance and targeting:

During development, connections among brain areas are formed by growing neural tubes (axons). In the prevalent picture of this process, each growing axon is independently guided to the proper target by sensing a spatially distributed chemical cue. We develop models in which axon-axon interactions play a dominant role, and proper targeting thus becomes a collective effect. In our basic model, each axon is represented as a directed random walk which has attractive contact interactions with other growing axons; this leads to the formation of axon fascicles. In the report on page 84, we characterize the dynamics resulting from the *turnover* of axons, a process in which the oldest fully grown axons die and are replaced by newly growing axons. This corresponds to the situation in the mammalian olfactory system, where the turnover of sensory neurons persists into adulthood, and the connectivity pattern between the nasal epithelium and the olfactory bulb reaches its steady state only after 3-5 turnover periods. We show how time scales much slower than the lifetime of an individual axon can emerge from the dynamics of the basic model, and discuss our findings in terms of an effective dynamics of axon fascicles. In our current work, we are relating the theoretical results to experimental observations of axonal growth in cell culture, and are extending our basic model with the goal of connecting to data from the developing olfactory system.

2. Regulation of insect flight by mechanosensory feedback:

The aim of this project is to understand how the fruit fly *Drosophila* uses mechanosensory input from its wings to enhance flight stability and maneuverability. Flies have approximately 100 mechanosensory receptors in each wing; the pattern of the deformation of the wing is thus encoded in the timing of action potentials generated by these sensory neurons. The flight apparatus of Drosophila may be viewed as consisting of the "engine" (a set of power flight muscles) and two "transmissions" (sclerite hinges with attached small control muscles) which couple the power muscles to the left and right wing. The control muscles are influenced by the activity of the mechanosensory neurons in the wings; each "transmission" is thus dynamically regulated by a mechanosensory feedback loop.

In our approach, we view the flight apparatus of the fly as a nonlinear oscillator, and use general tools from nonlinear dynamics to characterize its properties. We ana-

lyze detailed flight recordings from the laboratories of S. N. Fry (ETH Zurich) and J. Howard (MPI-CBG, Dresden). Using wavelet-based analysis, we classify the distinct dynamical regimes which occur spontaneously during unstimulated tethered flight, and characterize in detail their phase coherence properties. To investigate the functional role of the mechanosensory neurons, we analyze the changes in wing dynamics resulting from externally delivered mechanical stimuli and from surgical perturbation of the mechanosensors. Observed effects include a partial entrainment of the the wingbeat cycle to external periodic force acting on the body of the fly, as well as changes in phase coherence following a resection of the wing nerve. In our theoretical treatment, we analyze analytically the dynamics of a Hopf oscillator element (representing the power muscles) coupled to linear mechanical elements with parameters controlled by the activity of the mechanosensors. The project is partially supported by a grant awarded by the VolkswagenStiftung (to J. Howard, S. N. Fry, and M. Zapotocky).

3. Signal transduction in olfactory sensory neurons:

In the cilia of olfactory sensory neurons, the initial external chemical signal (odorant identity and concentration) is transduced into an electrical signal. The corresponding signal transduction pathway is well characterized biochemically, and is known to include several feedback loops mediated by intra-ciliar calcium. The group has proposed and analyzed dynamical models of the calcium-mediated feedback and its functional role in the neuronal signaling. In the past year, we have concentrated on obtaining analytical results for a simplified model that takes into account both fluctuations in intracellular calcium and its diffusion along the cilium.

Cooperations

With biology groups:

S. N. Fry, Institute of Neuroinformatics, ETH Zurich
(mechanosensory control of insect flight)

J. Howard, MPI for Cell Biology and Genetics, Dresden
(mechanosensory control of insect flight)

P. Feinstein, City University of New York
(axon guidance in the olfactory system)

J. E. Schwob, Tufts University, Boston
(axon guidance in cell culture)

With theorists:

P. Borowski, University of British Columbia, Vancouver

M. Gopalakrishnan, Indian Institute of Technology, Madras

P. Marsalek, Charles University, Prague

G. Sibona, Universidad Nacional de Cordoba, Argentina

P. K. Mohanty, Saha Institute of Nuclear Physics, Kolkata

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

Fluctuations and noise have strong effects on the dynamics and function of many biological systems. We study stochastic models that incorporate dynamical noise in the theoretical description of systems from neuroscience (neurons and sensory organelles) and of systems from cell biology (molecular motors). In particular, we are interested in (i) the spontaneous activity of and signal transmission by single and coupled stochastic neurons and neural receptors and (ii) the transport properties (velocities and diffusion coefficients) of phenomenological models of active motility and of coupled molecular motors. Our main focus is on the nontrivial interactions between noise and nonlinearities in these systems. By means of novel analytical approaches and numerical simulations, we explore how biological systems cope with or even benefit from the inevitable fluctuations which they are prone to. In the last two years our research has been devoted to the following topics:
Stochastic Neural Activity. The spiking of nerve cells is inherently noisy. Synaptic transmission failures, channel noise and, most importantly, quasi random input from other neurons cause fluctuations in the subthreshold membrane voltage and the spontaneous generation of action potentials. This stochastic process is furthermore shaped by adaptation, synaptic plasticity, and synaptic filtering. We study analytically the statistics of subthreshold fluctuations, spike intensity, spike variability, and of information transfer in the framework of simple linear and nonlinear integrate-and-fire neurons using different models of noisy synaptic input. Furthermore, we investigate effects of short-term synaptic plasticity and of interspike interval correlations on the properties of neural signal transfer. We are also interested in the characterization of input-output correlations in neural networks and in the application of basic theorems for stochastic processes (e.g. the Novikov theorem) to problems from neuroscience.
Stochastic Dynamics of Hair cells. Sensory signals from the outside world are transduced by receptor cells into electrical currents that can be processed by the brain. One well-studied example of such a signal transducer is the hair cell in the inner ear organs of vertebrates. It possesses a small organelle, the hair bundle which is the key element in the transduction process. In vitro experiments on hair cells have shown that the hair bundle is an active element capable of producing noisy periodic deflections, a sharply tuned response to weak periodic signals, and a compressive nonlinearity with respect to strong periodic signals. Hair bundles in the cochlea and in other hearing organs are often coupled by an overlying membrane. We study biophysical models of coupled hair bundles in order to clarify under which conditions such a mechanical coupling of hair bundles enhances their active properties. We also use simplified models of nonlinear noisy oscillators to uncover the underlying mechanism and the limits for such a potential enhancement.
Active Brownian motion of self-propelled particles. Self-propelled motion is one of the most vivid indications of living systems. This motion can be observed on various spatial and temporal levels ranging from motion of proteins within single cells (molecular motors) to swarming behavior in groups of animals. One class of phenomenological models for biological motility comprises active Brownian motion. We study the diffusive behavior of active Brownian particles in different situations (subject to a bias force or to a spatially periodic force field). We also work on approximation schemes

which permit to map more detailed biophysical models of motility (as, for instance, for coupled molecular motors) to the simple active Brownian particle model.

Cooperations

Experimental groups:

- Jan Benda, LMU München, Germany
- John E. Lewis, University of Ottawa, Canada
- Pascal Martin, Institut Curie Paris, France

Theoretical groups:

- Anders Carlsson, Washington University, St. Louis, USA
- Debashish Chowdhury, I.I.T. Kanpur, India
- Frank Jülicher, mpi**pks** Dresden, Germany
- Andre Longtin, University of Ottawa, Canada

We have a number of collaborations with experimental groups studying the stochastic activity of and providing us with data from neurons (Benda and Lewis) and sensory hair cells (Martin). We also collaborate with other theory groups to explore stochastic problems in diverse biophysical systems, e.g. in neurons and synapses (Longtin), in RNA polymerase (Chowdhury), in isolated and coupled hair cells (Jülicher), and in the dynamics of actin polymerization (Carlsson).

Division: Electronic Correlations
(Head: Prof. Dr. P. Fulde (until 9/07))

The division "Electronic Correlations" terminated officially with the retirement of Prof. P. Fulde in October 2007. Nevertheless a number of activities continued thereafter and are still going on. Some of them are described in the following:

In the field of superconductivity it was explained why the filled skutterudite $Pr_2Os_4Sb_{12}$ has a transition temperature which is more than twice as high as that of $La_2Os_4Sb_{12}$. The only difference between the two systems are the two 4f electrons of Pr^{3+} which are well localized. It was shown with the help of inelastic neutron scattering data that intra-atomic quadrupolar excitations of the $4f^2$ shell provide the additional glue for Copper pairing. Furthermore the observed resonances in $CeCu_2Si_2$, $CeCoIn_5$ and YbB_{12} were explained. Our work has made clear that they are a general phenomenon in superconductors with unconventional order parameters (see report I. Eremin).

The work on charge degrees of freedom in geometrically frustrated lattices with strongly correlated electrons was continued. It was demonstrated that for a kagome lattice with one-third filling a ferromagnetic ground-state may result solely due to kinetic effects (F. Pollmann, principal investigator). With the Nagaoka state in the half filled Hubbard model and with Thouless' ring exchange in ^{3}He this is the third example of kinetic ferromagnetism. Also in the field of frustrated lattices by extensive numerical calculations we showed for the first time the existence of an extended U(1) liquid phase in a three-dimensional quantum dimer model (O. Sikora, principal investigator). The origin of the heavy quasiparticles in the spinel LiV_2O_4 was explained (V. Yushankhai, principal investigator). This has been a controversial issue. We were able to explain the neutron scattering data by calculating the spin susceptibility using a realistic bandstructure, supplemented by correlation effects, whereby the frustrated lattice structure plays an important role.

We collaborated with the experimental group of R. Mohanty at Boston University who did an incredible experiment by measuring with a nanomechanical device the torque generated when a current is flowing from a spin polarized, i.e., ferromagnetic metal into a non-magnetic metal. This effect was calculated by us ten years ago. The experiments took 5 years and in the torque measurement a sensitivity of 10^{-22} N·m was achieved, a world record. The paper made it to the front cover of *Nature Nanotechnology* (G. Zolfagharkhani, principal investigator).

Considerable progress was also made in the field of wavefunction based electronic structure calculation. For the first time we were able to calculate energy bands of solids with strongly correlated electrons by quantum chemical methods which are based on fully controlled approximations. The Fermi surface of doped Cu-O planes was determined this way. Also we were able to calculate energy gaps of insulators together with conduction and valence bands, here for MgO and BN by quantum chemical techniques. This makes us optimistic that those methods will gain in importance. They are computationally more expensive than density functional based methods, but they do not face problems of arbitrariness as the latter do (principle investigator L. Hozoi for Cu-O - see separate report - and MgO and A. Stoyanova for BN).

Cooperations

Quantum Chemical Methods: H. Stoll (Univ. Stuttgart), A. Shukla (IIT, Bombay), K. Rosciszewski (Univ. Krakow)

Strongly Correlated Electrons: P. Thalmeier (MPI-CPfS), different collaborators (CPfS), G. Zwicknagl (Univ. Braunschweig)

Frustrated Lattices: K. Shtengel (UC Riverside), K. Penc (Univ. Budapest), N. Shannon (Univ. Bristol), E. Runge (TU Ilmenau), G. Hotta (Aoyama Gakuin Univ.), J. Betouras (Univ. of St. Andrews, Scotland)

GdI_2: A. Taraphder (IIT, Kharagpur)

Spin Transport: P. Mohanty (Boston Univ.), S. Kettemann (Jacobs Univ.)

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

Dynamically generated complexity has many facets. We are tackling several of these, where we restrict our efforts to classical systems, both deterministic and stochastic, few and many degrees of freedom. A particular focus of the past two years was on the origin of long range correlations and on extreme events, mechanisms and forecasts.

The literature is full of papers reporting long range temporal correlations in many systems and data sets. Such correlations give rise to unexpected clustering of events which has to be distinguished from true instationarity due to drifting parameters, but which also leads to new classification schemes for data. The origin of such correlations is usually not discussed. We have studied two prototypic classes of intermittent dynamics as possible mechanisms. In Hamiltonian dynamics with mixed phase spaces, trajectories stick to regular islands and hence give rise to power laws in the decay of autocorrelations. A particular feature of this type of intermittency is that it is robust against perturbations of the system's dynamics by noise. Maps of the Manneville-Pomeau type are a mathematical idealization of another type of intermittency, which under suitable conditions leads to weak ergodicity breaking: Even if formally the ergodic theorem is valid, the invariant measure is singular and therefore the times for convergence are infinite. Therefore, physical realizations of such dynamics suffer from convergence of expectation values and hence seem to be non-ergodic. We represent the dynamics by its induced map which is ergodic, and which, after introduction of an operational time, enables us to map the process onto an anomalous diffusion process formulated as a continuous time random walk (CTRW). In the framework of time series analysis, the reconstruction of memory kernels in terms of a Mori-Zwanzig equation turned out not to be a suitable approach, since the form of the kernel depends sensitively on the observable (i.e., is not invariant under transformation of variables), such that the temporal decay of such a kernel is not a good characterization of long range correlations of the underlying process. Due to its hierarchical structure, also hydrodynamic turbulence displays long range temporal correlations. In the lower atmospheric boundary layer, turbulence is strongly affected by the interaction with the surface by thermal and roughness effects, which introduce additional structures and instationarity. In a data analysis project, we could show that real boundary layer turbulence can be thought of as being a concatenation of ideal turbulence of different intensity. A suitable model for boundary layer turbulence is a simple geometric autoregressive process.

We continued our efforts to understand dynamical mechanisms which lead to extreme deviations in complex dynamics, and to predict these extreme events based on time series data. A particular such process is self organized criticality (SOC), which in finite systems leads to a repulsion of extreme events. This temporal structure can be exploited for predictions. For the studied system, events of larger magnitudes are better predictable than small amplitude events, which is in agreement with theoretical considerations. "Extreme Events" was also the topic of a workshop which we organized jointly with the Mallorca institute IFISC in November 2008.

As a future perspective, we plan to extend our work related to predictions and predictability to the context of complex weather and climate models. It is common knowedge that error doubling times in low dimensional dynamics are controlled by

the spectrum of Lyapunov exponents. In atmospheric processes, however, large scale structures are much more robust than the small scales, such that the maximal Lyapunov exponent of the system, whose value is dominated by dynamics on small spatial scales, is irrelevant for, e.g., weather prediction with its prediction horizon of several days. Also, the role of model inaccuracy calls for a deeper understanding: Different models of the atmosphere employ different types of approximations, so that the (divergent) results of multi-model runs require more than just a linear average of the individual results. In a collaboration with Klaus Fraedrich, a meteorologist at the University of Hamburg, we are going to organize a workshop on model and prediction errors in summer 2009. This includes the issues of model accuracy, of skill scores, of data assimilation for initial conditions, of interpretations of multimodel runs, and of ensemble breeding.

Cooperations

- W. Just, University of London; G. Radons, University of Chemnitz: Dynamical systems versus statistical physics, fluctuation theorems.
- J. Peinke, University of Oldenburg: Surface wind, turbulence, and wind power turbines (consortium together with R. Friedrich, Münster; K. Schaffarzyk, FH Kiel; C. Wagner, DLR Göttingen)
- S. Albeverio, University of Bonn: Stochastic processes.
- N. Vitanov, IMB Sofia: extreme events in the ocean and the atmosphere.
- K. Fraedrich, University of Hamburg: accuracy and errors in weather and climate models.

1.9 Junior Research Groups

Emmy Noether Junior Research Group: Many-Body Effects in Mesoscopic Systems
(Head: Dr. M. 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 are mesoscopic systems and phenomena. Besides the focus on many-body effects in electronic mesoscopic systems, the group also investigates questions in the field of quantum chaos in optical microcavities as a second research topic. During the period 2007/08, the research was carried out by two PhD students (funded, as the group leader and one Postdoc, by the Emmy-Noether Program of the DFG) and three to five Postdocs from the mpi**pks** Visitors Program. Additional funding is received via the DFG Research Group 760 "Scattering Systems with Complex Dynamics" that was approved in April 2007. The group leader was awarded a two-year fellowship in the "Fast Track Programme" (that supports 20 young women scientists across Germany) of the Robert-Bosch Foundation in September 2008. Our research results have been presented on a number of international conferences and workshops (including invited and key note talks). The group runs the seminar series "Mesoscopic Systems" at mpi**pks**. In addition, the group leader has co-initiated the "Scientific Jam Session", a discussion forum for the young scientists (Postdocs and advanced PhD students) of the institute and was its chief organizer from June 2006 to February 2008. She was also one of the main organizers of the international conference "New Frontiers of Quantum Chaos in Mesoscopic Systems" that took place at the mpi**pks** May 15-30, 2008.

Many-body effects have always been a core interest in condensed matter physics. The objective of the group's research is their investigation in the mesoscopic regime, where the finite number of particles in the system, its small size, the resulting complex wave phenomena and the geometry dependence of the energy level and wave function statistics as well as intrinsic mesoscopic fluctuations, are known to 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, mainly because of (quasi-)degeneracies of the energy levels in the integrable case. 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. Another research topic is the Kondo effect in mesoscopic systems. We have also investigated the influence of breaking of spatial symmetries at graphene zigzag edges and found that they change the density of states in a characteristic way. This also explains recent experimental observations within the Dirac theory.

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. In collaboration with Jan Wiersig (University of Magdeburg) we have

predicted that cavities of so-called Limacon shape show directional emission. This idea was very soon verified by three different experimental groups. In another work we have in detail investigated the conditions for achieving directional emission from microlasers of spiral shape. This work was published in Optics Letters together with a Press Release that triggered further interest. Deviations from the naively expected ray-wave correspondence occur when the wavelength becomes of the order of characteristic system length scales. Including the resulting 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.

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 on small scales. One focus will be the dependence of the photoabsorption cross section on the density of states. The latter can, to a certain extent, be customized in the mesoscopic regime, for example in graphene via edge-state engineering via impurities or 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 the breaking of edge symmetries. Another research topic will be the interplay of Kondo and x-ray edge physics in quantum dots. Eventually, questions of quantum chaos in optical microcavities, including the effects of nonlinear materials and lasing cavities, will remain another focus of the group's research interests.

Cooperations

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 Eduardo Mucciolo (University of Central Florida, Orlando, USA) on the mesoscopic Kondo box.
- 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) group of Federico Capasso (Harvard University, Cambridge, USA) on the far-field characteristics of microlasers with different (spiral, Limacon, 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 (Kyoto, Japan) and Chil-Min Kim (Seoul, Korea).

Junior Research Group: Computational Nonlinear and Relativistic Optics
(Head: Dr. S. Skupin (since 10/07))

The Junior Research Group *Computational Nonlinear and Relativistic Optics* started to operate in fall 2007 at the mpi**pks**. Together with the group leader Stefan Skupin, Mickael Grech started as a long-term postdoc. From April 2009, Stefan Skupin will also be appointed as *Carl Zeiss* Junior Professor for *Computational Photonics* at the Friedrich-Schiller-University in Jena. The group is currently working on four topics.

Ultrashort filaments of light in weakly ionized, optically transparent media In the mid-1990's, first experiments on the meter-range propagation of femtosecond (fs) laser pulsed beams were performed. In these experiments, infrared laser pulses with a duration of about 100 fs produced narrow filaments of several meters. More than 10 % of the energy was observed to be localized in the near-axis area. Similar results, but on smaller length scales, are known for pulse propagation in dense media like silica or water. This so called filamentation is attributed to initial self-focusing of laser radiation, which originates from the Kerr response of air and leads to an increase of the light intensity. This growth is then saturated by the defocusing action of the electron plasma created by photoionization of the medium. The understanding of the complex dynamics of these filaments is crucial for potential applications. Pulse compression in pressurized cells filled with noble gases by femtosecond filaments is one prominent example. The impressively simple setup and the high compression rates achieved so far attracts much interest at recent international conferences. Fully space-time resolved simulations can give insight into the details of the compression mechanisms which are not accessible in experiments (see also MPG Jahresbericht 2008). The recent experimental verification of Terahertz (THz) emission from high intense laser matter interaction also attracts a lot of interest. We plan to extend our numerical model to provide a more accurate description of the underlying physics. For example, strong focusing geometries require to go beyond paraxial approximation, while considering few-cycle or multi-color pulses requires the use of a field-dependent ionization rate. On this topic, we collaborate with Luc Bergé (CEA/DAM, Arpajon, France) and the group of Günter Steinmeyer (MBI, Berlin).

Nonlinear localized waves in nonlocal media and their interaction 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 modes is determined by the interplay of the wave-field with the functional form of the nonlinearity. In the case of optical beams the nonlinear response can be described in terms of the induced change in the refractive index, often approximated as a local function of the wave intensity. However, in many real physical systems the nonlinear response is spatially nonlocal, i. e., the refractive index in one spatial point depends on the beam intensity in the neighborhood of this point. Nonlocality occurs, for instance, when the nonlinearity is associated with some 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. Nonlocal media may support formation of stable complex localized structures, even long-lived rotating solutions, so called azimuthons. We were able to link these azimuthons to internal modes of non-rotating solitons. In perspective, especially the potentially three-dimensional nonlocal systems in BEC are promising candidates to observe interesting novel solutions and effects. Here we are especially interested to see modulational instability in self-defocusing media, as well as the formation of bound states of otherwise repelling bright or dark solitons. On this topic, we collaborate with Wieslaw Królikowski (ANU, Canberra, Australia) and Mark Saffman (Wisconsin, USA).

Nanosecond laser plasma interaction (LPI) in the context of inertial fusion (ICF) The control of laser beam coherence properties is crucial to optimize the coupling between laser beams and target in the ICF context. It is achieved by optical smoothing techniques that provide a laser intensity distribution in the focal spot made of many randomly distributed peaks, the speckles. Coherence properties of such beams can be reduced by the LPI. While the reduction of temporal coherence is interesting to limit the reflectivity due to parametric instabilities, reduction of the spatial one is associated with angular spreading of the laser beam. This beam spray can modify the energy balance on the target and thus must avoided. At high intensity, plasma induced incoherence follows from the laser beam filamentation, whereas at lower intensities, forward stimulated Brillouin scattering (FSBS) is responsible. We have developed a statistical model for FSBS driven by a spatially incoherent, monochromatic beam and successfully verified it against numerical simulations. We have shown that FSBS induced beam spray occurs when the average power in a speckle exceeds a threshold value, well below the one for filamentation. This threshold value depends on the ion acoustic damping rate. An experiment has been proposed (accepted and scheduled for 06/2009) to study this dependence at the ALISE facility (CEA/CESTA, France). We will continue to develop statistical and numerical tools for the simulation of the LPI in the ICF context. On this topic, we collaborate with Denis Pesme (CPhT, Paris, France), Gilles Riazuelo (CEA/DAM, Arpajon, France), and Vladimir Tikhonchuk (CELIA, Bordeaux, France).

Laser based charged particle acceleration The possibility of using high power lasers to generate multi-MeV proton beams is extremely interesting for applications in physics, engineering or medicine. Such beams can be used to initiate thermonuclear reactions in the so-called fast ignitor scheme for ICF. Due to their good laminarity, collimation and short duration, they are also used for time resolved radiography in plasma experiments. Potential medical applications are hadron therapy and isotope creation. Last but not least, laser based particle acceleration may provide table-top accelerators. While the production of proton beams with energy up to a few tens of MeV has already been demonstrated experimentally, the control of the beam properties remains the principal problem for most applications. The standard mechanism of ion acceleration occurs in the electrostatic field generated by hot electrons escaping into the vacuum surrounding the target. This mechanism provides proton beams with broad (quasi-thermal) energy distribution. We are currently working on alternative mechanisms of ion acceleration that allow a better control of the ion beam properties. In particular, we are considering the possibility to generate ion beams with narrow energy spectrum and well controlled emittance and angular aperture. These schemes rely on

the interaction of PW laser pulses with nano-structured targets. The polarization of the incident laser pulse also plays a crucial role. Moreover, at ultra-high intensities (above $10^{21}\,\mathrm{W/cm^2}$), new effects, such as radiation friction and electron-positron pair generation, must be included in our simulation tools. On this topic, we collaborate with the group of Erik Lefebvre (CEA/DAM, Arpajon, France), Roland Sauerbrey and Ulrich Schramm (Forschungszentrum Dresden Rossendorf), and Vladimir Tikhonchuk (CELIA, Bordeaux, France).

Joint research program mpipks 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 mpi**pks** 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 how molecular machines function collectively to perform the dynamics that are seen within the living cell. 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; while progress in experimental biology continues to elucidate the networks on the molecular level, the widespread use of novel forms of electronic communication provides plentiful 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. We focus in particular on three areas that correspond to three conceptually different classes of networks.

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.

The approach of generalized modeling has been developed in the past by members of the group. At present we work on numerical tools to extract more information from

generalized models. However, our main effort is currently focused on demonstrating the applicability of the method to paradigmatic examples on different scales. Two recent systems that were successfully studied in this way are ecological food webs and the cellular MAPK signaling cascade. In addition we have started to collaborate with mathematicians to clarify the conceptual foundations of generalized modeling. This collaboration has opened up many promising prospects for future research. In particular we will investigate whether generalized models can be used to formulate a model reduction scheme for conventional models, that reduces the model's complexity while leaving the local dynamics unchanged.

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 directions 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 we have mainly focused on adaptive networks in which the network nodes assume discrete states. We have developed an approximation scheme allowing to capture the dynamics of adaptive networks by a low-dimensional system of differential equations. At present this approximation is used to study systems from different fields including models of swarming, epidemic spreading, and social cooperation. In addition we are currently developing an approach to the dynamics of weighted adaptive networks. While these are much more complicated than their discrete counterparts, we were able to show in an example that many properties of the long-term dynamics can be computed analytically. Future will focus on linking different forms of self-organization in order to obtain a coherent picture. In parallel we will move toward more realistic biological models to understand the role of adaptive networks in nature. A first result has already been achieved in neural networks where we were able to explain several empirical observations with a realistic model.

Numerical Coarse-graining. The third area in which the group is active is numerical coarse-graining of individual-based models. Traditionally biological models are based on systems of equations, which can be analyzed by advanced mathematical tools. By contrast individual-based models allow for a more direct and more realistic description of biological processes but can only be studied by simulation. However, even in an individual-based model the relations connecting emergent properties can in principle be described by equations. While the derivation of these equations is often prohibitively difficult, only limited information is needed to study the unknown set of equations by the powerful tools of numerical dynamical systems theory.

In the past year we have adapted a previously proposed approach for the efficient analysis of individual-based models to the investigation of biological evolution. In this approach the information needed to study the system on the emergent level is generated on-demand from multiple bursts of individual-based simulation. Our results show that this multi-level approach can be used to speed up simulations significantly (factor 10^3 in our example) and extract information that is not usually accessible by simulation

alone. A major challenge for future applications of this technique is to come up with automated procedures that can identify emergent-level in simulation data. For this purpose we have started to work on the development of data analysis techniques such as new clustering and segmentation algorithms. After testing these methods mostly on benchmark examples we are now actively seeking collaborations with biologists to apply them to current questions.

Cooperations

Generalized Models:
Ulf Dieckmann, IIASA, Laxenburg, Austria.
Simon Levin, Princeton University, Princeton, NJ, USA.
Ralf Steuer, University of Manchester, UK.
Stefan Siegmund, TU Dresden, Germany.

Adaptive Networks:
Hiroki Sayama, Binghampton University, NY, USA.
Cristian Huepe, independent NSF-grantee, Chicago, IL, USA.
Kevin Bassler, Houston University, Houston, TX, USA.
Chen-Ping Zhu, Nanjing University, CN.

Coarse-graining and Data Analysis:
Iva Tolić-Nørrelykke, MPI-CBG, Dresden, Germany.
Ioannis Kevrekidis, Princeton University, Princeton, NJ, USA.
Boaz Nadler, Weizmann Institute of Science, Rehovot, IL.

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. We have proposed a mechanism of these oscillations based on collective behavior of dynein motors, which link dynamic microtubules and the cell cortex. By combining quantitative live cell imaging and laser ablation with a theoretical description, we have shown that dynein dynamically redistributes in the cell in response to load forces, resulting in more dynein attached to the leading than to the trailing microtubules. The redistribution of motors introduces an asymmetry of motor forces pulling in opposite directions, leading to the generation of oscillations. This work provides the first direct *in vivo* observation of self-organized dynamic dynein distributions, which, due to the intrinsic motor properties, generate regular large-scale movements in the cell.

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 recent 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 have proposed 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.

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 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. Our recent experiments using live-cell imaging and optical tweezers have shown that this pushing force is responsible for irregular oscillations of the bundle position along the cell axis, and for nuclear centering. However, the physics of these irregular oscillations and its relation to the process of nuclear centering in not yet fully understood. In order to describe nuclear centering by pushing forces in fission yeast, we have started to develop a physical model. The model reproduces oscillations of a single bundle, as well as the movements of the cell nucleus. This work should be relevant to a variety of other systems where forces are generated by microtubules pushing against the cell cortex or a physical barrier in general.

Aging. Aging can be defined as a decrease in fitness with time and an increased probability of death. In replicative aging, cells lose their ability to replicate as the total number of divisions increases, undergoing a limited number of divisions. It was hypothesized that asymmetry is required for aging, which is in agreement with what is observed in prokaryotic and eukaryotic asymmetrically dividing cells. Even morphologically symmetrically dividing prokaryotic cells have a limited replicative potential. However, it is not known if morphologically symmetrically dividing eukaryotic cells age. We have shown that the fission yeast *Schizosaccharomyces pombe* does not exhibit aging. We found that as the total number of divisions increases, no decrease in replicative fitness occurs. The cells followed for more than 30 consecutive divisions maintain their replicative fitness. Furthermore, cell morphology does not change, and the probability of cell death does not increase, with the total number of divisions. Siblings did not show any replicative fitness differences when the division number increased. Our results suggest the existence of an immortal unicellular organism. Replicative immortality might be achieved by the equal distribution of damaged components during division, efficiently kept under a threshold that would result in a cumulative deleterious effect. Comparative studies of the mechanisms underlying this different life strategy will help to understand what limits the number of divisions a cell can undergo.

Cooperations

Frank Jülicher, Max Planck Institute for the Physics of Complex Systems, Dresden: Modeling of nuclear oscillations and centering

Nenad Pavin, University of Zagreb, Croatia, and mpi**pks**: Modeling of nuclear oscillations

Thilo Gross, Max Planck Institute for the Physics of Complex Systems, Dresden: Aging in symmetrically dividing organisms

Stefan Diez, Max Planck Institute of Molecular Cell Biology and Genetics, Dresden: *In vitro* reconstitution of nuclear oscillations

Frank Bradke, Max Planck Institute 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, collectively function to give rise to the complex dynamical processes observed in living organisms. We focus on the physical mechanisms underlying the generation, coordination and regulation of force and movement in biological systems. This is achieved via a combination of theoretical and experimental approaches, focusing on two systems that reach from the scale of a single molecule to that of a single cell.

Transcriptional Systems. RNA polymerase is the molecular machine responsible for reading out the genetic code stored within DNA in the form of a 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. In the past two years, we have shed light on how this machine moves along the DNA template, and how it ensures that a minimum number of copy mistakes is made. We have focused on rate-limiting off-pathway events during transcription, examining the dynamics of backtracking, a state which is thought to be crucial for detecting and removing copy errors. We have proposed that the polymerase performs a one-dimensional random walk while it is in this backtracked state and engaged in error correction. As a consequence, pause lifetimes follow a $t^{-3/2}$ power law, giving rise to two asymptotic subsets of pauses distinct both in duration and trajectory. Both classes of pauses have been observed in experiments, but we now suggest that they are caused by a single process. Furthermore, the ability of the machine to move backwards along the copy template allows for retrospective proofreading of past copy errors. Together with the 2008 Gutzwiller fellow Juan M. R. Parrondo, we have investigated this dedicated mechanism of diffusive proofreading within the general framework of kinetic proofreading schemes. Finally, we have studied the role of base-pairing in the RNA strand in the context of the early stages of transcription, during which the polymerase is prone to premature and irreversible stalling. Specifically, we have examined the hypothesis that the absence of long transcripts contributes to stalling in the vicinity of the promoter. In a statistical mechanics treatment we have utilized numerical and analytical approaches to calculate the average number of consecutive unpaired bases adjacent to the polymerase, representing the space available for backtracking. We have found that the length-dependent equilibrium fold attributed to the nascent strand poses a marked barrier to a backtracking polymerase within length scales commensurate with observed early stalling events. These theoretical investigations are complemented by the construction of a high-resolution dual-trap optical tweezer apparatus which is nearing completion. This microscope will be used to test theoretical predictions regarding the transcriptional progress of polymerase molecules, by monitoring and manipulating one molecule at a time.

Cytoskeletal Systems. A multitude of morphological movements must occur in the development of each and every animal. These movements arise through stresses that are generated within the cellular cytoskeleton. A striking example is the large-scale flows of cortical cytoskeletal material that are observed in the early development of the *Caenorhabditis elegans* embryo. These flows are required to move particular cellular components to specific cellular regions, for the purpose of establishing distinct domains with different protein compositions, a process that is referred to as polarization. We have investigated the properties of the cortex that are essential for the observed flow behavior. We find that on the time scale of flows, the cortex may be described as a thin layer of viscous fluid that consumes energy through ATP hydrolysis. With this simple description, we have found that variation in myosin activity yields a gradient in actively generated stresses, which counteracts viscous dissipation to drive flow. Subsequently, we examined the nature of cortical stresses within the single cell stage *C. elegans* actomyosin cortex and their relation to cortical flows. We have measured stresses by severing the cortex in a living embryo with a pulsed UV laser. Analyzing the kinetics of the elastic response of the cortex to this cut has allowed us to quantify local stiffness

and stress, which we have found to vary across different regions of the *C. elegans* embryo. Active stresses are under control of the Rho-GTPase cycle, a prominent switch-like regulator of cellular activity, which we have shown by laser-cutting under conditions where the embryo is genetically perturbed. Finally, we have found that there are anisotropies but no gradients in cortical stress, which suggests that resistance to compression and expansion dominates over all other sources of viscous dissipation. In summary, this combined experimental and theoretical approach has shed light on how active stresses are regulated, and how a local down-regulation is translated into cortical flow.

Interestingly, this flow serves to localize a particular set of interacting proteins to specific cortical regions of the cell, and their localization pattern persists even after the flows cease. We have investigated how this might come about, by putting forward a series of components that are able to interact via reaction-diffusion-advection. By including a global coupling that arises from the conservation of the total number of components, we have found a particular form of nonlinear interactions that allow for the switching from a homogeneous and unpolarized state to an inhomogeneous and persistently polarized state, with dynamics close to what we observe in the experiment. These findings describe a novel mechanism by which cortical flows are able to localize the components that specify which end of the cell is which, ultimately allowing for proper animal development.

Cooperations

C. Bustamante, Howard Hughes Medical Institute and at the University of California, Berkeley, U. S. A. : Transcription by RNA Polymerase II

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

A. A. Hyman, Max Planck Institute of Molecular Biology and Genetics: Cortical polarization in *C. elegans*

J. Howard, Max Planck Institute of Molecular Biology and Genetics: Single cell perturbation experiments

J. M. R. Parrondo, Universidad Complutense de Madrid, Spain: Diffusive Proofreading during Transcription

F. Jülicher, Max Planck Institute for the Physics of Complex Systems, Dresden: Active Polar Gels

1.10 Advanced Study Groups

Localizing Energy through Nonlinearity, Discreteness and Disorder
(Head: Prof. Serge Aubry, 2007)

Classical Problems

- *Diffusion of a wavepacket in Random Nonlinear Systems* It was proven analytically that diffusion cannot be complete in some family of Random Nonlinear models with norm conservation and large enough initial amplitude wavepacket. Numerical investigations [1–3] were done on Random Nonlinear Systems for understanding the effect of nonlinearities on Anderson Localization. There is absence of diffusion or incomplete diffusion in more situations than those fulfilling our theorem while in other situations there is apparently complete diffusion. This problem is not yet fully understood. Further investigations continue.

- *Disordered linear FPU model*

  The divergency of the second moment of the energy distribution, is not a good criteria for energy spreading. In the disordered linear FPU model (neglecting nonlinearity), there is no possible energy diffusion but nevertheless the second moment of a wave packet diverges as a function of time (due to acoustic modes) and there is a well defined limit energy profile with no second moment [4].

- *Transmission Threshold in time-periodically driven Nonlinear Random Systems*

  How a plane wave could be transmitted through nonlinear random systems? In the linear case, no transmission is possible because of Anderson localization. This problem has been investigated numerically in the nonlinear case for random Klein-Gordon, random DNLS and random FPU chains [5] initially at zero degree and submitted to a time periodic driving force at one edge. It has been found in all three models that there is a critical amplitude for the driving force beyond which energy transmission occurs. The existence of this threshold is explained analytically.

- *Anomalous Thermostat*

  A general model consisting to a finite anharmonic system coupled to an infinite linear system (phonon bath) is investigated [6]. The harmonic degrees of freedom can be explicitly eliminated and the energy dissipation through the phonon bath calculated. The nature of the phonon spectrum was shown to be essential for determining its dissipative properties. There may be absence of dissipation when the phonon spectrum is discrete and for some kind of driving force of the phonon bath. Then the anharmonic subsystem coupled to the phonon bath) could sustain in principle Discrete Breathers, Quasiperiodic Discrete Breathers or (perhaps?) singular continuous Breathers.

- *Energy spreading of a localized excitation in the FPU-model* A simplified FPU model consisting of a single anharmonic bond which initially excited is studied [7]. This is a special case of the above model where explicit calculations can be

done. A sharp continuous transition in the initial amplitude of the excitation has been found. Beyond this initial amplitude, the asymptotic solution is a Discrete Breather and below the wavepacket spreads to zero amplitude.

- *Discrete Breathers in Alkali Halides* Discrete breathers in the context of their formation in stressed, doped alkali halide crystals were studied. The breather explanation for an anomaly in the decay of luminescence in these substances was further tested against theoretical and experimental issues [8, 9].

- *Nonequilibrium statistical mechanics* The exploration of applications of the "observable representation" (OR) was continued. Work and power production was investigated in nonequilibrium systems [10, 11].

Quantum Problems

- *Position and observation dependent quantum tunneling*

  Quantum tunneling of a single anharmonic bond at site M with symmetric double well potential embedded in a harmonic chain is studied [12]. The phonon bath consists of a 1d system of a finite length and a transition to the infinite length from superOhmic to Ohmic was described.

- *Boson scattering* Scattering of boson by groups of bound identical bosons were studied. An essential progress has been achieved and study is an ongoing project. E. Kot has defended his Masters thesis with distinction.

- *Nonlinear Tunneling* The problem of tunneling in nonlinear systems (BEC or nonlinear optics) and the behavior of the matter wave which remains localized within the trap have been investigated. PhD student of VF Gali Dekel was involved [13].

- *Other Quantum Problems* Finally, fundamental aspects of quantization were studied in [14]

[1] G. Kopidakis, S. Komineas, S. Flach and S. Aubry, *Phys. Rev. Lett* **100**, 084103 (2008)

[2] S. Flach, D. O. Krimer and Ch. Skokos, Phys. Rev. Lett. 102, 024101 (2009)

[3] G. Kopidakis and S. Aubry in preparation

[4] R. Schilling and S. Aubry in preparation

[5] M. Johansson, G. Kopidakis, S. Lepri and S. Aubry, preprint (2008)

[6] S. Aubry and R.Schilling, in preparation

[7] D. Hajnal and R. Schilling, preprint (2008)

[8] L. S. Schulman and E. Mihokova, *Phys. Rev.* **E78** 026212 (2008)

[9] L. S. Schulman and E. Mihokova preprint (2008)

[10] B. Gaveau, M. Moreau and L. S. Schulman *Physics Letters* **A372** 3415 (2008)

[11] L. S. Schulman, J. P. Bagrow, and B. Gavea, to appear in Systems Epigenomics, A. Benecke, ed.

[12] V.Fleurov, R.Schilling, B.Bayani, *Phys. Rev.* **B78** 184301(2008)

[13] G. Dekel, O.V. Farberovich, A. Soffer and V. Fleurov to appear Physica D and `http://dx.doi.org/10.1016/j.physd.2008.06.013`

[14] M. Roncadelli and L. S. Schulman *Phys. Rev. Lett.* **99** 170406 (2007)

Time: Quantum and Statistical Mechanics Aspects
(Head: Prof. Lawrence S. Schulman, 2008)

The advanced study group (ASG), "Time: quantum and statistical mechanics aspects," dealt with several issues centering about the physical nature of time. The members of the group were L. S. Schulman, A. Bohm, B. Gaveau, J. Halliwell and J. G. Muga. In addition visitors and seminar speakers were invited for periods of a few days to several weeks. Principal areas of study were as follows:

Arrows of time. Why does coffee cool? The clash between the (near) time-symmetry of Nature's dynamical laws and the asymmetry of thermodynamics has been a concern since an understanding of these subjects first emerged. During the course of this ASG an extremely simple explanation was articulated which was related to physical processes occurring at the time of "decoupling" (380000 years into the history of the universe). More details are given in the research portion, section 2.26. A second problem in this area dealt with signaling and information transmission. Some years ago it was shown that regions with opposite thermodynamic arrows could co-exist in weak contact. What was not clear was whether signals could be sent. A modeling program was initiated to study this question.

Quantum operators for time and arrival time. Pauli famously proved that there could be no time operator in quantum mechanics, the essential point being that its putative conjugate variable, energy, is bounded from below. This is ironic in view of the fact that in contemporary technology time is the most precisely measured of physical quantities. Taking a cue from actual measurements, one proposal has been to look at "time of arrival," a quantum-symmetrized version of the operator combination mx/p, basically distance over velocity. Because inverse momentum is singular, the notion of operator must be generalized to that of "Positive Operator Valued Measure" (POVM) and a useful operator formulation has been developed. The weakening of the operator notion has as a consequence the introduction of distributions of arrival times, most notably that discovered by Kijowski. In a surprising development, it was discovered during the course of the ASG that an ostensibly different approach *also* leads to the Kijowski distribution. One of our visitors, Y. Strauss, gave a talk on what he conceived to be necessary to define a time operator in quantum mechanics, in particular that it should be monotonic for all wave functions as they evolved in time. Strauss calls these Lyapunov operators, and considered examples and resultant properties. G. Hegerfeldt, another participant, heard of this talk after Strauss had left, and began to generalize and extend these results. Enter Muga, who realized that a consequence of Hegerfeldt's extension was the introduction of distributions—indeed the Kijowski distribution!

Image courtesy of the Greek Mythology Link.

$Χρόνος$

Unstable "fundamental" particles. Unstable particles are different. They are born and they die. Unlike stable particles you cannot translate them backward indefinitely in time. It turns out that they are not all that different, and just as stable particles can be classified (by mass and spin) using Wigner's representation theory of the Poincaré group, the same can be done if one allows only *forward* translations in time, and analyzes the Poincaré *semi*group. The states to be associated with these representations are nevertheless problematic; they grow exponentially large at spatial infinity. By extending quantum mechanics to include *Hardy spaces*, a consistent mathematical framework can be developed. The advantage of this approach is that it allows a clear relation between resonance widths and lifetimes, an issue left ambiguous in other approaches and having experimental significance in classifications of high energy particles.

Non-equilibrium thermodynamics. If you only knew thermodynamics you would think that aiming for maximum Carnot efficiency would be a good idea. But that efficiency obtains only for reversible processes, which, to achieve this ideal, must take place infinitely slowly. What's the best you can do if *time* is important? For example, how much dissipation is forced upon you if you want to maximize *power*, rather than efficiency? The approach to non-equilibrium thermodynamics taken by members of the ASG uses stochastic dynamics as a general description of natural processes. It was found, using this framework, that by and large you must dissipate as much power as you draw from the system. Another problem tackled by members of the group had to do with currents. Non-equilibrium complex systems invariably have *flows*. In fact, practitioners use flow diagrams to describe everything from ecology to cell biology. Such currents naturally arise in the stochastic dynamics formulation. A problem solved during the course of the ASG was a modeling issue: to what extent can the observed currents characterize the underlying stochastic dynamics.

Other topics. Several of the lectures gave rise to lively discussion outside the topics indicated above. Creswick was concerned with a particular experimental way to reverse an apparent arrow, a more complex variation of the Hahn spin-echo experiment. Rost reviewed work by himself and Briggs in which time became a derived quantity. My interpretation was that time was not *measured* by the pendulum, it *was* the pendulum. There were similar ideas put forth in the context of quantum gravity, with one of the ASG participants (Halliwell) an early architect of that viewpoint. Price, a philosopher, contributed a rather physical model illustrating retro-causality. The talk of Strauss, mentioned above (which was part of the unstable particles program) gave rise to a satisfying bit of synergy from which one can see that the topical division in this description is only a low order approximation.

Chapter 2

Selection of Research Results

2.1 Magnetic Monopoles in Spin Ice

Claudio Castelnovo, Roderich Moessner, Shivaji L. Sondhi

Electrically charged particles, such as the electron, are ubiquitous. By contrast, no elementary particles with a net magnetic charge have ever been observed, despite intensive and prolonged searches [1]. We pursue an alternative strategy, namely that of realizing them not as elementary but rather as *emergent* particles, i.e., as manifestations of the correlations present in a strongly interacting many-body system. The most prominent examples of emergent quasiparticles are the ones with fractional electric charge $e/3$ in quantum Hall physics. Here we show that magnetic monopoles *do* emerge in a class of exotic magnets known collectively as spin ice [2]: the dipole moment of the underlying electronic degrees of freedom fractionalizes into monopoles. These monopoles can in principle be detected in an experiment modelled after the celebrated Stanford magnetic monopole search [3].

The spin-ice $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ materials are characterized by the presence of magnetic moments $\vec{\mu}_i$ residing on the sites of a pyrochlore lattice (Fig. 1).

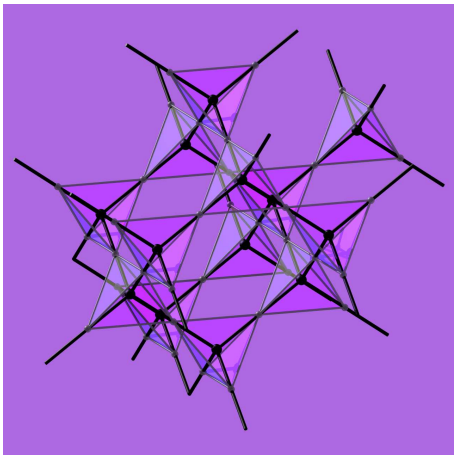


Figure 1: The pyrochlore and diamond lattices. The pyrochlore lattice consists of corner-sharing tetrahedra. These are at the same time the midpoints of the bonds of the diamond lattice (black) formed by the centres of the tetrahedra. The Ising axes point along the respective diamond lattice bonds.

These moments are constrained to point along their respective local Ising axes $\hat{e}_i$ (Fig. 1), and they can be modelled as Ising spins $\vec{\mu}_i = \mu S_i$, where $S_i = \pm 1$ and $\mu = |\vec{\mu}_i|$. Our model accounts for a nearest neighbour exchange and the long ranged dipolar interactions [2]:

$$H_D = Da^3 \sum_{(ij)} \left[\frac{\hat{e}_i \cdot \hat{e}_j}{|\mathbf{r}_{ij}|^3} - \frac{3\,(\hat{e}_i \cdot \mathbf{r}_{ij})\,(\hat{e}_j \cdot \mathbf{r}_{ij})}{|\mathbf{r}_{ij}|^5} \right] S_i S_j \quad .$$

The distance between spins is r_{ij}, $a \simeq 3.54$ Å the pyrochlore nearest-neighbour distance, and $D = \mu_0 \mu^2/(4\pi a^3) = 1.41$K the strength of the dipolar interaction.

Spin ice was identified as a very unusual magnet when it was noted that it does not order to the lowest temperatures, T, even though it appeared to have *ferromagnetic* interactions. Indeed, spin ice was found to have a residual entropy at low T, which is well-approximated by the famous Pauling entropy for (water) ice, $S \approx S_P = (1/2)\log(3/2)$ per spin. Pauling's entropy measures the huge ground state degeneracy arising from the so-called ice rules [2].

Our central result is: the excitations above this ground state manifold, i.e., defects that locally violate the ice rule, are magnetic monopoles [4]. From the perspective of the seemingly local physics of the ice rules, the emergence of monopoles would at first sight seem rather surprising.

Their origin becomes transparent through a modest deformation of Eq. (1): replace the interaction energy of the magnetic dipoles living on pyrochlore sites by that of dumbbells consisting of equal and opposite magnetic charges that live at the ends of the diamond bonds.

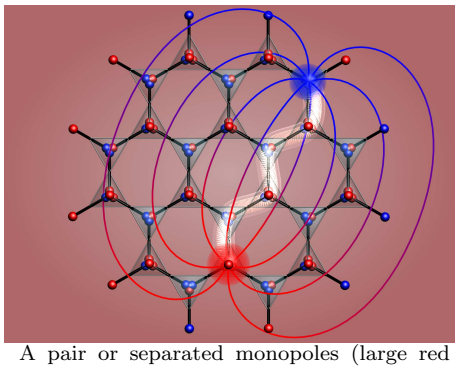


Figure 2: A pair or separated monopoles (large red and blue spheres). A chain of inverted dipoles ('Dirac string') between them is highlighted, and the magnetic field lines are sketched.

The two ways of assigning charges on each diamond bond reproduce the two orientations of the original dipole. Demanding that the dipole moment of the spin be reproduced quantitatively fixes the value of the charge at $\pm\sqrt{\frac{2}{3}}\frac{\mu}{a}$.

The energy of a configuration of dipoles is computed as the pairwise interaction energy of magnetic charges, given by the magnetic Coulomb law

$$V(r_{\alpha\beta}) \;=\; \begin{cases} \frac{\mu_0}{4\pi}\frac{Q_\alpha Q_\beta}{r_{\alpha\beta}} & \alpha \neq \beta \\ \frac{1}{2} v_o Q_\alpha^2 & \alpha = \beta \end{cases} , \qquad (1)$$

where Q_α denotes the total magnetic charge at site α in the diamond lattice, and $r_{\alpha\beta}$ is the distance between

two sites. The finite "self-energy" $v_0/2$ is required to reproduce the net nearest neighbour interaction correctly. This expression is equivalent to the dipolar energy up to corrections which vanish at least as fast as $1/r^5$.

The total energy is minimized if each diamond lattice site is net neutral, i.e., we must orient the dumbbells so that $Q_\alpha = 0$ on each site. But this is just the ice rule. Thus, one of the most remarkable features of spin ice pops right out of the dumbbell model: the measured low-T entropy agrees with the Pauling entropy (which follows from the short-distance ice rules), even though the dipolar interactions are long-ranged.

Naively, the most elementary excitation involves inverting a single dipole / dumbbell to generate a local net dipole moment 2μ. However, this is misleading in a crucial sense. The inverted dumbbell in fact corresponds to two adjacent sites with net magnetic charge

$$Q_\alpha = \pm Q_m = \pm 2\mu/a_d \quad , \tag{2}$$

a nearest neighbour monopole-antimonopole pair. As shown in Fig. 2, the monopoles can be separated from one another without further violations of local neutrality by flipping a chain of adjacent dumbbells. A pair of monopoles separated by a distance r experiences a Coulombic interaction, $-\mu_0 Q_m^2/(4\pi r)$, mediated by monopolar magnetic fields, see Fig. 3.

This interaction is genuinely magnetic, hence the presence of the vacuum permeability μ_0, and not $1/\epsilon_0$. It takes only a finite energy to separate the monopoles to infinity (i.e., *they are deconfined*), and thus they are the true elementary excitations of the system: the local dipolar excitation fractionalizes!

The magic of spin ice arises from its exotic ground states. The ice rule can be viewed as requiring that two dipole strings enter and exit each site of the diamond lattice. In a typical spin ice ground state, there is a "soup" of such strings: many dipole strings – of arbitrary size and shape – can be identified which connect a given pair of sites. Inverting the dipoles along any one such string creates a monopole-antimonopole pair on the sites at its ends. The associated energy cost does not diverge with the length of the string, unlike the case of an ordered ferromagnet, as no domain walls are created along the string, and the monopoles are thus deconfined.

Notice that we did not make reference to the famous Dirac condition [5] that the fundamental electric charge e and any magnetic charge Q must exhibit the relationship $eQ = nh/\mu_0$ whence any monopoles in our universe must be quantized in units of $q_D = h/\mu_0 e$. This follows from the monopole being attached to a Dirac string which has to be un*observable*. By contrast, the string soup characteristic of spin ice at low temperature makes the strings energetically un*important*, although they are observable and thus not quantized.

Indeed, the monopoles in spin ice have a magnitude

$$Q_m = \frac{2\mu}{a_d} = \frac{2\mu}{\mu_b}\frac{\alpha\lambda_C}{2\pi a_d} q_D \approx \frac{q_D}{8000} \quad , \tag{3}$$

where λ_C is the Compton wavelength, and α the fine-structure constant. Amusingly, the charge of a monopole in spin ice can even be tuned *continuously* by applying pressure, as this changes the value of μ/a_d.

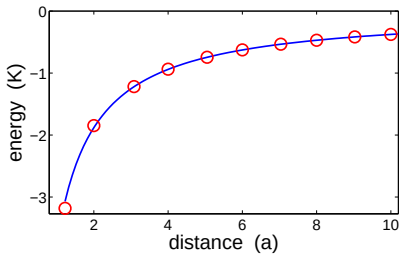


Figure 3: Monopole interaction. Comparison of the magnetic Coulomb energy $-\mu_0 Q_m^2/(4\pi r)$ (Eq. (1), solid line) with the monopole interaction energy in dipolar spin ice (open circles), as a function of monopole separation.

The magnetic monopoles would in principle show up in one of the best-known monopole searches, the Stanford experiment to detect fundamental magnetic monopoles from cosmic radiation. This experiment is based on the fact that a long-lived current is induced in a superconducting ring when a monopole passes through it [3]. The presence of the Dirac string of flipped dipoles is immaterial to the establishment of a current.

Our central qualitative results are: ice-rule-violating defects are deconfined monopoles of **H**, they exhibit a genuine magnetic Coulomb interaction, and they produce Faraday electromotive forces in the same way as elementary monopoles would. Their attraction is further heightened by this being a rare instance of high-dimensional fractionalization, a phenomenon of great interest in fields as diverse as correlated electrons and topological quantum computing.

[1] K. A. Milton, Rep. Progr. Phys. **69** (2006) 1637.

[2] S. T. Bramwell, M. J. P. Gingras, Science **294** (2001) 1495.

[3] B. Cabrera, Phys. Rev. Lett. **48** (1982) 1378.

[4] C. Castelnovo, R. Moessner, S. L. Sondhi, Nature **451** (2008) 42.

[5] P. A. M. Dirac, Proc. Roy. Soc. A **133** (1931) 60.

2.2 Graphene: From Condensed Matter to Quantum Optics

Balázs Dóra, Roderich Moessner

Introduction Graphene, a single sheet of carbon atoms in a hexagonal lattice, has attracted enormous interest recently [1]. Its quasiparticles obey to the relativistic Dirac equation, with the speed of light c replaced by the Fermi velocity $v_F \approx c/300$, opening up the possibility to investigate "relativistic" phenomena in a condensed matter experiment. Associated peculiarities include the unconventional quantum Hall effect, the Klein paradox and Zitterbewegung [2]. Further research is expected to continue to result in interesting new physics and the technological potential of graphene devices makes this field especially worth pursuing.

In a half-filled graphene monolayer, the energy spectrum vanishes at certain points in the Brillouin zone, giving rise to two non-equivalent Dirac points (K and K'), which is sketched in Fig. 1. The low energy excitations around the K point are described by the two-dimensional Dirac equation

$$H_g = v_F \left(\sigma_x p_x + \sigma_y p_y\right) + \sigma_z \Delta \qquad (1)$$

where the σ's are Pauli matrices (pseudospin variables) stemming from the two-sublattice structure of the honeycomb lattice. Finally, Δ represents a possible excitonic gap or a substrate induced bandgap in epitaxial graphene.

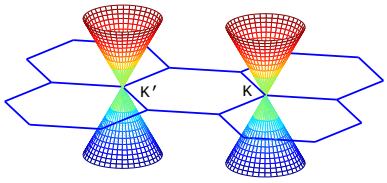


Figure 1: Two inequivalent Dirac cones at K and K' for $\Delta = 0$. The inequidistant isoenergetical lines on the cones denote the Landau level energies in a perpendicular magnetic field.

Relation to Quantum Optics Coupling of a (pseudo)spinor to an external quantum field is a common feature in quantum optics, which deals with the interaction of electromagnetic fields and matter. The simplest, fully quantum mechanical model is the Jaynes-Cummings (JC) Hamiltonian [3]

$$H_{JC} = V(a^+\sigma^- + \sigma^+ a) + \Delta\sigma_z \ , \qquad (2)$$

describing a single two-state atom, represented by the Pauli matrices, interacting with a (single-mode quantized) electromagnetic field. a^+ (a) are the photon creation (annihilation) operators, and V is the coupling strength between the atom and the electromagnetic field. The interaction leads to a periodic exchange of energy between the electromagnetic field and the two-level system, known as Rabi oscillations. A very similar situation occurs for the Landau levels of graphene. In terms of the Hamiltonian in Eq. (2), the two level atom in the JC model (represented by σ's) corresponds to a pseudospin 1/2 due to the two sublattices in graphene, and the photon operators a^+ and a are translated to operators in graphene that are acting on Landau levels [2]: $a^+ = \pi^+/\sqrt{2eB}$ and $a = \pi^-/\sqrt{2eB}$, where $\pi^\pm = \pi_x \pm \pi_y$ with $\boldsymbol{\pi} = \mathbf{p} + e\mathbf{A}$ are the (Peierls substituted) momentum operators with the vector potential $\mathbf{A}$. Formally, they act as creation and annihilation operators of a harmonic oscillator. The coupling constant V depends on the magnetic field strength B and the Fermi velocity in graphene through $V = v_F\sqrt{2eB}$. The eigenenergies are $E_{n\alpha} = \alpha\sqrt{\Delta^2 + V^2(n+1)}$ with n non-negative integer, $\alpha = \pm$. In addition, there is a special eigenstate from the Landau level at the Dirac point with $E^* = -\Delta$.

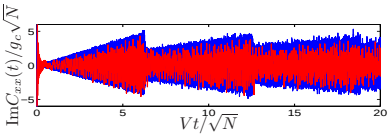


Figure 2: The real time evolution of $C_{xx}(t)$ is shown for long times for $T = \Delta = 0$ around half-filling, g_c is the degeneracy of Landau levels. The number of levels is measured as $D = V\sqrt{N+1}$, corresponding to different magnetic field strengths with $N = 10000$ (blue) and $N = 100$ (red). Collapse and revival shows up with time similarly to the thermal field Jaynes-Cummings model. The revivals gradually get wider and overlap. The presence of thermal revivals are related to the finite average boson number in the Jaynes-Cummings model, which translate to a finite cutoff in the Dirac case.

Interestingly, σ_x is the current density in x direction and plays the role of the dipole operator in quantum optics. Thus, the correlation function $C_{xx}(t) = \langle\sigma_x(t)\sigma_x(0)\rangle$ corresponds to current autocorrelation function of Dirac particles and at the same time to the symmetric dipole-dipole correlator of the JC model. Therefore, we expect the Rabi oscillations of quantum optics to be observable in the response functions of Landau quantized Dirac fermions.

The real time evolution of the current correlation function [4] is shown in Fig. 2. Similarly to observations in quantum optics, the initial collapse is followed by a revival. For longer times, the additional collapses and revivals gradually become wider and overlap. This revival time depends on the value of the cutoff (D) like $2\pi\sqrt{N+1}/V = \pi D/v_F^2 eB$, as is apparent from the figure, and is controllable by the magnetic field. In quantum optics, similar chaotic Rabi oscillations are observed when the electromagnetic field is prepared in a

thermal state and the atom in its excited state. Due to the very wide range of boson numbers, the broad distribution of Rabi frequencies leave almost no trace of coherent oscillations after ensemble averaging.

Entanglement Skyrmions [5] An additional attraction of graphene is presented by its multi-component nature: in a magnetic field, each Landau level comes in four copies corresponding to spin up/down and valley index K/K'.

In quantum Hall ferromagnets near integer filling, the lowest charged excited states can be topological defects, called Skyrmions, which in turn are fascinating in their own right. They are spin textures carrying a topological quantum number and which necessarily carry a quantized net charge. The Hamiltonian appropriate for these excitations can have an effective symmetry group as large as SU(4). In order to obtain a physically transparent parameterization of the internal state of the electrons, it is rather natural to express the internal state at site $\mathbf{r}$ in a way that treats both spin and pseudospin degrees of freedom on an equal footing. This is achieved by the Schmidt decomposition

$$|\Psi(\mathbf{r})\rangle = \cos\frac{\alpha}{2}|\psi_S\rangle|\psi_I\rangle + \sin\frac{\alpha}{2}e^{i\beta}|\chi_S\rangle|\chi_I\rangle$$

where α and β are functions of $\mathbf{r}$, and the local two-component spinors $|\psi_{S/I}\rangle, |\chi_{S/I}\rangle$ are up and down spinors for spin and isospin, respectively, e.g. $|\psi\rangle = (\cos\ \theta/2, \sin\ \theta/2\ e^{i\phi})^T$.

One can now read off directly the reduced density matrices as well as the local spin density:

$$\begin{aligned} \rho_S &= \mathrm{Tr}_I|\psi\rangle\langle\psi| = \cos^2\frac{\alpha}{2}|\psi_S\rangle\langle\psi_S| + \sin^2\frac{\alpha}{2}|\chi_S\rangle\langle\chi_S| \\ m_S^a &= \mathrm{Tr}\rho_S S^a = \cos\alpha\langle\psi_S|S^a|\psi_S\rangle = \cos\alpha\, n^a(\theta_S,\phi_S) \end{aligned}$$

Notice that for the case $\alpha \neq 0$ or π (i.e. $\cos^2\alpha < 1$), the local densities are no longer normalized, but are of length $|\mathbf{m}_{S/I}|^2 = \cos^2\alpha$. Thus, in a semiclassical picture, the (pseudo)spin dynamics is no longer restricted to the surface of the Bloch sphere, but explores the entire volume enclosed by the sphere (Fig. 3).

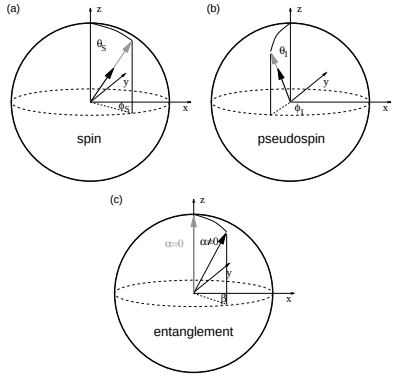


Figure 3: Bloch spheres for entangled spin-pseudospin systems. Bloch sphere for the spin *(a)*, pseudospin *(b)*, and a third type of spin representing the entanglement *(c)*. In the case of spin-pseudospin entanglement ($|\cos\alpha| \neq 1$), the (pseudo)spin-magnetizations explore the interior of their spheres, respectively (black arrows).

It turns out that spin and pseudospin can be perfectly entangled. This is most simply the case for an 'entanglement Skyrmion', where $|\psi_S\rangle = \binom{1}{0}$, $|\chi_S\rangle = \binom{0}{1}$, $|\psi_I\rangle = (1/\sqrt{2})\binom{1}{1}$ and $|\chi_I\rangle = (1/\sqrt{2})\binom{-1}{1}$ for all $\mathbf{r}$, and the Skyrmion is a texture in $\alpha(\mathbf{r})$ and $\beta(\mathbf{r})$ only, with the same form as θ, ϕ in a spin Skyrmion. In this case, $\langle\sigma^x\rangle \equiv 0$ throughout as this operator is off-diagonal in this basis but has no matrix elements between $|\psi_S\rangle|\psi_I\rangle$ and $|\chi_S\rangle|\chi_I\rangle$. At the same time, $\langle\sigma^z\rangle = \cos\alpha(\mathbf{r})$ has the same profile as in a standard spin Skyrmion.

The vanishing of the expectation value of the transverse spin components is a consequence of their entanglement with the pseudospin, quantified by:

$$\Xi := 1 - \sum_a \langle\sigma^a\rangle^2 = 1 - \sum_\mu \langle\tau^\mu\rangle^2 = \sin^2\alpha \quad . \qquad (3)$$

For the entanglement texture, local entanglement is maximal ($\Xi = 1$) when $\alpha = \pi/2$, that is at the a distance from the origin given by the overall size of the texture. Note that at a maximally entangled point, the moduli of both spin and pseudospin vanish.

Crucially, even in the presence of symmetry reduction due to anisotropies such as the Zeeman field acting on the spin, *families* of degenerate Skyrmions remain which differ in their degree of entanglement. These should therefore be visible in experiment.

[1] K. S. Novoselov, A. K. Geim, et al., Science **306** (2004) 666.

[2] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, A. K. Geim, Rev. Mod. Phys. **81** (2009) 109.

[3] B. W. Shore, P. L. Knight, J. Mod. Opt. **40** (1993) 1195.

[4] B. Dóra, K. Ziegler, T. Thalmeier, M. Nakamura, arXiv:0807.4794 (Phys. Rev. Lett. in press).

[5] B. Douçot, M. O. Goerbig, P. Lederer, R. Moessner, Phys. Rev. B **78** (2008) 195327.

2.3 Magnetism and Superconductivity in Iron-based Superconductors

Ilya Eremin and Maxim Korshunov

The relation between unconventional superconductivity and magnetism is one of the most interesting topics in the condensed matter physics. Recent discovery of superconductivity in the iron-based layered pnictides with T_c ranging between 26 and 55K generated enormous interest in the physics of these materials [1]. Like the cuprates, the pnictides are highly two-dimensional, their parent material shows antiferromagnetic long-range order below 150K, and superconductivity occurs upon doping of either electrons or holes into the FeAs layers. In our studies, we have addressed three important issues for the pnictides: which interactions cause SDW order and superconductivity, what is the gap symmetry, and what are the implications of the gap symmetry for the experiments in the superconducting (SC) state.

We have modeled the iron pnictides by an itinerant electron system with two electronic orbitals, and we assume that the hybridization between the orbitals leads to small hole (c-fermions) and electron (f-fermions) pockets located near $(0,0)$ and (π,π), respectively in the folded BZ (two Fe atoms per unit cell) of nearly equal sizes (Fig.1(a)). We assume that electron-electron interaction is short-range (Hubbard-like) and involves two couplings – between fermionic densities from the same orbital and from different orbitals. In itinerant systems, the interactions are expected to be small compared to the fermionic bandwidth, and the physics is dominated by fermions near the Fermi surface (FS). The projection of the Hubbard interaction term onto c and f fermions leads to five different interactions. They include intraband interactions for electrons (u_4) and for holes (u_5), which we assume to be equal, inter-band interactions u_1 and u_2 with momentum transfer 0 and (π,π), respectively, and the pair hopping term u_3.

We searched for possible density-wave and Cooper-pairing instabilities for our model, and found that the ones which may potentially occur are spin density wave (SDW) ($\Gamma^{(r,i)}_{sdw}$) and charge density wave (CDW) ($\Gamma^{(r,i)}_{cdw}$) instabilities with momentum $\mathbf{Q}_{AFM}$ and with either real or imaginary order parameter, and superconducting (SC) instability either in pure s channel (the gaps Δ_c and Δ_f have the same sign) ($\Gamma^{(s)}_{sc}$), or in s^+ channel (the gaps Δ_c and Δ_f have opposite sign) ($\Gamma^{(s^+)}_{sc}$). The SC instabilities requires an attraction (a negative $\Gamma^{(s,s^+)}_{sc}$) and do not occur at this level because both $\Gamma^{(s)}_{sc}$ and $\Gamma^{(s^+)}_{sc}$ are *positive*. The instabilities with momentum-dependent order parameter, like a nematic instability also do not occur simply because we set all interactions to be momentum-independent and weak, and will neglect regular (non-logarithmic) corrections which give rise to the momentum dependence of the scattering amplitude in a Fermi liquid.

Beyond mean-field, the potential SDW and SC instabilities are determined by u_i at energies below the Fermi energy E_F, and generally differ from bare u_i^0 defined at energies comparable to the bandwidth, W. For small size of the FS, $W >> E_F$, and the intermediate range is quite large. At $u_i^0 < 1$ the renormalization can be considered in one-loop approximation. The one-loop diagrams contain particle-particle and particle-hole bubbles [2]. The crucial element of our analysis is the observation that, for $\epsilon^c_{\mathbf{p}} = -\epsilon^f_{\mathbf{p}+\mathbf{q}}$, particle-hole channel is indistinguishable from particle-particle channel, such that the renormalization in both channels are logarithmical and interfere with each other. h channels are logarithmical and interfere with each other. The presence of the logarithms in both channels implies that the one-loop perturbation theory must be extended to one loop RG analysis for the running u_i (in the diagrammatic language, one needs to sum up series of logarithmically divergent parquet diagrams). The derivation of the RG equations is straightforward and collecting combinatoric pre-factors for the diagrams, we obtain:

$$\begin{aligned} \dot{u}_1 &= u_1^2 + u_3^2,\ \dot{u}_2 = 2u_2(u_1 - u_2), \\ \dot{u}_3 &= 2u_3(2u_1 - u_2 - u_4), \\ \dot{u}_4 &= -u_3^2 - u_4^2. \end{aligned} \tag{1}$$

where the derivatives are with respect to $L = \log W/E$, and E is the running energy scale. One could clearly sees that once u_3^0 is finite, the system moves into the basin of attraction of a fixed point, at which $u_3 \propto \frac{u}{1-|u|\ln\frac{W}{E}}$, $u_1 = -u_4 = \frac{|u_3|}{\sqrt{5}}, u_2 \propto |u_3|^{1/3}$, where u depends on the bare values of the couplings. For positive $u_3^0 \approx u_2^0$, this result implies that $\Gamma^r_{sdw} = u_1 + u_3$ remains positive and the largest out of density-wave vertices (see Fig. 1(b)). The interaction in the s^+ SC channel, $\Gamma^{(s+)}_{sc} = u_4 - u_3$, becomes

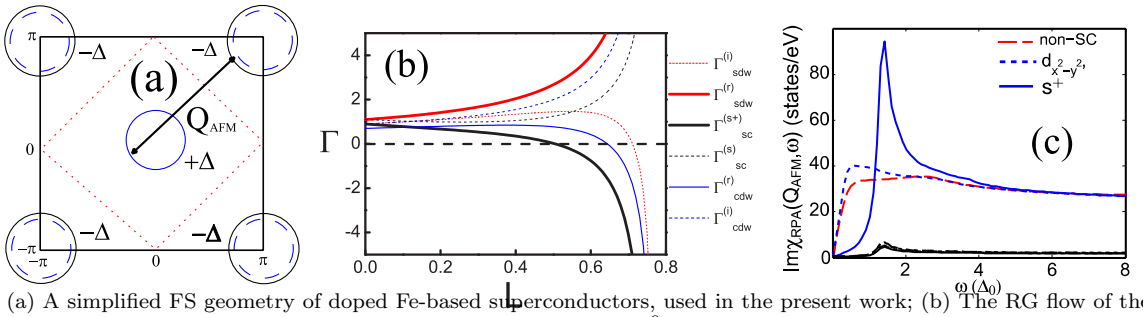


Figure 1: (a) A simplified FS geometry of doped Fe-based superconductors, used in the present work; (b) The RG flow of the effective couplings in various density-wave and superconducting channels vs $L = u^0 \log W/E$; (c) Calculated imaginary part of the RPA spin susceptibility at the AFM wave vector $\mathbf{Q}_{AFM}$ as a function of frequency.

negative (attractive) below some scale (Fig. 1(b)), while $\Gamma_{sc}^{(s)}$ remains repulsive. We emphasize that the density-density vertex u_4 changes sign under renormalization, becomes attractive and also supports SC. Moreover, the interactions in the SDW and the $s+$ SC channel $\Gamma_{sdw}^{(r)} = u_1 + u_3$ and $\Gamma_{sc}^{(s+)} = u_3 - u_4$, become comparable to each other. The implication is that the SDW order and s^+ superconductivity are *competing orders, determined by effective interactions of comparable strength.*

The SC s^+ state that we found has two features similar to a conventional isotropic s-wave state. First, the superconducting gaps on the hole and electron FS are opposite in sign, but equal in magnitude. They, however, become unequal when E_F on the two FS become is different, which happens once the doping increases (or when intraband density-density interactions u_4 and u_5 become unequal). Second, solving the non-linear gap equation, we immediately find that the gap Δ obeys the same BCS relation $2\Delta = 3.53T_c$ as for an isotropic $s-$wave state simply because the pairing kernel contains either two $c-$fermions or two $d-$fermions, but no cf pairs.

The s^+ and s SC states, however, differ qualitatively in the presence of non-magnetic impurities. For $s-$state, non-magnetic impurities do not affect T_c and non-linear gap equation. For s^+ state, the impurity potential $U_i(\mathbf{q})$ has intra and interband components $U_i(0)$ and $U_i(\pi)$, respectively. The $U_i(\pi)$ components scatter fermions with $+\Delta$ and $-\Delta$ and acts as a "magnetic impurity".

One other interesting consequences of the s^+-wave superconducting order parameter concerns the behavior of the dynamical spin susceptibility [3]. In a superconducting state it is given by an RPA-type formula $\chi_s(\mathbf{q},\Omega) = \frac{\chi_s^0(\mathbf{q},\Omega)}{1-\Gamma_{sdw}^{(r)}\chi_s^0(\mathbf{q},\Omega)}$, where $\chi_s^0(\mathbf{q},\Omega)$ is the (dimensionless) susceptibility of an ideal s^+ SC. In our case, when the gap changes sign between hole and electron FS, one can easily verify that $\chi_s^0(\mathbf{q} \approx \mathbf{Q}_{AFM},\Omega)$ coincides with the particle-particle susceptibility for either $c-$ or $f-$ fermions. Furthermore, in the superconducting state, $\chi_s(\mathbf{Q}_{AFM},\Omega)$ has a resonance below 2Δ. Indeed, at $T = 0$, in the clean limit and at small Ω and $\mathbf{q} - \mathbf{Q}_{AFM}$, $\chi_s^0(\mathbf{q},\Omega) = \log\frac{E_F}{E_0} + \frac{1}{4\Delta^2}\left(\Omega^2 - v^2(\mathbf{q}-\mathbf{Q}_{AFM})^2\right)$ where $v = v_F/\sqrt{2}$ is the velocity of the Anderson-Bogolyubov mode in two dimensions (2D), and E_0 is the largest of Δ and the cutoff energy associated with non-equivalence of the two FS. Substituting this into $\chi_s(q,\Omega)$, and assuming $\Gamma_{sdw}^{(r)} \log E_F/E_0 < 1$, we find the resonance at $\Omega = \sqrt{(v^2(\mathbf{q}-\mathbf{Q}_{AFM})^2 + \Omega_0^2}$, where $\Omega_0 = 2\Delta(1/\Gamma_{sdw}^{(r)} - \log E_F/E_0)^{1/2}$. The results are shown in Fig.1(c).

To conclude, we presented Fermi liquid analysis of SDW magnetism and superconductivity in $Fe-$pnictides. We considered a two-band model with small hole and electron pockets located near $(0,0)$ and $\mathbf{Q} = (\pi,\pi)$ in the folded BZ. We argued that for such geometry, particle-hole and particle-particle channels are nearly identical, and the interactions logarithmically increase at low energies. We found that the interactions in the SDW and extended $s-$wave channels ($\Delta_{\mathbf{k}} = -\Delta_{\mathbf{k}+\mathbf{Q}}$) become comparable in strength due to the increase of the intraband pair hopping term and the reduction of the Hubbard-type intraband repulsive interaction. We argued that at zero doping, SDW instability comes first, but at a finite doping, s^+ superconducting instability occurs at a higher T.

We also analyzed spin response of a clean and dirty s^+ superconductor and found that (i) it possess a resonance mode which disperses with the same velocity as Anderson-Bogolyubov mode, (ii) intraband scattering by non-magnetic impurities is harmless, but interband scattering affects the system in the same way as magnetic impurities in an $s-$wave superconductors.

[1] Y. Kamihara *et al.*, J. Am. Chem. Soc. **130** 3296 (2008).

[2] A.V. Chubukov, D.V. Efremov, and I. Eremin, Phys. Rev. B **78**, 134512 (2008).

[3] M. M. Korshunov, and I. Eremin, Phys. Rev. B **78**, 140509(R) (2008); *ibid* Europhys. Lett. **83**, 67003 (2008).

2.4 Pairing Properties of Population Imbalanced Fermions in an Optical Lattice

Andreas Läuchli

Introduction: Attractive interactions between fermions are known to drive transitions to superconducting or superfluid states of matter. The understanding of the situation where two-component fermions (such as up and down spins of electrons, or two hyperfine levels of a neutral fermionic atom) share a common Fermi surface is rather complete, based on the description provided by the Bardeen-Cooper-Schrieffer (BCS) theory [1]. The key objects are Cooper pairs which have zero center of mass momentum. In contrast, if the Fermi surfaces of the two components are different, the situation is subtler because not all of the fermions can easily form pairs. The question thus arises as to whether a superfluid phase exists in this setup and if so, what its properties are. On the theoretical side, different answers to this question have been proposed ranging from exotic superfluid phases to more conventional phase separation. Particular attention has been devoted to the so-called Fulde-Ferrell-Larkin-Ovchinnikov (FFLO, sometimes also denoted LOFF in the literature) state, in which fermion pairs with nonzero momentum form an inhomogeneous superfluid phase [2, 3]. Initially developed for superconductors in magnetic fields, this theory has been applied to heavy fermion systems [4] and dense quark matter [5].

Population imbalanced two component Fermi gas: Recent advances in methods for trapping and controlling ultracold atoms have opened up the possibility of experimentally observing population imbalanced mixtures of ultracold fermions with attractive interactions [6]. Compared to solid state materials, cold gases allow an unprecedented control over the Fermi surface mismatch by adjusting the population imbalance

$$p = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} \, .$$

Here N_σ denotes the number of particles in one of two hyperfine states labeled by a pseudo-spin index $\sigma \in \{\uparrow, \downarrow\}$. So far, these experiments have not revealed any of the proposed exotic superfluids, but have concluded that the system either phase separates, forming an unpaired normal state immersed in a BCS superfluid, or forms pairs that do not condense. Although theoretical studies of the stability and extent of the FFLO state in the phase diagram have not yet reached a consensus, it is currently believed that it is best realized at low temperatures and in quasi one-dimensional (1D) geometries. Given the disagreement between theoretical predictions and the difficulty of unambiguously identifying exotic phases encountered in experiments, we believe it lends insight to study the simplest possible system that could exhibit FFLO-type pairing: the 1D Hubbard model with attractive interactions.

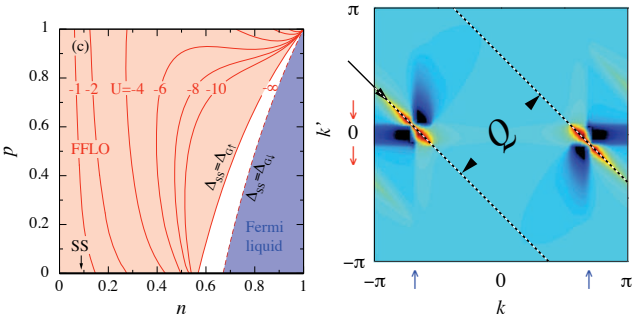


Figure 1: Left: Pairing phase diagram of an array of attractive Hubbard chains as a function of density n and polarization p. The red region denotes dominant FFLO type pairing, while the blue region indicates an unpaired Fermi liquid regime. Right: Signature of the FFLO paring in the atomic shot noise correlation pattern. The diagonal separation of the ridges is precisely given by the momentum Q of the FFLO Cooper pairs.

In our recent work [7] we have exploited the Bethe Ansatz solution of the 1D Hubbard model to derive the strength of various correlation functions as a function of density, interaction and population imbalance. As a key result we could show that among all particle-particle and particle-hole correlators, the FFLO pairing correlations are always dominant for finite imbalance, while the pairing wave vector is directly related to the population imbalance p.

In a next step we investigated the case of weak interchain couplings in an array of chains, by comparing the correlation exponents of the FFLO pairing and the one-particle Green's function. The dominant correlation will determine whether the system will flow towards a FFLO fixed point or a 2D Fermi liquid. The resulting overall phase diagram is presented in the left panel of Fig. 1.

We have also analyzed a possible detection scheme for the FFLO pairing phase in experiments, the so called "noise correlations" put forward by Altman et al. [8], and a typical pattern obtained by Density Matrix Renormalization Group (DMRG) simulations is shown in the right panel of Fig. 1. The structure of the noise pattern reveals pairing tendencies with a characteristic center of mass momentum Q directly related to the population imbalance p.

Finally we put imbalanced systems in an experimentally relevant trapping potential and could show that the noise correlation pattern is basically unaffected, therefore offering an unambiguous and promising way to de-

tect FFLO phases in current experiments on attractive two component Fermi gases in 1D optical lattices.

Population imbalanced three component Fermi gas:

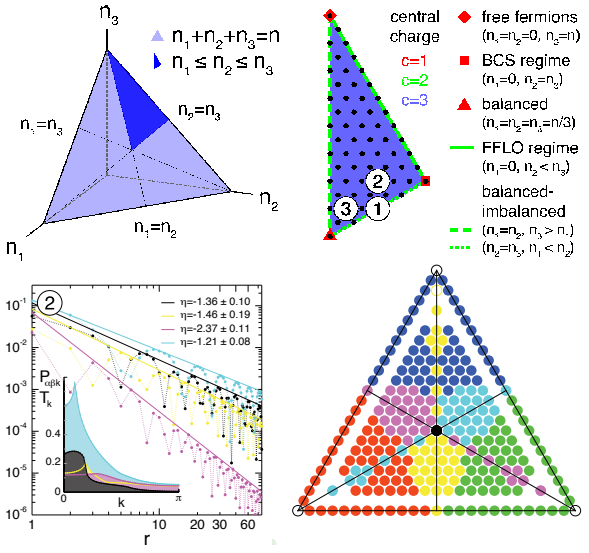


Figure 2: *Top:* Density configurations for a given filling n form a triangle in n_1-n_2-n_3 space. *Bottom left:* Real space and reciprocal space pairing correlation functions. *Bottom right:* Phase diagram for $U/t = -4$ showing the dominant correlation functions at total density $n = 3/4$. The primary colors indicate dominant single particle Green's functions, while the mixed colors (yellow, cyan, magenta) indicate dominant FFLO type pairing of two colors. The white regions denote phase separated or collapsed mixtures.

Motivated by the significant FFLO phase uncovered in the two-component case we turned our attention to the three-component case, which has been introduced theoretically [9] and more recently shown to be accessible experimentally [10] by populating three hyperfine levels of ^{6}Li atoms with mutual attractive interactions. Interestingly the three component situation might mimic some aspects of QCD [11].

We thus considered the three-component attractive Hubbard model on a 1D chain at conserved individual densities n_α which add up to total density $n = 3/4$ (c.f. top panel of Fig. 2) and performed an extensive DMRG study to determine gaps and pairing correlation functions [12].

We find that there are many different phases competing with each other in this system: i) if all densities are equal there is a molecular phase in which the three fermion species form bound molecules (trions), opening a gap to single- and two-particle excitations. ii) a BCS pairing phase involving two balanced species in the presence of a third fermionic flavor at a different density which simply acts as a spectator. iii) for generic imbalance all pairing correlations are of FFLO type and decay algebraically (bottom left panel of Fig. 2), but with different center of mass momentum and decay exponent depending on the two flavors involved. The dominant FFLO mode depends on interaction and density imbalance as is illustrated in the phase diagram presented in the bottom right panel of Fig. 2. As in the two-component case the wave vector of a FFLO pairing mode here scales with the density difference. iv) Finally we observed that at very strong attractive interactions there is a significant tendency for the system to phase separate or to collapse, depending on the imbalance.

[1] J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[2] P. Fulde and R.A. Ferrell, Phys. Rev. **135**, A550 (1964).

[3] A.I. Larkin and Y.N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **47**, 1136 (1964) [Sov. Phys. JETP **20**, 762 (1965)].

[4] H.A. Radovan, N.A. Fortune, T.P. Murphy, S.T. Hannahs, E.C. Palm, S.W. Tozer, and D. Hall, Nature (London) **425**, 51 (2003); A. Bianchi, R. Movshovich, C. Capan, P.G. Pagliuso, and J.L. Sarrao, Phys. Rev. Lett. **91**, 187004 (2003).

[5] R. Casalbuoni and G. Nardulli, Rev. Mod. Phys. **76**, 263 (2004).

[6] M.W. Zwierlein, A. Schirotzek, C.H. Schunck, and W. Ketterle, Science **311**, 492 (2006); G.B. Partridge, W. Li, R.I. Kamar, Y. Liao, and R.G. Hulet, Science **311**, 503 (2006).

[7] A. Lüscher, R.M. Noack, and A.M. Läuchli, Phys. Rev. A 78, 013637 (2008).

[8] E. Altman, E. Demler, and M. D. Lukin, Phys. Rev. A **70**, 013603 (2004).

[9] C. Honerkamp and W. Hofstetter, Phys. Rev. Lett. **92**, 170403 (2004); R.W. Cherng, G. Refael, and E. Demler, Phys. Rev. Lett. **99**, 130406 (2007).

[10] T.B. Ottenstein, T. Lompe, M. Kohnen, A.N. Wenz, and S. Jochim, Phys. Rev. Lett. **101**, 203202 (2008).

[11] F. Wilczek, Nature Physics **3**, 375 (2007).

[12] A. Lüscher and A.M. Läuchli, submitted to Phys. Rev. Lett.

2.5 Optical Slingshots

Ulf Saalmann and Jan M Rost

The interaction of intense laser fields with atoms leads to efficient absorption of many photons resulting, e.g., in *high harmonic generation* which can be understood in surprisingly simple terms of classical mechanics. Here, we describe, analytically, how for a cluster this picture gets replaced by a similarly simple one [1]. It is akin to the mechanism by which space crafts gain velocity through gravitational slingshots [2].

Non-perturbative light-matter interaction typically occurs if the binding energy E_I of an electron is smaller than its ponderomotive energy U_p. The latter is the kinetic energy $\dot{\mathbf{x}}(t)^2/2$ of an electron oscillating in a laser field $\mathbf{F}(t) = \mathbf{F}_0 \cos\omega t$ with the velocity $\dot{\mathbf{x}}(t) = -(\mathbf{F}_0/\omega)\sin(\omega t)$ averaged over one laser cycle $T = 2\pi/\omega$, $U_\mathrm{p} = F_0^2/(4\omega^2)$. The velocity follows through classical mechanics from the Hamiltonian

$$H_F = \frac{\mathbf{p}^2}{2} + \mathbf{x}\,\mathbf{F}(t) \qquad (1)$$

since H_F contains only linear and quadratic operators (Ehrenfest theorem). We treat the light field classically which is justified since the intensity is high enough to be in the limit of large photon numbers. Hence, the light field is essentially a source of photons which does not change if it exchanges some of them with the atom.

In the presence of a potential $H = H_F + V$ no longer fulfills the Ehrenfest theorem. The generally quite complicated strong field dynamics must be solved for quantum mechanically. Moreover, the linear coupling of the light field in Eq. (1) is now an approximation, well justified, since the wavelength of typical intense light, 800nm, is much larger than the electron orbitals it couples to. Another simplification arises: On the atomic time scale (introduced by the potential V), the light induced dynamics is adiabatically slow with a photon energy of 1.2 eV (800 nm) corresponding to an optical period of $T = 2.6$fs. Atoms are in this case simply field ionized, either through tunneling or above-the-barrier ionization at suitable phases of the electric field of the laser [3].

Atoms: The principle of energy absorption from a strong laser pulse A free electron continuously exchanges energy with a light field without net gain. This can be easily seen by calculating the energy difference $\Delta E(t_\mathrm{f}, t_\mathrm{i}) = \int_{t_\mathrm{i}}^{t_\mathrm{f}} \dot{H}_F\, dt$, where we assume that the electron was initially at rest, i.e., $\dot{\mathbf{x}}(t) = -(\mathbf{F}_0/\omega)[\sin(\omega t) - \sin(\omega t_\mathrm{i})]$. Then

$$\begin{aligned}\Delta E(t_\mathrm{f}, t_\mathrm{i}) &= -\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t\, \dot{\mathbf{x}}\,\mathbf{F}(t) \\ &= 2U_\mathrm{p}(\sin\phi_\mathrm{f} - \sin\phi_\mathrm{i})^2 \qquad (2)\end{aligned}$$

with $\phi = \omega t$ and corresponding definitions for $\phi_\mathrm{i,f}$. For n full laser periods $t_\mathrm{f} - t_\mathrm{i} = 2\pi n/\omega$ we get $\Delta E = 0$, i.e., for net energy absorption, the coupling to the light must be limited to incomplete laser cycles.

An example is high harmonic generation, where many photons of low frequency are absorbed by an atomic electron through tunneling ionization (see above). However, the field is strong enough to push the electron back to the ion with which it recombines releasing its kinetic energy and (ionization) potential energy by emitting a high energy photon with a maximum energy of E_HHG. Numerical calculation with Eq. (1) and Eq. (2) leads to $E_\mathrm{HHG} = 3.17\hbar\omega + E_\mathrm{I}$, realized by a trajectory which starts slightly after the maximum of the laser field from the nucleus and returns to it close to the next but one zero crossing of the electric field [4].

Hence, the essence of energy gain from a periodic field is to interrupt the motion of the charged particle through some perturbation in order to effectively limit the exposure to the light to an incomplete field cycle. This simple picture is surprisingly accurate and has been coined the "simple man's approach" [5]. The (Coulomb) potential does not play a crucial role. Note, that the field property (ponderomotive energy U_p) and the atomic property (ionization potential E_I) enter additively in the energy gain of Eq. (2). This differs qualitatively from the situation for clusters as shown below.

Clusters: Optical slingshots While the same quasi-classical principles of light absorption can be carried over to clusters, the simple rescattering from a point-like potential (ion) does no longer happen. Instead, in an idealized way, an electron with velocity v_i traveling through an extended cluster potential can be thought of passing two potential steps, first, when entering the cluster, and second when leaving it again. Both these potential steps (and if the potential is constant otherwise *only* these steps!) give rise to possible energy absorption since they interrupt the exposure to full laser cycles. The classical dynamics of an electron in such a potential under a laser field is stepwise free motion and can be solved analytically in one dimension [1]. In the limit of a deep potential, $v \equiv \sqrt{2V} \gg v_\mathrm{i}$ and $v \gg A$, the final velocity v_f of the exiting electron defines also the energy gain through $\Delta E = {v_\mathrm{f}}^2/2$,

$$\Delta E(\phi) = 4Ap\sin[L\omega/(2v)]\cos[\phi/2]\,, \qquad (3)$$

where L is the extension of the potential (see Fig. 1) and $\phi = \phi_\mathrm{f} + \phi_\mathrm{i}$ is the sum of the phases of the field when the electron enters and exits the potential. As one can easily see, Eq. (3) gives rise to a "double resonance", i.e.,

a maximum energy gain if both trigonometric functions are unity. One condition can be met with all potentials since it restricts the dynamics of the electron: energy gain is maximized for symmetric phases $\phi = 0$ with the result, rewritten in terms of U_p and V,

$$\Delta E_\mathrm{max} = 4\sqrt{U_\mathrm{p}}\sqrt{2V}\,\sin(L\omega/\sqrt{8V})\,. \qquad (4)$$

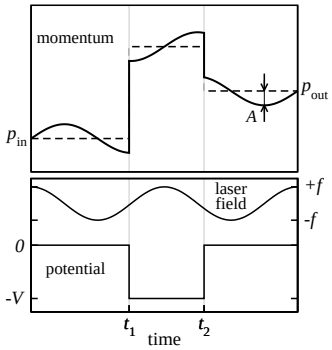


Figure 1: Schematic picture of the scattering process. The upper part shows the momentum of the electron, the lower part the potential V and the electric field $F(t)$ (assumed to be homogeneous in space) as a function of time, respectively, after [1].

If in addition for $L\omega/\sqrt{8V} = \pi/2$, the absorption is resonant in the sense that from entrance to exit of the potential, exactly half a laser cycle is completed (as sketched in Fig. 1) which results quite generally in optimum absorption, see Eq. (2). Compared to atomic systems, the qualitative difference is obvious: Now the field (U_p) and system (V) properties enter *multiplicatively* rendering clusters very efficient absorbers of intense light. Figure 2 illustrates the validity of this simple model by comparing experimental data and microscopic calculations with the outcome from the model, Eq. (4).

In general, (see Eq. (2)), a particle with high velocity absorbs most efficiently energy from an external field. Hence, when passing the center of a realistic cluster where the potential is deepest, the electron should feel the largest field. The phase $\phi = 0$ (Eq. (4)) ensures exactly this condition, making the model quite robust.

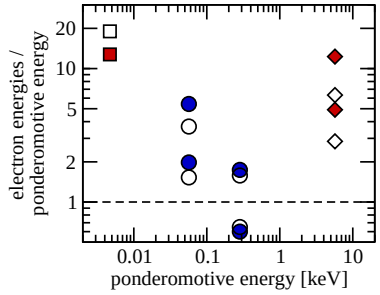


Figure 2: Electron energies as a function of the ponderomotive energy U_p from various clusters. The filled symbols show E_kin for experiments (red) and microscopic calculations (blue): Ag_{1000} (square, [6]), Ar_{1700} and Ar_{33000} (diamonds, [7]), Xe_{1151} and Xe_{9093} (circles). The corresponding estimates ΔE from the rescattering model (4) are shown by open symbols. The dashed line indicates the atomic limit, from [1].

A similar mechanism called "gravitational slingshot" is known in space science: The precious thrust for acceleration of a space craft is systematically applied when flying close by a planet which carries a large gravitational field, where the space craft has a large velocity (similar to the effect of a deep cluster potential on the electron). The thrust (in analogy to the acceleration caused by the laser field) yields optimum increase of speed if the velocity is already high [2]. Acknowledging the analogy, we call the optimum energy absorption from light fields "optical slingshots".

One can also view the resonant absorption in clusters from a more general perspective. In comparison to point-like atomic systems extended systems have a length scale, the extension L, which can give rise to *resonant* absorption when having the right value in relation to the depth of the potential and the light, as can be seen from the argument of the sin-function in Eq. (4): Absorption is maximized for $L\omega/\sqrt{8V} = \pi/2$, i.e., if the potential of extension L is transversed by the electron with momentum $p = \sqrt{2V}$ in the time $(\pi\omega)^{-1}$, half a period of the light. This is reminiscent of the resonant heating in a large but finite plasmas [8].

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

[1] U. Saalmann and J. M. Rost, Phys. Rev. Lett. **100**, (2008) 133006.

[2] A. F. B. A. Prado, J. Guid. Control Dynam. **19**, (1996) 1142.

[3] M. V. Ammosov, N. B. Delone, and V. P. Krainov, Sov. Phys. JETP **64** (1986) 1191.

[4] J. W. Cooper, Phys. Rev. A **47** (1993) 1841.

[5] M. Lewenstein, P. Balcou, M. Y. Ivanov, A. L'Huillier, and P. B. Corkum, Phys. Rev. A **49** (1994) 2117.

[6] T. Fennel, T. Döppner, J. Passig, C. Schaal, J. Tiggesbäumker, and K.-H. Meiwes-Broer, Phys. Rev. Lett. **98** (2007) 143401.

[7] L. M. Chen, J. J. Park, K.-H. Hong, J. L. Kim, J. Zhang, and C. H. Nam, Phys. Rev. E **66** (2002) 025402 (R).

[8] T. Taguchi, J. T. M. Antonsen, and H. M. Milchberg, Phys. Rev. Lett. **92** (2004) 205003.

2.6 Femtosecond Photoionization under Noise

Kamal P. Singh, Anatole Kenfack and Jan M Rost

Adding noise to a strong femtosecond laser pulse irradiating an atom or molecule can lead to dramatic enhancement of ionization [1]. The mechanism is akin to classical stochastic resonance [2]. Intense noise will be available as broad band chaotic light from attosecond sources.

Stochastic resonance is a frequent phenomenon in nonlinear classical systems which are periodically stimulated [2]. Its key feature is an amplification of the desired response of the system if the right amount of noise is added. The system must have at least two states, and for such minimal systems stochastic resonance has been successfully translated into quantum mechanics with a number of realizations. However, does stochastic resonance also exist for the more generic situation of a quantum system with a partially continuous spectrum, such as all atoms and molecules?

Coupling to intense light and noise can realize the corresponding scenario. The simplest is a one-electron atom (hydrogen) described by the Hamiltonian

$$H(x,t) = \frac{\hat{p}^2}{2} + V(x) + x\{F(t) + \xi(t)\} \qquad (1)$$

in one dimension, where the potential $V(x) = -(x^2 + a^2)^{-1/2}$ is the so called soft core potential. It approximates the Coulomb interaction in one dimension and gives a ground state energy of $E_g = -0.5$ with $a = 2$. (We use atomic units if not stated otherwise.) In fact, the exact form of the potential is not so important as long as it allows for a mixed discrete and continuous spectrum. Laser field and noise, $F(t) = f(t)F_0 \sin(\omega t + \delta)$ and $\xi(t)$, respectively, are dipole-coupled to the atom. The Gaussian white noise $\xi(t)$ with intensity D has zero mean and is $\delta-$correlated [3],

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = 2D^2\, \delta(t - t')\,. \qquad (2)$$

Ionization with chaotic light Intense white noise with $D \sim F_0$, where F_0 is of the order of 10^{13}W/cm^2, is difficult to generate. On the other hand, pulse shaping is developing fast and allows to generate almost arbitrary wavefronts. Since any specific atom or molecule only absorbs in a limited frequency range $\Delta\omega$, white noise can be replaced by chaotic light with N modes ω_n which cover $\Delta\omega$,

$$Z(t) = \sqrt{\frac{2}{N}} \sum_{n=1}^{N} F_{\rm rms} \sin(\omega_n t + \phi_n)\,. \qquad (3)$$

Each mode is assumed to have the same strength while the phases ϕ_n are randomly distributed. The inset of Fig. 1 shows an example for chaotic light with $N = 1024$ in a chosen bandwidth (BW) of 0.75 (corresponding to a pulse of 32 attoseconds length) [4]. The overall strength is given by $F_{\rm rms}$, the root-mean-square amplitude of $Z(t)$.

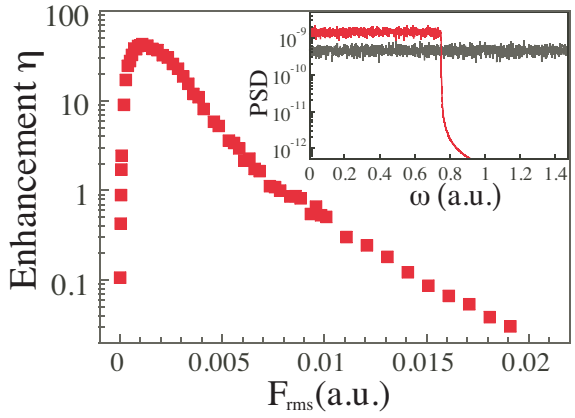


Figure 1: Enhancement η (Eq. (4)) for atomic photoionization (Eq. (1)) induced by a broadband chaotic light. The peak amplitude and frequency of the 20 cycle laser pulse are $F_0 = 0.02$ and $\omega = 0.057$, respectively. The bandwidth of the chaotic light is $\Delta\omega = 0.75$ with central frequency $\omega_0 = 0.375$. Inset: power spectral density (PSD) of the chaotic light compared to the one for the white noise.

We solve the time-dependent Schrödinger equation with many deterministic realizations of $Z(t)$ from Eq. (4) in the Hamiltonian Eq. (2), and average the results to obtain the stochastic solution. Of particular interest is the total ionization probability. If $F_0 \gg F_{\rm rms}$ or $F_0 \ll F_{\rm rms}$, the ionization is close to exclusive ionization P_l by the femtosecond laser or the noise P_n, respectively. The ionization enhancement factor

$$\eta = \frac{P_{l+n} - P_0}{P_0} \qquad (4)$$

subtracts these two limits with $P_0 = P_l + P_n$ and isolates the enhancement due to the combined ionization by laser and chaotic light, P_{l+n}. Figure 1 shows η as a function of $F_{\rm rms}$ for the hydrogen atom with an ionization enhancement of almost two orders of magnitude.

Time- versus frequency-domain In contrast to many classical systems which exhibit stochastic resonance phenomena, an atom has a well defined resonance spectrum which provides frequencies where it responds strongly to external perturbations. To demonstrate, that the stochastic enhancement is not only a simple two-photon absorption where a noise photon with appropriate energy leads to a (resonant) transition from the ground to an excited state while some IR photons

from the femtosecond laser pulse carry the electron further to the continuum, we exclude from the chaotic light frequencies which correspond to the three strongest transitions in the atom, shown in Fig. 3. Only excluding large intervals of $W \geq 0.1$ around each of the resonances from the chaotic light reduces the enhancement significantly, see Fig. 2. However, with $W = 0.15$ almost the entire range of frequencies where the atom can absorb are discarded from the chaotic light. We may conclude that it is indeed the non-linear nature of the light-electron interaction in the atom which leads to the stochastic enhancement – an interpretation which is reinforced by the absorption spectrum of the atom which is no longer restricted to the atomic resonance frequencies (black) but considerably broadened under the intense laser pulse (red, Fig. 3).

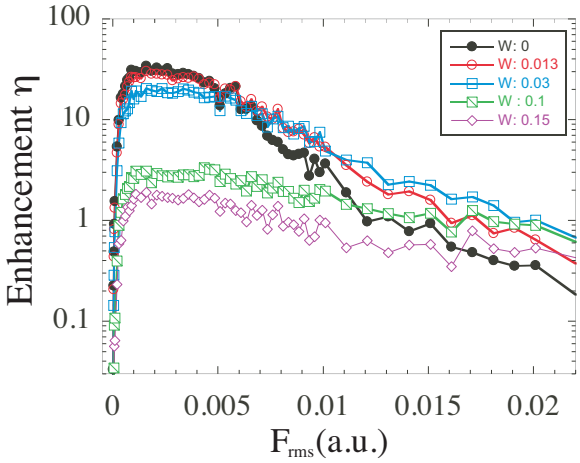


Figure 2: Enhancement due to a "perforated" chaotic light spectrum with holes of width W at the first three resonances of the hydrogen atom in Eq. (1). The curves correspond to increasing widths $W = 0, 0.013, 0.03, 0.1$ and 0.15, at which the last case essentially discards all frequencies, where the hydrogen atoms absorbs significantly, see Fig. 3.

Diatomic molecules We have found an even more dramatic enhancement due to non-linear photo absorption in the combination of chaotic light and a driving femtosecond pulse for diatomic molecules [5] which is illustrated in the parameter plane of light and noise amplitude, (F_0, D) in Fig. 4. Since it is rather difficult to dissociate a molecule with a strong laser pulse without ionizing it, noise offers an interesting possibility to increase the efficiency of dissociation. One can use structured white noise, which can be thought of as random kicks in time by short light pulses, but with an average delay Δt between two pulses: If Δt is of the order of molecular vibrational periods, the electronic motion will hardly couple to the noise, but the nuclear motion is sensitive to it which allows a dissociation of up to 30% [6].

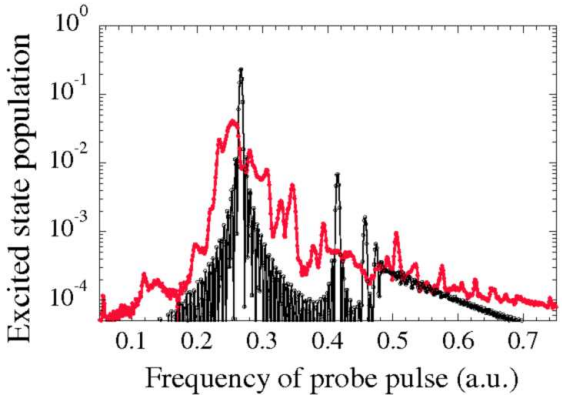


Figure 3: Frequency-resolved gain profile of the atom which is driven by a 10 cycle laser pulse with the same strength and frequency as in Fig. 1. The atomic gain (black) is probed by a synchronized weak probe beam ($F_p = 0.0005$) of tunable frequency ω_p. The gain of the driven atom is shown in red.

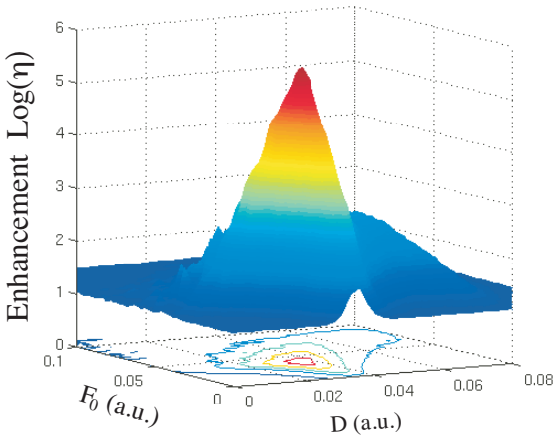


Figure 4: The enhancement landscape $\eta(D, F_0)$ with noise amplitude D (Eq. (2)) and the peak amplitude $F_0 = 0.04$ of a 15 cycle laser pulse with frequency $\omega = 0.007$ illuminating an HF molecule which is described by a Morse potential [5].

[1] Kamal P. Singh and Jan M. Rost Phys. Rev. Lett. **98** (2007) 160201; Phys. Rev. **76** (2007) 063403.

[2] L. Gammaitoni, P. Hänggi, P. Jung, and F. Marchesoni, Rev. Mod. Phys. **70** (1998) 223.

[3] C. Gardiner, Handbook of Stochastic Processes (Springer-Verlag, Berlin, 1983).

[4] R. L. Martens *et al.*, Phys. Rev. Lett. **94** 033001 (2005).

[5] Kamal P. Singh, Anatole Kenfack and Jan M. Rost, Phys. Rev. **A 77** (2008) 022707.

[6] A Kenfack, F Grossmann and Jan M. Rost, New J. Phys. **10** (2008) 013020.

2.7 Attosecond Coherent Control

Feng He, Camilo Ruiz and Andreas Becker

Understanding the nature of inter- and intra-molecular dynamics, visualizing the creation and breaking of molecular bonds and observing and controlling in real time a chemical reaction has been and is still one of the major goals in physics and chemistry. Bond breaking and bond forming in a molecule is an ultrafast dynamical process involving the motion of electrons and nuclei. Using the time resolution of femtosecond laser pulses it has become possible to control the dynamics on the timescale of the nuclear motion. Currently we are observing another technological breakthrough with the advent of phase-stabilized few-cycle pulses and subfemtosecond pulses. Such light pulses provide a temporal resolution beyond the limit of nuclear motion and pave the way to observe, probe and control the correlated electronic and nuclear motion in a molecule.

The first concepts of controlling electron dynamics in a reaction using these new laser technologies were proposed recently. They deal with the simplest process in a molecular bond, namely the localization of the electron in the dissociating hydrogen molecular ion. The control over the electronic motion has been achieved either by the carrier-to-envelope phase of a few-cycle laser pulse at Ti:sapphire wavelengths [1–4] or by two coherent time-delayed ultrashort laser pulses [5–7].

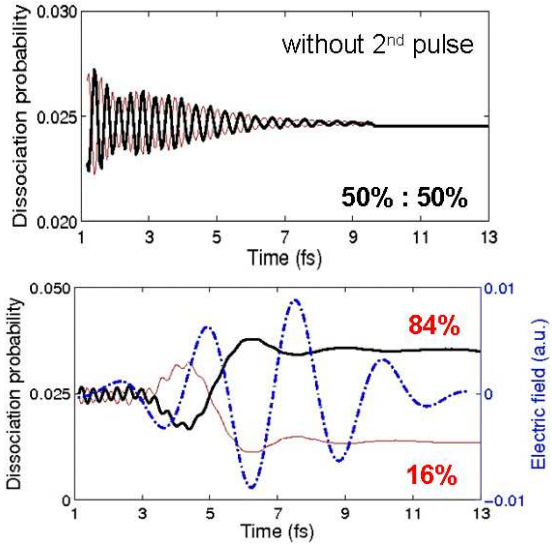


Figure 1: Electron localization probabilities at the two protons in a dissociating hydrogen molecular ion as function of time. The dissociation is initiated by a transition from the $1s\sigma_g$ ground state to the $2p\sigma_u$ excited state via an attosecond pulse. Without further interaction the electron is found with the same probability at either one of the nuclei (upper panel). Application of a time-delayed infrared laser pulse, shown by its electric field (blue line), leads to a control over the electron localization (lower panel) [5].

The latter scenario, proposed by us, is an extension of the pulse timing control technique, known from the control of fragment selectivity in femtochemistry [8, 9], to the regime of electron dynamics on the (sub-)femtosecond time scale. According to our scheme the dissociation of the hydrogen molecular ion (or other molecules) is initiated by a transition from the electronic ground state to a dissociative excited state of the molecule using an attosecond laser pulse. While the distance between the protons increases, the internuclear Coulomb barrier acts as an ultrafast shutter and traps the electrons at either one of the two nuclei with equal probabilities as long as there is no further interaction (Figure 1, upper panel). By applying a second few-cycle ultrashort pulse during the shutter time the electron is driven by the oscillating electric field of the laser and can be located with high probability at one of the nuclei (Figure 1, lower panel). The control is achieved via the parameters of the second laser pulse, namely its wavelength, pulse duration, carrier-to-envelope phase as well as its time delay to the initiation of the dissociation by the first pulse.

Next, we have extended the pulse timing control strategy by using attosecond pulse *trains* instead of an isolated single attosecond pulse for the excitation step [7]. Isolation of a single attosecond pulse can be realized today with state of the art experiments by either selecting high-energy cutoff harmonics from a few-cycle pulse or by using the polarization gating technique. More easily obtained are the attosecond pulse trains, as they are produced in infrared laser pulses of many-cycles. In this case the pulses are separated by either half a period or the full period of the driving pulse. In both cases a train of electron wave packets is generated in the excitation step, which can be controlled by the time-delayed infrared pulse. A high degree of control over the total localization probability can be achieved if the pulses in the train are separated by *a full cycle* of the infrared laser, but a considerably lower one if the separation is just *half a cycle*. Our analysis (c.f. Figure 2) has shown that this is due to the fact that in the former scenario each electron wave packet is directed to the same direction (nucleus) while in the latter subsequent wave packets are steered in opposite directions (nuclei). As a result the asymmetry and the degree of control in the *total* localization probability over the two nuclei almost vanishes for trains of attosecond pulses separated by half a period of the driving pulse. In contrast, full control over the asymmetry remains present in the scenario, where the attosecond pulses are separated by a full period of the driving pulse.

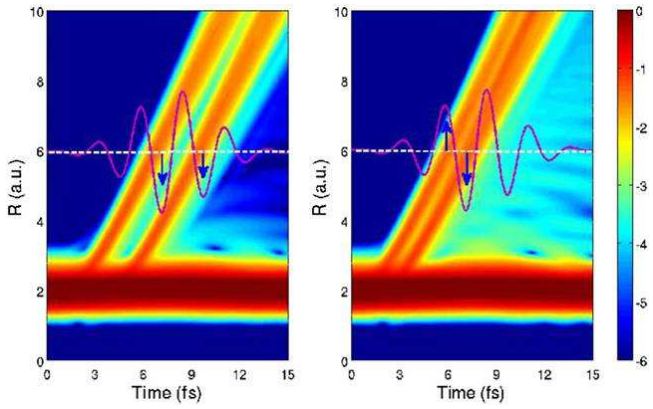


Figure 2: Results of numerical simulations of the hydrogen molecular ion interacting with a sequence of two attosecond laser pulses [7]. In the panel on the left the time delay of the two attosecond pulses was doubled as compared to the scenario considered for the results shown in the right hand panel. Shown are probability distributions $P(R,t) = \int\int |\phi(R,z,\rho;t)|^2 dz\rho d\rho$, where R is the internuclear distance and ρ and z are the coordinates of the electron. In both cases, the distribution is initially located around the equilibrium distance at about R=2 a.u., before due to the interaction with the attosecond pulses two dissociating wave packets are created which propagate to larger internuclear distance. The electric field plotted at about $R = 6$ a.u. schematically indicates how the two wave packets can be located at one of the two nuclei by application of another laser pulse.

The present pulse timing control scheme is found [6] to be more effective than the previously proposed [1] (and experimentally studied [2]) control scheme based on the variation of the carrier-to-envelope phase of a few-cycle infrared laser pulse. In the latter case a dissociative wave packet with a rather broad distribution over the internuclear distance R is generated due to two effects. Since the laser pulse contains a few cycles, several dissociative wave packets are created. Furthermore dissociation occurs via different pathways and the sub-wave packets overlap during further propagation. It is therefore not very likely that the resulting widely spread dissociative wave packet can be controlled to a high degree as it passes the critical internuclear distance during the shutter time. To obtain a high degree of control of the electron localization, it is desirable to confine the dissociative wave packet as much as possible. This is achieved in the pulse timing control scheme due to the excitation of electron wave packet(s) with attosecond laser pulse(s) directly to the excited dissociative state (c.f. Figure 2).

Finally, we have shown that at high intensities of the infrared laser pulse the electronic dynamics in a diatomic molecule driven by a strong field is even more complex and potentially counterintuitive [10]. Depending on the laser intensity, the direction of the electron's motion between the two nuclei is found to follow or oppose the classical laser-electric force. Our interpretation of this effect in phase space is based on the passage of electronic flux through diffracting momentum gates in the diatomic molecule that may or may not allow the electron to transfer to the other nucleus. The external laser field dynamically shifts the gates, causing the electron to explore different gates at different laser intensities, i.e. at different times during the varying electric field of the laser. This leads to a sensitive dependence of the electron-nuclear dynamics on the combined effect of both the external laser field and the diffraction gates. We expect that the dynamics and control of electronic motion at a sub-fs time scale in any other molecule should also be affected by at least these two effects. Indeed, diffraction effects have been found to play an important role in the phenomenon of suppressed molecular ionization in fullerenes [11].

Part of this work has been done in collaboration with U. Thumm (Kansas State University, USA).

[1] V. Roudnev, B. D. Esry, and I. Ben-Itzhak, Phys. Rev. Lett. **93** (2004) 163601.

[2] M. F. Kling, Ch. Siedschlag, A. J. Verhoef, J. I. Khan, M. Schultze, Th. Uphues, Y. Ni, M. Uiberacker, M. Drescher, F. Krausz, and M. J. J. Vrakking, Science **312** (2006) 246.

[3] X. M. Tong and C. D. Lin, Phys. Rev. Lett. **98** (2007) 123002.

[4] S. Graefe and M. Yu. Ivanov, Phys. Rev. Lett. **99** (2007) 163603.

[5] F. He, C. Ruiz, and A. Becker, Phys. Rev. Lett. **99** (2007) 083002.

[6] F. He and A. Becker, J. Phys. B **41** (2008) 074017.

[7] F. He, C. Ruiz, and A. Becker, J. Phys. B **41** (2008) 081003.

[8] D. J. Tannor and S. A. Rice, J. Chem. Phys. **83** (1985) 5013

[9] D. J. Tannor, R. Kosloff, and S. A. Rice, J. Chem. Phys. **85** (1986) 5805.

[10] F. He, A. Becker, and U. Thumm, Phys. Rev. Lett. **101** (2008) 213002.

[11] A. Jaroń-Becker, A. Becker, and F. H. M. Faisal, Phys. Rev. Lett. **96** (2006) 143006.

2.8 High Harmonic and Attosecond Pulse Generation at Mid-Infrared Laser Wavelengths

Marcello Ciappina, Feng He, Camilo Ruiz and Andreas Becker

Recent upsurge in the development and application of ultrafast intense laser sources at mid-infrared wavelengths is related to the semiclassical rescattering picture [1], which predicts a scaling of strong-field phenomena with the wavelength of the laser. According to this picture an electron tunnels out of the atom or molecule in the quasistatic laser field and propagates away from the core, like a classically free electron. As the direction of the field changes the electron returns to the core region, where it can recombine with the core (leading to higher-order harmonic generation) or it is elastically (leading to acceleration to high energies) or inelastically (leading to nonsequential double and multiple ionization) scattered from the core. The maximum classical energies for the harmonics and the electrons are found as $I_p + 3.17U_p$ and $10U_p$, respectively. Here, I_p is the ionization potential of the target atom or molecule and $U_p = I/4\omega^2$ is the cycle-averaged kinetic energy (or ponderomotive energy) of the oscillating motion of a free electron in a field of intensity I and frequency ω. These scaling laws show that a control of the energies of the returning and the outgoing (backscattered) electron can be achieved via the ponderomotive potential, i.e. the intensity and the frequency or wavelength of the laser pulse.

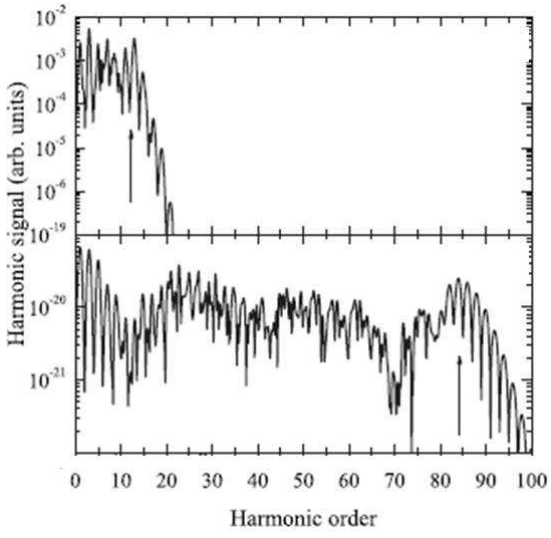


Figure 1: Theoretical predictions [2] using an extension of the so-called Lewenstein or three-step model [3] to molecules, for high-order harmonic spectra generated in C_{60} at $\lambda = 800$ nm (upper panel) and $\lambda = 1800$ nm (lower panel) and an intensity of $I = 5\times10^{13}$ W/cm^2. The arrows indicate the cutoff of the plateau as predicted from the semiclassical model [1, 3].

Figure 1 shows a comparison of theoretical predictions of the high harmonic spectra of the C_{60} fullerene at 800 nm (upper panel) and 1800 nm (lower panel), but the same intensity [2]. It is clearly seen, that the spectrum extends to higher harmonics in case of the longer wavelength in the mid-infrared regime. The corresponding maximum harmonic orders predicted by the semiclassical rescattering picture are indicated by the arrows in the Figure. We have studied how these new laser sources can be utilized to image the nuclear frame of large fullerenes and to generate attosecond pulses.

Molecular imaging One of the exciting goals in intense laser science is that of imaging dynamical changes in molecular structure and molecular reactions on an ultrafast time scale. A promising tool for such investigations is high-harmonic generation (HHG). This perspective becomes obvious from the physical mechanism, mentioned above, in which an electron is steered back in the linearly polarized field to its origin and recombines under the emission of a high-energy photon. An unique aspect of HHG is its sensitivity to the orientation and structure of the molecule and the symmetry of the highest occupied molecular orbital [4].

We have studied high-order harmonic generation in fullerenes with icosahedral symmetry interacting with a linearly polarized intense short laser pulse at near- and mid-infrared wavelengths [2, 5], using an extension of the so-called three-step or Lewenstein model [3] to the molecular case. The results exhibit modulations in the plateaus of the spectra at the longer wavelengths, as shown in Figure 1 (lower panel) for the C_{60} fullerene. These modulations are due to a multislit interference effect [6] arising from the contributions of the different atomic centers in the fullerene to the dipole moment. Unlike in the case of di- and other polyatomics, the interference patterns do not disappear for molecular ensembles oriented randomly with respect to the polarization axis of the laser. This is due to the high symmetry of the nuclear cage of C_{60}. The modulations are found in the results obtained in both the length as well as the velocity gauge.

It has been further shown that the positions of the interference minima are related to the zeros of the matrix element in the recombination step. In view of the correspondence we have applied a simple spherical model for the fullerenes [7] to derive a formula for an estimation of the radius of the fullerene cage from the interference pattern in the harmonic spectra. The estimates are in rough agreement with the average distance of the atoms

from the center of the fullerene. Thus, the observation of high harmonic spectra may establish a way to image the fullerene cage during the interaction with a strong pulse. This option may be interesting in view of recent experimental observations and theoretical predictions of oscillations of the nuclear frame during the interaction of C_{60} with an intense laser pulse [8, 9].

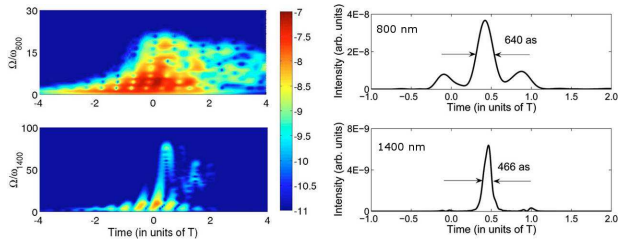


Figure 2: Panels on the left: Time-frequency analysis (on a logarithmic scale) using a wavelet transform for driving laser pulses at 800 nm (upper panel) and 1400 nm (lower panel) in an ellipticity modulated electric field. Panels on the right: Attosecond laser pulses generated from the harmonics near the end of the harmonic plateau from 800 nm (upper panel) and 1400 nm (lower panel) driving pulses [11].

Attosecond pulse generation Attosecond pulses are produced by high harmonic generation (HHG) from a driving laser pulse at high intensity. In an oscillating field this process repeats every half cycle, which leads in a multicycle driving pulse to a train of attosecond pulses. Isolated single attosecond pulses have been realized using e.g. a polarization gating technique [10]. The polarization gating method is based on the strong dependence of the generation of high harmonics on the ellipticity of the driving pulse. The transverse field component causes the ionized electron wave packet to be driven away from the parent ion. Consequently, the high-harmonic signal falls off rapidly with increasing ellipticity. This feature of HHG has been used by modulating the driving laser pulse such that it is only linearly polarized during its central part while elliptically polarized elsewhere.

We have studied theoretically high-harmonic order and single attosecond pulse generation with elliptically polarized laser pulses at wavelengths ranging from the visible to the mid-infrared [11]. Results of ab-initio simulations of the time-dependent Schrödinger equation of the hydrogen atom interacting with an elliptically polarized intense laser pulse show that the ellipticity dependence of the high harmonic signal intensifies with increasing wavelength of the driving pulse and saturates in the mid-infrared. It is further found that the generation of a single attosecond pulse via the polarization gating technique using mid-infrared driving pulses is indeed promising.

This can be seen from the results presented in Figure 2 in which we show on the left a time-frequency analysis of the harmonic response at 800 nm (upper panel) and 1400 nm (lower panel) in ellipticity modulated fields with the same number of field cycles. While for the near-infrared laser pulses there are several bursts at high-harmonic energies, in the mid-infrared just one significant burst occurs. Consequently, just a single attosecond pulse is generated at the mid-infrared wavelength (lower panel on the right), while at 800 nm (upper panel on the right) a train of three attosecond pulses is seen. Thus, at the longer wavelength side bands are effectively suppressed. Furthermore, the duration of the (central) attosecond pulse is shorter in the midinfrared, however the intensity is reduced compared with the generation at 800 nm.

Part of this work (molecular imaging) has been done in collaboration with A. Jaroń-Becker (Technical University Dresden).

[1] P. B. Corkum, Phys. Rev. Lett. **71** (1993) 1994.

[2] M.F. Ciappina, A. Becker and A. Jaroń-Becker, Phys. Rev. A **76** (2007) 063406.

[3] M. Lewenstein, P. Balcou, M. Y. Ivanov, A. L'Huillier, and P. B. Corkum, Phys. Rev. A **49** (1994) 2117.

[4] M. Lein, J. Phys. B **40** (2007) R135.

[5] M.F. Ciappina, A. Becker and A. Jaroń-Becker, Phys. Rev. A **78** (2008) 063405.

[6] A. Jaroń-Becker, A. Becker and F.H.M. Faisal, Phys. Rev. Lett. **96** (2006) 143006.

[7] S. Hasegawa, T. Miyamae, K. Yakushi, H. Inokuchi, K. Seki, and N. Ueno, Phys. Rev. B **58** (1998) 4927.

[8] R. Sahnoun, K. Nakai, Y. Sato, H. Kono, Y. Fujimara, and M. Tanaka, Chem. Phys. Lett. **430** (2006) 167.

[9] T. Laarmann, I. Shchatsinin, A. Stalmashonak, M. Boyle, N. Zhavoronkov, J. Handt, R. Schmidt, C.P. Schulz, and I.V. Hertel, Phys. Rev. Lett. **98** (2007) 058302.

[10] G. Sansone, E. Benedetti, F. Calegari, C. Vozzi, L. Avaldi, R. Flammini, L. Poletto, P. Villoresi, C. Altucci, R. Velotta, S. Stagira, S. De Silvestri, and M. Nisoli, Science **314** (2006) 443.

[11] F. He, C. Ruiz, and A. Becker, Opt. Lett. **32** (2007) 3224.

2.9 Entanglement-Screening by Nonlinear Resonances

Ignacio García-Mata, André R. R. Carvalho, Florian Mintert and Andreas Buchleitner

So far, little is known about entanglement in open quantum systems – where "open" refers to the unavoidable coupling to uncontrolled degrees of freedom in the "environment", which eventually induces decoherence in the system dynamics. However, it is a well established common belief that coherence and entanglement gets more and more fragile with increasing system size. In our present contribution, we will show that also exactly the opposite can happen. This can be understood from generic features of quantum dynamics with underlying mixed, regular-chaotic phase space structure, i.e., from quantum chaos [1]. We will see that nonlinear resonances, which are ubiquitous in classical Hamiltonian systems [2], naturally define robust strongly entangled multipartite quantum states, and the robustness of the associated multipartite entangled states is found to *increase* with the number of particles, i.e., in the semiclassical limit.

We start out with a system of k qubits that lives on a Hilbert space with tensor structure $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_k$, where each factor space $\mathcal{H}_j$ has dimension two. The "computational basis" $\{|i\rangle\}$, which spans $\mathcal{H}$, is given by the k-particle product states (i.e., by binary k-strings, which we identify with the binary representations of $i = 0 \ldots N-1$), and has dimension $N = 2^k$. Maps on classical phase space can be implemented efficiently in such systems after suitable identification of the computational with the position basis $\{|q_i\rangle\}$, upon the substitution $q_i = i/N$ [3–5]. Then, the corresponding momentum basis $\{|p_i\rangle\}$ is given by the discrete Fourier transform of $\{|q_i\rangle\}$ [6]. Thus, the phase space is wrapped on a torus, with a phase space area $1/N$ occupied by a single position basis state. Coherent (or minimum uncertainty) states are obtained as Gaussian wave packets of width $1/\sqrt{N}$ both in position and momentum [7]. Accordingly, the effective Planck constant is given by $\hbar_{\rm eff} = 1/2\pi N$, and the semiclassical limit $\hbar_{\rm eff} \to 0$ of arbitrary phase space resolution by a single quantum state is approached as the particle number k tends to infinity.

Given this quantum coarse graining of phase space, we will now monitor the time evolution of the multipartite entanglement of a quantum state initially prepared as a minimum uncertainty Gaussian wave packet, launched at different positions on the torus (which we will unfold as a unit square, for the ease of illustration). We propagate the wave packet by the unitary operator

$$U^t = (e^{iN\chi_2 \cos(2\pi\hat{q})} e^{iN\chi_1 \cos(2\pi\hat{p})})^t \,, \qquad (1)$$

(with t integer) which follows from the quantization of the classical Harper map

$$\begin{aligned} p' &= p - \chi_1 \sin(2\pi q) \\ q' &= q + \chi_2 \sin(2\pi p') \end{aligned} \quad (\mathrm{mod} 1) \,. \qquad (2)$$

Equation (2) describes a particle subject to a periodic impulse, with a position-dependent amplitude [8], and exhibits a transition from regular to chaotic dynamics as the kicking strengths χ_1, χ_2 are tuned from $\chi_1, \chi_2 \lesssim 0.11$ to $\chi_1, \chi_2 \gtrsim 0.63$. Here, we employ the fixed values $\chi_1 = \chi_2 = \chi = 0.4964$, what defines a mixed phase space structure as depicted in the inset of Fig. 1.

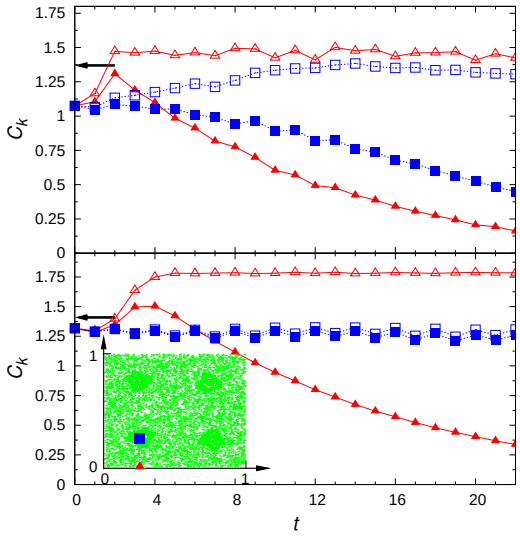


Figure 1: Evolution of multipartite concurrence C_k for two different numbers of qubits: $k = 5$ (top), $k = 8$ (bottom). Open symbols refer to unitary dynamics, while filled symbols represent the evolution under the diffusive noise. Squares correspond to an initial condition inside the nonlinear resonance island, triangles to initial conditions within the chaotic sea, in the classical phase space spanned by p and q (see inset).

The quantum evolution (1) modifies the decomposition of the evolved state $|\psi_t\rangle$ in the computational basis, and thus the entanglement of the k degrees of freedom defined by the constituent qubits. In order to assess the nonclassical correlations inscribed into the evolved state, we use the k-partite concurrence C_k as defined in [9].

We start out with a short inspection of the entanglement dynamics under purely coherent dynamics, to set the scene. The evolution is generated by application of U^t, where the integer t counts the number of applications and defines a discrete time. The open symbols in Fig. 1 represent $C_k(t)$, for two different initial positions

(also indicated by filled triangles and squares in the inset) of the initial minimum uncertainty state in phase space – either within an elliptic island ($q = p = 0.25$; open squares), or within the chaotic phase space component ($q = 0.25$, $p = 0.0$; open triangles).

Since, on the quantum level, chaotic dynamics is tantamount of strong coupling in any basis, it immediately follows that C_k will increase rapidly for the initial condition placed in the chaotic domain, and saturate once equilibrated over the chaotic eigenstates of the quantized Harper map – this is indeed observed in the figure.

For $k = 5$, the initial coherent state cannot be well accommodated within the elliptic island in phase space (due to the finite size of $\hbar_{\rm eff}$), and exhibits non-negligible tunneling coupling to its chaotic environment. Consequently, as time proceeds, the coherently evolved state spreads more and more over the chaotic phase space component, and its entanglement finally reaches essentially the same value as for the initial condition within the chaotic domain, just after considerably longer time.

In contrast, for $k = 8$, tunneling from the island into the chaotic sea occurs on a much longer time scale (which, on average, increases exponentially with $\hbar_{\rm eff}$), and remains invisible on the time scale covered in Fig. 1. The small oscillations of $C_{k=8}(t)$ are due to the spreading of the initial wave packet along the regular island's tori.

This screening of the initial state from the chaotic sea when initially placed within the elliptic island, more and more efficient with increasing particle number, has an immediate consequence for the robustness of the state's multipartite entanglement under the influence of decoherence, as illustrated by the filled symbols in Fig. 1: For chaotic initial conditions, an initial rise of C_k is rather quickly overruled by the loss of multiparticle coherence and hence of entanglement, and this is once again largely independent of k. However, for initial conditions within the island, $k = 5$ again leads to asymptotically the same behaviour as for the chaotic initial condition, while $k = 8$ induces entanglement dynamics almost completely unaffected by the noise. Thus, for sufficiently large k, equivalent to sufficiently small $\hbar_{\rm eff}$, and correspondingly suppressed tunneling rates, the classical nonlinear resonance creates strongly entangled multipartite states which, in addition, are robust against noise. This is further illustrated in Fig. 2, where $C_{k=8}(t = 16)$ is plotted for different initial conditions, in the absence and in the presence of noise:

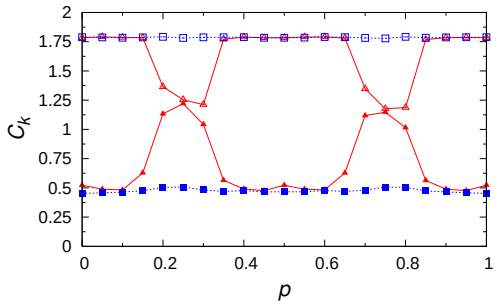


Figure 2: Eight-partite concurrence $C_{k=8}$ as a function of initial momentum ($p = 0.0, 0.05, \ldots, 0.95, 1.0$), after 16 iterations of the Harper map, with $\chi = 0.4964$. Open symbols correspond to unitary evolution, while filled symbols refer to unitary evolution amended by diffusive noise. Squares represent the initial position $q = 0.5$, and triangles $q = 0.25$. Peaks and dips of $C_{k=8}(t)$ are located exactly at the center of the nonlinear resonance island in classical phase space.

Clearly, entanglement is robust when shielded by the resonance island. While chaotic dynamics produce slightly stronger entanglement, this is significantly more fragile under decoherence.

Given the robust entanglement evolution for initial conditions within a regular island, also those eigenstates of the Harper Hamiltonian which are anchored to the classical regular island exhibit the same robustness properties. Thus, robust multipartite entangled states can be defined through the resonance condition which defines the regular island, a ubiquitous feature of Hamiltonian systems with mixed classical phase space structure.

[1] J. Madronero *et al.* Advances in Atomic, Molecular, and Optical Physics, Elsevier (2006).

[2] A. J. Lichtenberg and M. A. Lieberman, Regular and Chaotic Dynamics, Springer-Verlag (1991).

[3] A. J. Scott and C. M. Caves, J. Phys. A: Math. Gen. **36**, 9553 (2003).

[4] C. Miquel, J. P. Paz and M. Saraceno, Phys. Rev. A **65**, 062309 (2002).

[5] J. P. Paz and A. J. Roncaglia, M. Saraceno, Phys. Rev. A **69**, 032312 (2004).

[6] J. H. Hannay and M. V. Berry, Physica **1D**, 267 (1980).

[7] S. Nonnemacher, Nonlinearity **10**, 1569 (1997).

[8] P. Leboeuf, J. Kurchan, M. Feingold and D. P. Arovas, Phys. Rev. Lett. **65**, 3076 (1990).

[9] F. Mintert, A. R. R. Carvalho, M. Kuś, and A. Buchleitner, Phys. Rep. **415**, 207 (2005).

[10] V. Vedral et al., Phys. Rev. A **54**, 147 (1996).

[11] C. Miquel et al., Phys. Rev. A **54**, 2605 (1996).

2.10 A Factorization Law for Entanglement Decay

Thomas Konrad, Fernando de Melo, Markus Tiersch, Christian Kasztelan, Adriano Aragão, Andreas Buchleitner

Introduction Whenever we contemplate the potential technological applications of quantum information theory [1], from secure quantum communication over quantum teleportation [2] to quantum computation [3], we need to worry about the unavoidable and detrimental coupling of any such quantum device to uncontrolled degrees of freedom – typically lumped together under the label "environment". Environment coupling induces decoherence [4–6], i.e., it gradually destroys the phase relationship between quantum states, and thus their ability to interfere. In composite quantum systems, these phase relationships (or "coherences") are at the origin of strong quantum correlations between measurements on distinct system constituents – which then are *entangled*. The promises of quantum information technology rely on exploring precisely these non-classical correlations.

Yet, entanglement is *not* equivalent to many-particle coherences: it is an even stronger property, and hard to quantify – all commonly accepted entanglement measures [7,8] are *nonlinear* functions of the density matrix which describes the state of the composite quantum system, and in particular the coherences. While an elaborate theory on the time evolution of quantum states under environment coupling is at our hands, virtually no general results on entanglement dynamics have been stated. Hitherto, the time evolution of entanglement always needed to be *deduced* from the time evolution of the state [9–18]. In the present manuscript, a *direct* relationship between the initial and final entanglement of a two-qubit state undergoing a incoherent dynamics is presented [19], which, as illustrated in Fig. 1, renders the solution of the corresponding state evolution equation obsolete.

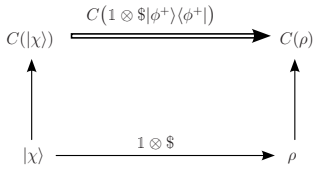


Figure 1: From state evolution to entanglement dynamics. Hitherto, the time evolution of entanglement C under open system dynamics had to be deduced from the time evolution of the state $|\chi\rangle$. However, it turns out that knowledge of the entanglement evolution of the maximally entangled state $|\phi^+\rangle$ under the channel $\mathbf{1}\otimes\$$ suffices to establish a direct mapping of $C(|\chi\rangle)$ onto $C(\rho)$, without detour over the state.

Main result Let us consider entangled states of qubit pairs, with one qubit being subject to an arbitrary channel $\$ – which may represent the influence of an environment, of a measurement, or of both. In order to illustrate the situation, we consider a source which emits a particle to the left and another one to the right (see Fig.2). Each particle on its own carries one qubit of quantum information (in general a superposition or mixture of two basis states $|0\rangle$ and $|1\rangle$).

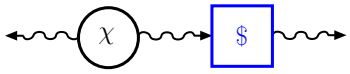


Figure 2: Entanglement decay scenario. One of the qubits of the initial pure state $|\chi\rangle$, the "right" one, undergoes the action of a general quantum channel $. The circle represents a source of entangled states, and the square symbolize the noisy channel.

In this scenario, the entanglement, as quantified by the concurrence C [20], evolves accordingly the simple factorization law:

$$C\left[(\mathbf{1}\otimes\$)\,|\chi\rangle\langle\chi|\right] = C\left[(\mathbf{1}\otimes\$)\,|\phi^+\rangle\langle\phi^+|\right]\; C(|\chi\rangle)\;; \quad (1)$$

The entanglement reduction under a one-sided noisy channel is *independent* of the initial state $|\chi\rangle$ and *completely determined* by the channel's action on a maximally entangled state. Thus, if we know the time evolution of the Bell state's entanglement, we know it for *any* pure initial state.

The factorization law (1) can be generalized for mixed initial states ρ_0, by virtue of the convexity of entanglement monotones such as concurrence, and given an optimal pure state decomposition $\rho_0 = \sum_j p_j|\psi_j\rangle\langle\psi_j|$, in the sense that the average concurrence over this pure state decomposition is minimal [21]. It then immediately follows, by convexity, that $C\left[(\mathbf{1}\otimes\$)\,\rho_0\right] = C\left[\sum_j p_j\,(\mathbf{1}\otimes\$)\,|\psi_j\rangle\langle\psi_j|\right] \le \sum_j p_j C\left[(\mathbf{1}\otimes\$)\,|\psi_j\rangle\langle\psi_j|\right]$, and application of (1) leaves us with

$$C\left[(\mathbf{1}\otimes\$)\,\rho_0\right] \le C\left[(\mathbf{1}\otimes\$)\,|\phi^+\rangle\langle\phi^+|\right]\; C(\rho_0)\;. \quad (2)$$

This inequality holds for all one-sided channels $, and has an immediate generalization for local two-sided channels $\$_1\otimes\$_2 = (\$_1\otimes\mathbf{1})(\mathbf{1}\otimes\$_\mathbf{2})$:

$$C\left[(\$_1\otimes\$_2)\,\rho_0\right] \le C\left[(\$_1\otimes\mathbf{1})\,|\phi^+\rangle\langle\phi^+|\right] \times C\left[(\mathbf{1}\otimes\$_\mathbf{2})\,|\phi^+\rangle\langle\phi^+|\right] C(\rho_0)\;. \quad (3)$$

The concurrence after passage through a two-sided channel is thus bounded from above, which immediately

implies a sufficient criterion for finite-time disentanglement [9, 10, 13] of *arbitrary initial states*, in terms of the evolution of the concurrence of the maximally entangled state under either one of the one-sided channels (e.g., choose $\$_1$ or $\$_2$ induced by infinite temperature or depolarizing environments).

Let us finally identify relevant cases when the inequality (2) saturates. For that purpose, we consider mixed states that are obtained after the application of a one-sided channel to an arbitrary pure state, $\rho_0 = (\mathbf{1} \otimes \$)|\psi_\mathbf{0}\rangle\langle\psi_\mathbf{0}|$. This occurs, for instance, if the qubit originally prepared in a pure state suffers amplitude decay, and the resulting mixed state again is subject to decay dynamics. This is tantamount to the concatenation of channels on one side, $(\mathbf{1} \otimes \$_\mathbf{2})\,(\mathbf{1} \otimes \$_\mathbf{1})\,|\psi_0\rangle\langle\psi_0|$, what can be lumped together as one channel which combines both actions, $(\mathbf{1} \otimes \$_\mathbf{2})\,(\mathbf{1} \otimes \$_\mathbf{1}) = \mathbf{1} \otimes \$_{\mathbf{2},\mathbf{1}}$. In a similar vein as for (2), and using the factorization relation (1) for pure states, we deduce

$$C\left[(\mathbf{1} \otimes \$_{\mathbf{2},\mathbf{1}})\,|\phi^+\rangle\langle\phi^+|\right] \leq C\left[(\mathbf{1} \otimes \$_\mathbf{2})|\phi^+\rangle\langle\phi^+|\right] \times C\left[(\mathbf{1} \otimes \$_\mathbf{1})|\phi^+\rangle\langle\phi^+|\right]\,. \quad (4)$$

The initial state's concurrence rescales both sides of the equation by the same amount, and therefore it is omitted in above equation. It is now sufficient to investigate the time dependence of the maximally entangled state's concurrence under the concatenated channels (much as for the evaluation of (1)): if all of these are of the form $C(t) = \exp(-\Gamma t)$ (which is the case, e.g., for $\$_1$ an amplitude decay and $\$_2$ a dephasing channel), then equality holds in (2), with $\$ = \$_1$, $\rho_0 = (\mathbf{1} \otimes \$_\mathbf{2})|\psi_\mathbf{0}\rangle\langle\psi_\mathbf{0}|$, and $C(\rho_t) = \exp(-\Gamma_1 t)C(\rho_0)$ (and, equivalently, for the roles of channels 1 and 2 interchanged).

Conclusion Equations (1,2,3,4) provide us with the first closed expression for the time evolution of a bipartite entangled state under general local, single- and two-sided channels, without recourse to the time evolution of the underlying quantum state itself. This is a general result inherited from the Jamiołkowski isomorphism [22], which is here "lifted" *from state to entanglement evolution* (see Fig. 1), and eases the experimental characterization of entanglement dynamics under unknown channels dramatically: instead of exploring the time-dependent action of the channel on *all* initial states, it suffices to probe the entanglement evolution of the maximally entangled state alone.

[1] C. Bennett and D. DiVincenzo, Nature **404**, 247 (2000).

[2] C. H. Bennett *et al.*, Phys. Rev. Lett. **70**, 1895 (1993).

[3] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, 2000).

[4] M. Schlosshauer, Rev. Mod. Phys. **76**, 1267 (2004).

[5] W. H. Zurek, Rev. Mod. Phys. **75**, 715 (2003).

[6] E. Joos *et al.*, *Decoherence and the Appearance of a Classical World in Quantum Theory* (Springer, 2003).

[7] F. Mintert *et al.*, Phys. Rep. **415**, 207 (2005).

[8] R. Horodecki *et al.*, (2007), quant-ph/0702225.

[9] K. Życzkowski *et al.*, Phys. Rev. A **65**, 012101 (2001).

[10] P. J. Dodd and J. J. Halliwell, Phys. Rev. A **69**, 052105 (2004).

[11] C. F. Roos *et al.*, Phys. Rev. Lett. **92**, 220402 (2004).

[12] A. R. R. Carvalho, F. Mintert, and A. Buchleitner, Phys. Rev. Lett. **93**, 230501 (2004).

[13] T. Yu and J. H. Eberly, Phys. Rev. Lett. **97**, 140403 (2006).

[14] M. F. Santos *et al.*, Phys. Rev. A **73**, 040305 (2006).

[15] W. Dür and H.-J. Briegel, Phys. Rev. Lett. **92**, 180403 (2004).

[16] M. P. Almeida *et al.*, Science **316**, 579 (2007).

[17] A. R. R. Carvalho *et al.*, Phys. Rev. Lett. **98**, 190501 (2007).

[18] M. Horodecki, P. W. Shor, and M. B. Ruskai, Rev. Math. Phys. **15**, 629 (2003).

[19] T. Konrad, F. de Melo, M. Tiersch, C. Kasztelan, A. Aragão, and A. Buchleitner, Nature Phys. **4**, 99 (2008).

[20] W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).

[21] C. H. Bennett *et al.*, Phys. Rev. A **54**, 3824 (1996).

[22] A. Jamiołkowski, Rep. Math. Phys. **3**, 275 (1972).

2.11 Formation of Atoms in Strongly Correlated, Ultracold Plasmas

Georg Bannasch and Thomas Pohl

The successful creation of ultracold neutral plasmas via photoionization of laser-cooled atoms [1] has tremendously stretched the parameter space of plasma physics. With their extremely low temperatures they open access to the domain of strongly correlated plasmas. Here we study the formation of atoms under such conditions. We demonstrate a break-down of its common description and show that recombination can be suppressed by several orders of magnitude.

Strongly coupled plasmas typically occur at high densities, such as in warm dense matter, produced by ionization of metal targets, or in astrophysical environments like the core of Jupiter. In classical systems the plasma state is uniquely characterized by the Coulomb coupling parameter

$$\Gamma = \frac{e^2}{a k_{\rm B} T_{\rm e}}, \qquad (1)$$

where e is the electron charge, $a = (4\pi\rho/3)^{-1/3}$ denotes the Wigner-Seitz radius at a plasma density ρ, and $T_{\rm e}$ is the electron temperature. The regime of strongly coupled plasmas is marked by $\Gamma \geq 1$, where the potential energy $\sim e^2/a$ exceeds that of thermal motion $\sim k_{\rm B}T_{\rm e}$. Because of their very low temperatures ultracold neutral plasmas (UNPs) potentially realize strong coupling conditions at densities that are many orders of magnitude smaller than in traditional plasmas. Thanks to these low densities they provide an ideal platform to study non-equilibrium plasma dynamics, as they offer "slow motion pictures" on a magnified spatial scale.

Formation of neutral atoms causes significant plasma heating [2,3], which limits the coupling strength achievable in UNPs. Current efforts to realize a strongly coupled electron component [4], thus, require an extension of recombination theory into the low-temperature domain.

At low temperatures atom formation is dominated by three-body recombination (TBR), in which two electrons collide in the vicinity of an ion to form a weakly bound Rydberg state. Subsequent electron-atom collisions drive the atom to deeper binding, and ultimately form a stably bound state upon passing a kinetic bottleneck (see below). The corresponding recombination rate ν is commonly described by [5]

$$\nu = C\rho_e^2\, T_{\rm e}^{-9/2} = 0.043\omega_{\rm p}\Gamma^{9/2}, \qquad (2)$$

where $C = 3.9 \cdot 10^{-9}{\rm cm}^6 s^{-1}$ is a numerical constant and $\omega_{\rm p} = \sqrt{e^2/a^3 m_{\rm e}}$ is the plasma frequency of electrons with mass $m_{\rm e}$. While eq.(2) is well confirmed at high and intermediate temperatures [5, 6], its validity becomes questionable at low temperatures. For $\Gamma > 1$ the temperature divergence predicted by eq.(2) implies a recombination time $1/\nu$ that is much shorter than the motional timescale of plasma electrons, and thus looses physical significance.

A consistent description of the recombination dynamics over a wide range of plasma parameters, consequently, requires to depart from the simplified three-body collision picture and account for correlated, many-body dynamics of the plasma electrons.

Classical particle simulations can provide a well suited framework for this problem. Here, we perform Monte-Carlo molecular dynamics simulations of a single ion embedded in an infinitely-extended electron background. Interactions between the electrons are determined via a Fast Multipole Method [7], to efficiently implement periodic boundary conditions.

The preparation of the initial state and in particular the inclusion of the ion requires some care, in order to assure energy conservation. First, we equilibrate the pure electron gas to produce a canonical ensemble characterized by a chosen value of Γ. Subsequently, we place a neutral electron-ion pair with positive relative energy at the box center. This procedure not only conserves energy during the ion insertion, but also yields a good description of the photoionization process used to produce UNPs.

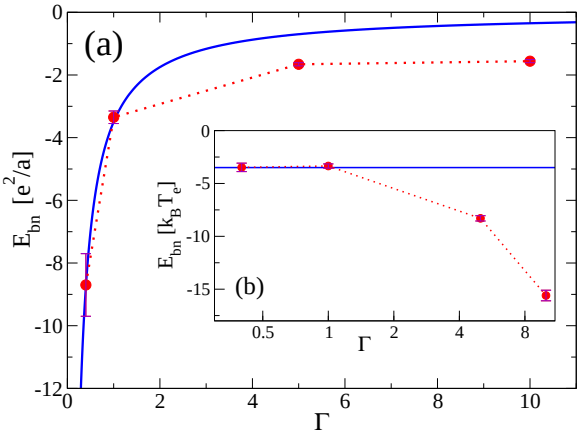


Figure 1: **Kinetic bottleneck energy** as a function of the Coulomb Coupling parameter Γ in units of the average potential (a) and kinetic (b) energy. The blue line shows the expected dependence of ideal plasmas as given by eq.(3).

As the plasma evolves the Rydberg state dynamics is monitored by recording the binding energy $E_{\rm b}$ of a formed atom as a function of time. Within a Monte Carlo scheme many realizations with randomly sampled

initial state configurations are then used to calculate ensembles averages of relevant observables from the obtained binding energy evolutions.

The kinetic bottleneck plays a crucial role in describing the dynamics of highly excited Rydberg states. The corresponding energy $E_{\rm bn}$ distinguishes between truly recombined and temporarily bound electrons. Once the binding energy of a loosely bound electron drops below this bottleneck energy re-ionization becomes less likely than a cascade to deeper binding. The recombination rate ν can, thus, be obtained as the phase space flux through the energy surface defined by $E_{\rm bn}$. In ideal plasmas, for which one obtains the recombination rate eq.(1), the bottleneck energy

$$E_{\rm bn} = -\alpha\, k_{\rm B} T_{\rm e} \tag{3}$$

is independent of density and has a simple linear temperature scaling, with a proportionality constant $\alpha \approx 4$ [5]. Fig.1 shows $E_{\rm bn}$, as obtained from our simulations, for four different values of the Coulomb coupling parameter Γ. For small Γ our numerical calculations well confirm the ideal-plasma prediction (3), with $\alpha \approx 3.5$. However, as Γ exceeds unity we find a significant departure from this behavior. For $\Gamma \gtrsim 5$ the bottleneck energy becomes independent of temperature and instead scales as

$$E_{\rm bn} = -\beta \frac{e^2}{a}\,, \tag{4}$$

with the proportionality constant $\beta \approx 1.7$. Despite the strongly correlated nature of the plasma dynamics, we, thus, arrive at the remarkably simple conclusion that the temperature, as the underlying energy scale, is replaced by the average interaction energy between electrons.

The recombination rate is obtained from the time dependent probability P to form a Rydberg state with a binding energy $E_{\rm b} \leq E_{\rm bn}$. Its typical time evolution is exemplified in the inset of fig.2 for $\Gamma = 1$. An exponential scaling $P = 1 - e^{-\nu t}$ provides a good fit to our data, from which we extract the recombination rate ν.

Fig.2 shows our calculated recombination rates for different values of the Coulomb coupling parameter. At

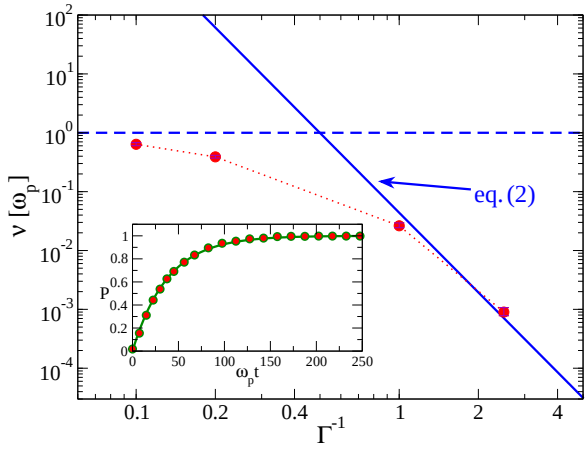


Figure 2: **Recombination rate** as a function of the Coulomb coupling parameter. The solid line shows the prediction of eq.(2) and the dashed line corresponds to $\nu = \omega_{\rm p}$. The insets exemplarily shows the recombination probability P for $\Gamma = 1$ fitted by $P = 1 - e^{-\nu t}$ (green line).

small Γ, i.e. in the weak-coupling domain, our simulations are in accord with the simplified three-body collision result [eq.(2)]. However, as Γ exceeds unity there is a strong departure from the predicted $\sim T^{-9/2}$ scaling. The data suggest that the recombination rate approaches the plasma frequency with increasing Coulomb coupling parameter, thus, removing the unphysical divergence predicted by eq.(2).

Discussion. The results discussed here represent an initial step towards a systematic description of collisional atom formation at ultra-low temperatures. A more refined analysis of the simulations will unravel the transition from the collisional regime to that of many-body interactions – extending deep into the strongly coupled region, where the plasma may even crystallize. We finally note that recent experiments that produce UNPs in a supersonic molecular beam [8] report unexpectedly long plasma lifetimes, inconsistent with the fast recombination predicted by eq.(2). The measured densities and temperatures imply a coupling parameter of up to $\Gamma \approx 10$, for which our calculations predict a dramatic suppression of the recombination rate by three orders of magnitude. However, a quantitative interpretation of these experimental findings will require a dynamical modeling of the plasma expansion, including additional influences of the molecular-beam environment.

[1] T. C. Killian, S. Kulin, S. D. Bergeson, L. A. Orozco, C. Orzel, and S. L. Rolston, Phys. Rev. Lett. **83**, 4776 (1999).

[2] R. S. Fletcher, X. L. Zhang, and S. L. Rolston, Phys. Rev. Lett. **99**, 145001 (2007).

[3] P. Gupta, S. Laha, C. E. Simien, H. Gao, J. Castro, T. C. Killian, and T. Pohl, Phys. Rev. Lett. **99**, 075005 (2007).

[4] S. D. Bergeson and F. Robicheaux, Phys. Rev. Lett. **101**, 073202 (2008).

[5] P. Mansbach and J. Keck, Phys. Rev. **181**, 275 (1969); J. Stevefelt, J. Boulmer, and J -F. Delpech, Phys. Rev. A **12**, 1246, (1975)

[6] T. Pohl, D. Vrinceanu, and H. R. Sadeghpour, Phys. Rev. Lett. **100**, 223201 (2008).

[7] H. Dachsel and I. Kabadshow, http://www.fz-juelich.de/jsc/fmm, (2008).

[8] J. P. Morrison, C. J. Rennick, J. S. Keller and E. R. Grant, Phys. Rev. Lett. **101**, 20 (2008)

2.12 Excitation Crystals in Ultracold Gases

Thomas Pohl, Eugene A. Demler and Mikhail D. Lukin

Owing to their exaggerated dimensions, highly excited Rydberg atoms are very susceptible to external fields and to interactions with each other. Here we demonstrate the utility of such strong interactions to form crystalline structures of regularly arranged Rydberg atoms out of disordered ultracold atomic gases. They are composed of localized collective excitations, which have an enhanced coupling to light and can be selectively excited by chirped laser pulses.

Strong interactions between Rydberg atoms can arise from electric field induced dipoles [1], resonant transition dipoles [2] or dipole-induced van der Waals potentials [3]. The latter scales as the eleventh power of the atoms principle quantum number, and for typical Rydberg states can, thus, be more then ten orders of magnitudes larger than for ground state atoms. Such strong interactions drastically affect their very creation through laser-excitation of cold atomic gases. For example a complete dipole blockade of multiple excitations enables the production of collective excitations [4, 5], with potential applications in quantum information processing. On the other hand, resonant excitation of larger systems resembles relaxation of disordered spins towards short-range correlated states [6]. Here we outline a scheme that avoids such relaxation processes and permits the preparation of well-defined many-body states of Rydberg excitations with similar degree of control as for the dipole blockade.

The basic idea rests on an adiabatic change of the many-body ground state as illustrated in fig.1. If the Rydberg atoms interact by repulsive van der Waals potentials $V = C/r^6$, the states with the lowest interaction energy maximize the spacing between Rydberg atoms for a given number n of excitations. Consequently, they arrange on regular crystals (fig.1b). Suppose that initially all atoms are in their ground states and the ensemble is excited into Rydberg states by a coherent laser field. For large negative detunings of the laser field Δ, the initial state coincides with the many-body ground state in the rotating frame of reference. However, as Δ increases to positive values, it effectively lowers the energy levels of excited many-body states (fig.1c). In a quasi one dimensional system of length $s_{||}$ they ultimately cross at critical detunings [7]

$$\Delta^n_{n+1} = \frac{C}{s_{||}^6}\left(n^7 - (n-1)^7\right) \overset{n\gg 1}{\to} 7\frac{C}{s_{||}^6}n^6; \qquad (1)$$

marking discrete jumps in the Rydberg atom number from n to $n+1$ (fig.1d), and inducing stepwise changes

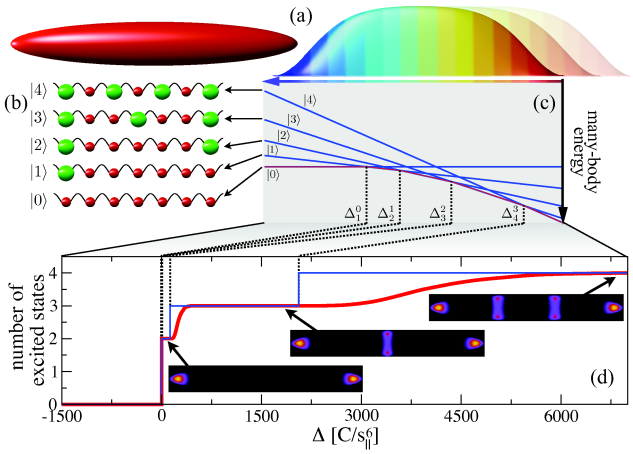


Figure 1: **Crystal state preparation.**(a) A cold atomic gas is illuminated by a chirped laser pulse, whose frequency changes from the blue ($\Delta < 0$) to the red ($\Delta > 0$) side of the driven Rydberg transition. (b) Schematics of the many-body energy spectrum as a function of the laser detuning Δ and for $\Omega = 0$. Shown are the lowest-energy states $|n\rangle$ for a given Rydberg atom number n. These states correspond to Rydberg atom (green spheres) lattices sketched in (c). Their energy crossings give rise to an excitation number staircase shown in (d) for a chain of $N = 31$ atoms (thin line) and a cigar-shaped condensate (thick line) with the same size and 500 atoms. The insets show the Rydberg atom densities resulting in the latter at the detunings marked by the arrows.

of the many-body state from the initial state $|0\rangle$ to regular chains of n excited Rydberg atoms ($|n\rangle$), during evolution of the chirped laser pulse. In essence, the detuning acts as a control parameter that decreases the energy difference between adjacent number states $|n\rangle$ and $|n+1\rangle$, allowing further Rydberg atoms to "enter" the excitation volume. The resulting "dipole-blockade staircase" bears resemblance to the Coulomb blockade staircase observed in nano-scale solid-state devices [8], where the number of electrons increases as a function of external lead-voltage. Compared to such solid state devices, the present systems permit dynamical manipulation in a highly coherent manner.

The excitation dynamics is obtained from a numerical solution of the underlying Schrödinger equation. For typical atom numbers this, in principle, requires to account for at least $\sim 10^{100}$ many-body states. To solve this problem we apply a truncation of the corresponding Hilbert space that exploits the dipole blockade of close atom pairs [7]. While this approach is limited in the number of Rydberg excitations it allows us to treat realistically large systems with up to several thousand atoms.
In fig.2 we show the excitation dynamics of a cigar-shaped Rubidium condensate excited to $65s$ Rydberg

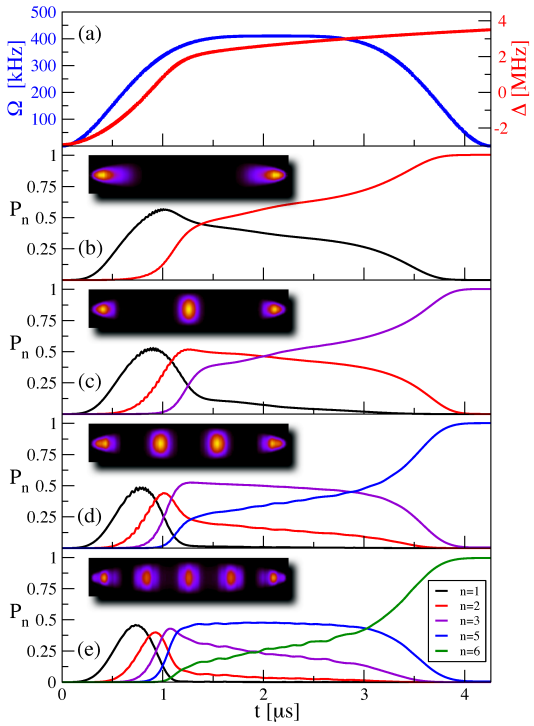


Figure 2: **Dynamic preparation of Rydberg lattices.** (a) Pulse envelope and chirp of the applied laser field, that excites a cigar-shaped Rb condensates to 65s states. (b)-(e) Resulting time dependence of the probabilities P_n to excite n atoms for $s_{||} = 15\mu$m (b), 22.5μm (c), 35μm (d), 45μ (e). The insets show the corresponding final Rydberg atom densities.

states (fig.2a). Increasing $s_{||}$ gives smaller critical detunings Δ^n_{n+1} [see eq.(1)], such that consecutively larger lattices are produced (fig.2b-2e). The depicted time evolution of the Rydberg atom number populations P_n demonstrates that – despite the disordered atom positions – the gas is transferred to a state with precisely n excitations, distributed over perfectly filled crystals.

Detection of the crystalline states can be done in several ways, such as position sensitive field ionization or Rydberg atom counting. Alternatively, the ordered Rydberg atom configurations can be mapped onto correlated states of light, and subsequently be detected as a pulse train of localized single photons.
Here a strong π-pulse is used to transfer the prepared Rydberg crystal to a crystal of atoms in another hyperfine ground state. Analogous to light stopping in an EIT medium such collective excitations – when driven by an adiabatic control pulse within a three-level Λ configuration – can be transferred to quantum states of light [7]. Fig. 3 shows the calculated propagation of a pulse produced from a three-Rydberg atom lattice. Albeit slight deformations due to a inhomogeneous group velocity, the Rydberg chain is mapped onto a clear triple-peak structure, which, for the chosen laser parameters, has well resolvable delay times of $\sim 1\mu$s.

Discussion. While the results discussed here are restricted to quasi one-dimensional systems, the presented scheme works equally well in higher dimensions. Such crystals naturally realize a network of localized collective excitations, without the need of extended micro-trap arrays. In this manner they form a suitable initial state to study quantum random walks in mixtures of different Rydberg states. Although our simulations are limited to comparably small excitation numbers, simple scaling laws suggest that large crystals can be prepared under typical experimental conditions. Chirped excitation of lattice-confined atoms to large Rydberg atom fractions would provide a platform to study magnetism of long-range interacting spins and explore their quench dynamics through quantum phase transitions. In this context, the described optical imaging offers a real-space probing technique of the system state. From another perspective, the presented scheme also provides a deterministic source that produces single-photon trains on demand with broadly tunable delay times.

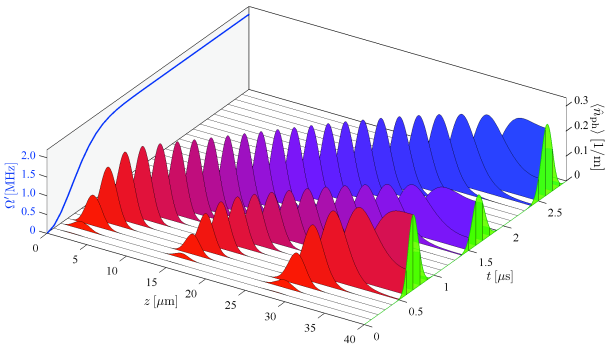


Figure 3: **Crystal state mapping.** Propagation of photon pulses produced from a three-atom crystal (see fig.2c). The outer-left blue curve shows the time evolution of the control Rabi frequency Ω', while the right green area gives the corresponding photon signal, detectable just outside the atom cloud.

[1] T. Vogt et al., Phys. Rev. Lett. **99**, 073002 (2007).
[2] T. Pohl and P. R. Berman, Phys. Rev. Lett. **102**, 013004 (2009).
[3] D. Tong et al., Phys. Rev. Lett. **93**, 063001 (2004).
[4] M.D. Lukin et al., Phys. Rev. Lett. **87**, 037901 (2001).
[5] E. Urban et al., Nature Phys. **5**, 110 (2009); Gaëtan, A. et al. Nature Phys. 5, 115 (2009).
[6] H. Weimer, R. Löw, T Pfau, and H.P. Büchler, Phys. Rev. Lett. **101**, 250601 (2008).
[7] T. Pohl, E.A. Demler and M.D. Lukin, to be published.
[8] *Mesoscopic Phenomena in Solids*, edited by B. Altshuler, P.A. Lee, and R.A. Webb (Elsevier, Amsterdam, 1991).

2.13 Dynamic Patterning of Two-dimensional Tissues

Thomas Bittig, Reza Farhadifar and Frank Jülicher

The emergence of morphologies and spatial patterns during the development of organisms from the fertilized egg remains a fundamental challenge in biology. Key mechanisms by which the morphology of cell arrangements, tissue size and shape are controlled remain unknown. An important model system are two dimensional sheets of cells, called epithelia. Epithelia form by repeated cell division from a small group of initial cells which have almost identical properties. Pattern formation in tissues involves signaling systems by which cells communicate. A key example are morphogens which are secreted by localized sources and form graded concentration profiles by a combination of diffusion and degradation [1]. These morphogens guide the position dependent expression of genes in the tissue.

Tissues consist of many cells which are packed in specific morphologies. These cell packings are inherently dynamic and are remodeled during development, in particular by cell division and cell death (called apoptosis). Of particular importance is the role of anisotropic cell division in this process. If cells divide predominantly along a preferred axis, the tissue grows anisotropically and the tissue shape is modulated. The cell division axis is indeed tightly controlled on the cellular level by local asymmetric cues and active rotation of the division apparatus using molecular motors [2]. By controlling the statistics of cell division orientation, the shape of a growing tissue then emerges as a collective behavior of many cells [3].

Cellular packings in two dimensional tissues can be characterized by the network of junctions, which are the adhesive lines along which neighboring cells are in close contact. We have studied the basic physical principles which govern morphological changes and dynamic rearrangements during isotropic and anisotropic growth of epithelia. These principles can be studied in coarse-grained descriptions on different scales. They range from vertex models to account for cell mechanics and shape [4] to the hydrodynamic limit where the tissue exhibits properties of an active visco-elastic fluid [3].

Cell packings in growing tissues. We have introduced a vertex model which describes the role of cell mechanics, cell adhesion as well as contractile ring structures to guide cell repacking and shape changes in developing epithelia [4]. This description is simplified by an important separation of time scales. Cell shapes relax in a time of the order of minutes as can be directly observed in experiments in which cell junctions are ablated by a UV laser pulse. This relaxation time is short compared to time scales of hours at which cells divide or tens of hours where spatial patterns form. Therefore, the junctional network is described as a force balanced configuration which adjusts quasistatically to slow changes in cell size and cell mechanical properties while the tissue develops.

The vertex model represents the network of cell junctions in a two dimensional packing. This network can be observed experimentally and is characterized by a set of cells $\alpha = 1, .., N_c$ and vertices $i = 1, ..., N_v$ with position $\mathbf{R}_i$ which are connected. Stable and stationary configurations are minima of a potential function [4]

$$E = \sum_\alpha \frac{K_\alpha}{2}(A_\alpha - A_\alpha^{(0)})^2 + \sum_{\langle ij \rangle} \Lambda_{ij} L_{ij} + \sum_\alpha \frac{\Gamma_\alpha}{2} L_\alpha^2 \,. \quad (1)$$

Here, A_α is the area and L_α the perimeter of cell α, L_{ij} is the length of bond $< ij >$. Cell elasticity is described by the modulus K_α, $A_\alpha^{(0)}$ denotes a preferred area. The bond tension is denoted Λ_{ij} and Γ_α is called perimeter contractility.

Figure 1: Cell packings resulting from repeated cell division in the vertex model. The statistical features of the cell packing depends on biophysical properties of cells and their interactions characterized by cell elasticity, junctional tension and perimeter contractility. Three different tissue types are shown which differ in these parameters. Case I is very similar to the morphology of cells in the developing wing of the fruit fly.

In large regions of parameter space, a perfect hexagonal network is the ground state of this potential. Starting with a small set of hexagonally packed cells, a tissue morphology is generated by introducing cell division. This is done by quasistatically increasing the preferred area of a randomly selected cell. After growth a new bond with isotropically or anisotropically distributed orientation is introduced and the network is relaxed. In this process topological changes called T1 and T2 transitions occur which remodel the junctional network and change cell neighbor relations. By repeating this process, an irregular cell packing with characteristic statistical features emerges. It can be characterized by several parameters such as neighbor number distribution and cell area distribution which can also be measured experimentally.

We find that the statistical properties of cell packings and thus tissue morphology crucially depend on the

biophysical properties of cells such as elasticity, junctional tension and contractility, see Fig. 1. We have estimated the biophysical parameters characterizing the tissue by using the vertex model to account for observed rearrangements that result from laser ablation of cell junctions. Using these parameter values, a simulation of growth generates a tissue morphology which indeed closely resembles the observed tissue. The vertex model can thus quantitatively account for cell shape and cell packing. It will provide the basis for future studies of the role of cell communication in growing epithelia during development.

Hydrodynamic limit. On large scales the slow modes of the system can be described in a generic hydrodynamic limit by a continuum description. This limit can be derived by general principles based on conservation laws and symmetries. The topological rearrangement described by the vertex model imply that on large scales the tissue can flow and behave as a complex fluid. Cell division induces active anisotropic stresses [3]. In the hydrodynamic limit we define the cell number density ρ which satisfies the balance equation

$$\partial_t \rho + \nabla(\rho \mathbf{v}) = (k_g - k_a)\rho\,, \tag{2}$$

where k_g and k_a denote the local rates of cell division and cell death, respectively, and $\mathbf{v}$ is the flow velocity of cells. Cell division introduces an active stress in the constitutive equations of the fluid. If cell division is on average aligned along a direction $\mathbf{p}$ which is a unit vector, the axial anisotropy can be characterized by a traceless symmetric tensor $\tilde{q}_{\alpha\beta} = p_\alpha p_\beta - (1/2)\delta_{\alpha\beta}$. We consider for simplicity the case where cells are incompressible which implies $\nabla \cdot \mathbf{v} = (k_g - k_a)$. Shear deformations, characterized by the traceless part $\tilde{u}_{\alpha\beta}$ of the velocity gradient tensor $u_{\alpha\beta} = (1/2)(\partial_\alpha v_\beta + \partial_\beta v_\alpha)$, are determined by force balances. Taking into account the active anisotropic stress generated by asymmetric cell division, the constitutive relation for the cellular material reads

$$2\eta \tilde{u}_{\alpha\beta} = \tilde{\sigma}_{\alpha\beta} + \mu k_g \tilde{q}_{\alpha\beta}\,. \tag{3}$$

Here, $\tilde{\sigma}_{\alpha\beta}$ is the traceless part of the stress tensor, η is the tissue viscosity and μ is a phenomenological coefficient with units of viscosity that describes stress generation by anisotropic cell division.

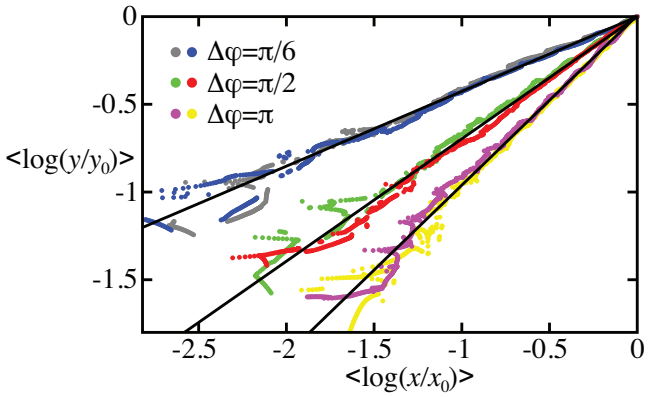


Figure 2: Averaged cell trajectories during anisotropic growth. The averages $\langle \log(x/x_0) \rangle$ and $\langle \log(y/y_0) \rangle$ of the cell positions (x, y) at different times during growth are displayed. The black lines reveal the power law behavior of the cell trajectories.

To illustrate the properties of growing tissues in the hydrodynamic limit, we discuss the simple case where the parameters as well as the rates k_g and k_a are position independent. From the force balance $\partial_\beta \sigma_{\alpha\beta} - \partial_\alpha P = 0$, where P is pressure, we obtain the flow field

$$\mathbf{v} = \begin{pmatrix} (k_0 + k_1)x \\ (k_0 - k_1)y \end{pmatrix}. \tag{4}$$

Here, $2k_0 = (k_g - k_a)$ is the area growth rate, while $k_1 = \mu k_g/(4\eta)$ characterizes anisotropic growth. As a consequence of anisotropies, the flow lines of cells scale as

$$y = y_0 x^{\frac{k_0+k_1}{k_0-k_1}}\quad . \tag{5}$$

The hydrodynamic theory can be studied numerically by a discrete description of the active fluid. We use a dissipative particle dynamics where cells are represented as deformable particles which interact with their neighbors by an interaction potential. Cell division is described by replacing a particle by two new particles, displaced by a small distance ϵ in a direction taken from an angular distribution.Viscosity is represented by relative friction between neighboring particles. The behavior of anisotropic growth in such a simulation is displayed in Fig. 2. It reveals emergent power laws in the cell trajectories which depend on cell properties and the angular distribution of cell division.

[1] A. Kicheva, P. Pantazis, T. Bollenbach, Y. Kalaidzidis, T. Bittig, F. Jülicher and M. González-Gaitán: Kinetics of morphogen gradient formation, Science **315**, 521 (2007)

[2] M. Théry, A. Jiménez-Dalmaroni, V. Racine, M. Bornens and F. Jülicher: Experimental and theoretical study of mitotic spindle orientation, Nature **447**, 493 (2007)

[3] T. Bittig, O. Wartlick, A. Kicheva, M. González-Gaitán and F. Jülicher: Dynamics of Anisotropic Tissue Growth, New J. Phys. **10**, 63001 (2008)

[4] R. Farhadifar, J.-C. Röper, B. Algouy, S. Eaton and F. Jülicher: The Influence of Cell Mechanics, Cell-Cell Interactions and Proliferation on Epithelial Packing, Curr. Biol. **17**, 2095 (2007)

2.14 Chemotaxis of Sperm Cells

Benjamin M. Friedrich and Frank Jülicher

In order to find the egg cell, sperm cells respond to chemical cues from the egg. They possess a sensory system which allows them to steer their swimming path. As a consequence, they move upwards a gradient of a chemoattractant. This process called chemotaxis is important for fertilization. Sperm chemotaxis is well established in marine invertebrates with external fertilization such as sea urchins [1] but also occurs in mammals including humans. Sperm cells are active microswimmers which are propelled in a liquid by the regular beat of their flagellum. In a two-dimensional experimental setup with sperm confined between two surfaces, sea urchin sperm cells swim on circular paths. The nonzero curvature of their swimming paths is a consequence of a chiral asymmetry of their flagellar beat. In a concentration gradient of a chemoattractant, the swimming paths resemble drifting circles (or trochoids) with a drift in the direction upwards the gradient. Chemoattractants stimulate an electro-chemical signaling system in the sperm flagellum which modulates the flagellar beat and thereby elicits a swimming response. Far from surfaces, sea urchin sperm cells swim on helical paths. In the presence of a chemoattractant concentration gradient, the helices bend, eventually leading to alignment of the helix axis with the gradient and net motion again upward the gradient. We have developed a general theory of sperm chemotaxis in two and three dimension which can account for the key properties and explains the reliability of the mechanism even in the presence of fluctuations [2–5].

Chemotaxis along circular paths in a plane. In two dimensions, chemotaxis can by studied by considering a planar swimming path $\mathbf{r}(t)$. The geometry of the path is characterized by its curvature $\kappa = |\dot{\mathbf{t}}|/v$ which characterizes the rotation rate of the tangent vector $\mathbf{t} = \dot{\mathbf{r}}/v$ with swimming speed $v = |\dot{\mathbf{r}}|$. If the curvature is constant, $\kappa = \kappa_0$, the swimming path is a circle with radius $r_0 = 1/\kappa_0$. The angular frequency of swimming in circles is $\omega_0 = v_0\kappa_0$ for constant swimming speed $v(t) = v_0$. In general, the curvature $\kappa(t)$ of a sperm swimming path changes with time t as a result of chemotactic steering. While swimming in a concentration field $c(\mathbf{x})$ of chemoattractant, receptors for the chemoattractant molecules, which are located on the flagellum surface, perceive a temporal concentration stimulus $s(t)$

$$s(t) = c(\mathbf{r}(t)). \tag{1}$$

This stimulus $s(t)$ triggers a response of the chemotactic signaling network which controls the activity of motor proteins in the flagellum and thereby modulates the curvature of the swimming path. We describe the dynamic dependence of the curvature $\kappa(t)$ on the chemotactic stimulus $s(t)$ by a generic signaling system which exhibits adaptation and relaxation [2, 3]. For a time-independent stimulus $s(t) = s_0$ the system reaches a steady state with $\kappa(t) = \kappa_0$ independent of the stimulus level s_0 due to its adaptation property. Small periodic variation of the stimulus $s(t) = s_0 + s_1\cos(\omega_0 t)$ evoke a periodic response $\kappa(t) = \kappa_0 + \rho_\kappa s_1 \cos(\omega_0 t + \varphi_\kappa)$ with amplitude gain ρ_κ and phase shift φ_κ.

An example of a swimming path in a linear concentration field is shown in Fig. 1. The swimming path can be described as circles whose centers $\mathbf{R}(t)$ drift along well defined trajectories. The corresponding chemotactic stimulus $s(t)$ comprises a periodic modulation with the frequency ω_0, and and a monotonic increase of its average value which results from the fact that the swimming circles drift gradient-upwards. The adaptive chemotactic signaling system processes this stimulus and causes a periodic modulation of the curvature. This results in the drift of the swimming circles. Due to the adaptive behavior of the signaling system, the monotonous increase of the stimulus is filtered out, there is thus no corresponding increase of the average curvature.

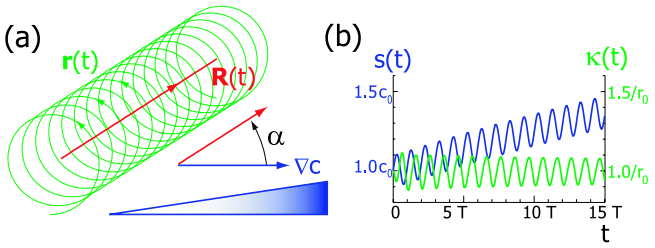


Figure 1: (a) Planar sperm swimming path in a linear concentration field obtained numerically from our theoretical description. The swimming path shown resembles a drifting circle; the drift direction encloses an angle α with the gradient direction ∇c. (b) Along its circular swimming path, the sperm cell traces a concentration stimulus $s(t)$ from the concentration field that comprises a periodic modulation with the frequency of circular swimming (blue). The signaling system processes this stimulus and modulates the curvature $\kappa(t)$ of the swimming path $\mathbf{r}(t)$ accordingly (green).

Many analytical results can be obtained in the limit case of a weak concentration gradient with $|\nabla c|r_0/c \ll 1$ [2]. We characterize the drift of the circle center by a drift speed $v_d = v_0 r_0^2 \rho_\kappa |\nabla c|/2$ and a drift direction at an angle α with respect to the gradient direction. The drift angle depends on the phase shift φ_κ

$$\alpha = 3\pi/2 - \varphi_\kappa. \tag{2}$$

Hence, a sperm cell will move gradient upwards whenever $\pi < \varphi_\kappa < 2\pi$. Our theoretical description of sperm chemotaxis can be extended to incorporating sources of fluctuations such as stochasticity of the chemotactic

stimulus $s(t)$ and internal noise of chemotactic signaling. We find that in the presence of fluctuations the chemotactic drift of the center of the swimming circles persists and is superimposed by effective diffusion with a diffusion coefficient that depends on chemoattractant concentration [3].

Chemotaxis along helical paths in three dimensions. The geometry of a path $\mathbf{r}(t)$ in three space dimensions is characterized by its curvature $\kappa(t)$ and torsion $\tau(t)$: For a planar swimming path, the binormal vector $\mathbf{b} = \dot{\mathbf{t}} \times \mathbf{t}/(v_0\kappa)$ is normal to the plane of swimming and torsion vanishes. In general, $\mathbf{b}$ may rotate around $\mathbf{t}$ resulting in non-zero torsion $\tau = \dot{\mathbf{b}} \cdot \dot{\mathbf{t}}/(v_0^2\kappa)$. For constant curvature $\kappa(t) = \kappa_0$ and torsion $\tau(t) = \tau_0$ the swimming path is a perfect helix with radius $r_0 = \kappa_0/(\kappa_0^2 + \tau_0^2)$ and pitch $2\pi h_0 = 2\pi\,\tau_0/(\kappa_0^2 + \tau_0^2)$. The angular frequency of helical swimming is $\omega_0 = v_0\,(\kappa_0^2 + \tau_0^2)^{1/2}$. Swimming along a helical path $\mathbf{r}(t)$ in a chemoattractant concentration field leads again to a time-dependent stimulus $s(t) = c(\mathbf{r}(t))$ as in the two dimensional case. The signaling system modulates both curvature and torsion of the swimming path. The response of the torsion to weak periodic stimuli is characterized by an amplitude gain ρ_τ and a phase shift φ_τ.

Fig. 2 shows an example of a swimming path in a radial concentration field which leads toward the origin of the concentration field. The swimming path $\mathbf{r}(t)$ is super-helical: It is a perturbed helix that winds around a curved centerline. The helix vector $\mathbf{h}$ which characterizes the direction of propagation of the centerline rotates with time t.

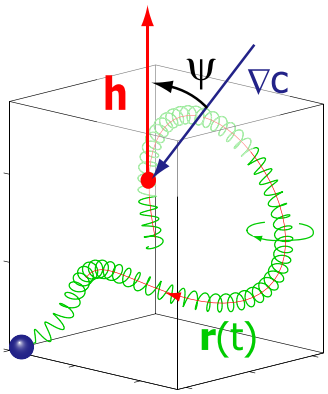


Figure 2: Numerical solution of a sperm swimming path (green) in the vicinity of a target (blue) that releases chemoattractant: The helical path bends to a super helix which winds towards the target. The bent of the helical path is characterized by a rotation of the helix vector $\mathbf{h}$.

As in the planar case, we can employ a perturbation calculation in order to characterize sperm swimming paths in the limit of a weak concentration gradient. As a result, we find an effective equation of motion for the angle ψ enclosed by the helix vector $\mathbf{h}$ and the direction of the concentration gradient ∇c in a linear concentration field

$$\dot{\psi} = -\beta \sin\psi. \qquad (3)$$

Depending on the sign of the alignment parameter $\beta = -\omega_0 r_0 |\nabla c|(h_0\rho_\kappa \cos\varphi_\kappa - r_0\rho_\tau \cos\varphi_\tau)/2$, the helical paths aligns parallel ($\beta > 0$) or anti-parallel ($\beta < 0$) with respect to the direction of the gradient. Again, we find a broad range of phase shifts $\varphi_\kappa, \varphi_\tau$ for which the helical path moves gradient-upwards. In a radial concentration field of chemoattractant established by diffusion from a single source, an equation of motion similar to (3) can be derived, which governs the dynamics of ψ and the distance R of the centerline $\mathbf{R}(t)$ to the origin of the concentration field. By analyzing fixed points and flow of the corresponding dynamical system, we obtained conditions for a sperm cell to generically find the source.

Within the general framework outlined, we can investigate the role of fluctuations for sperm chemotaxis [4,5]. In the presence of noise, the helix vector $\mathbf{h}$ performs a stochastic motion on the unit sphere. This motion can be characterized as a superposition of deterministic chemotactic alignment of the helix vector towards the concentration gradient with diffusion on the unit sphere. The steady state distribution of helix vector orientation is formally equivalent to the distribution of a thermally fluctuating dipole in an external field.

Discussion. Helical swimming paths are ubiquitous in nature and are a direct result of an asymmetric propulsion mechanism. In addition to sperm, it has been observed for ascidian larvae, for eukaryotic flagellates such as *Chlamydomonas*, and even for some bacteria. Our work demonstrates that temporal sampling of a concentration field along a helical path provides a robust strategy for chemotaxis if curvature and torsion are modulated in response to the stimulus. The robustness of this chemotaxis mechanism relies on an effective average over several helical turns. This mechanism can work reliably over a large concentration range and depends only on a few generic properties of the signaling network.

[1] U. B. Kaupp *et al.*: Mechanisms of sperm chemotaxis. Annu. Rev. Physiol., **70**, p. 93-117, 2008.

[2] B. M. Friedrich, F. Jülicher: Chemotaxis of sperm cells, Proc. Natl. Acad. Sci., **104**(33), p. 13256-13261, 2007.

[3] B. M. Friedrich, F. Jülicher: The stochastic dance of circling sperm cells, New J. Phys, **10**, p. 123035, 2008.

[4] B. M. Friedrich: Search along persistent random walks, Phys. Biol., **5**, p. 026007(6), 2008.

[5] B. M. Friedrich, F. Jülicher: Steering chiral swimmers along noisy helical paths, arXiv:0903.0930, 2009.

2.15 Dynamics of Axon Fasciculation in the Presence of Neuronal Turnover

Debasish Chaudhuri and Martin Zapotocky

Introduction: Sensory neurons located in peripheral tissues connect to the brain via *axons*. The direction of growth of these neuronal extensions is controlled by the *growth cone* structure at the tip of each axon, which probes the environment in its vicinity. In the absence of external signals, each growth cone maintains an approximately constant average growth direction, while exploring stochastically the environment in the transverse direction [1].

In this report, we study the collective effects that arise from *direct contact interactions* among the growing axons. When the interaction is attractive, the resulting dynamics leads to the formation of fascicles of axons – a common and essential feature of the developing nervous system. An important aspect included in our model is that of *neuronal turnover*: during development, a significant portion of sensory neurons with fully grown axons may die, and be replaced by younger sensory neurons which attempt a new connection to the brain. Our study is motivated by the properties of the mammalian olfactory system, in which the birth (and also death) events persist throughout the life of an animal, leading to a dynamical steady state pattern of connectivity between the olfactory epithelium and the olfactory bulb [2]. Here we restrict our attention to the fundamental properties of the basic version of our model.

The main contribution of this report is a detailed discussion of the slow time scales that emerge from the dynamics of our model. While the stationary properties of the system (such as the fascicle size distribution in the steady state) may be approximately understood using an analogy to one-dimensional diffusion with aggregation, the dynamical properties (time scales of approach to steady state, and correlation times in steady state) are undefined in the 1-dimensional analogy, and require understanding based on the full 2-dimensional model (see the discussion of fascicle basin dynamics).

Model and numerical implementation: Each growing axon is represented as a directed random walk in two spatial dimensions (Fig. 1*a*). The random walkers (representing the growth cones) are initiated at the periphery ($y = 0$, random x) with a birth rate α, and move towards the target area (large y) with constant velocity $v_y = 1$. In the numerical implementation on a tilted square lattice, at each time step the growth cone at (x, y) can move to $(x-1, y+1)$ (left) or $(x+1, y+1)$ (right). The probability $p_{\{L,R\}}$ to move left/right is evaluated based on the axon occupancy at the $(x-1, y+1)$ and $(x+1, y+1)$ sites and their nearest neighbors (see Fig. 1*a*). In the simplest version of the model, all axons belong to the same type, and their interaction is governed by the "always attach, never detach" rule: $p_L = 1$ when among the sites $(x \pm 1, y+1)$, $(x \pm 3, y+1)$ only $(x-3, y+1)$ is already occupied; $p_R = 1$ when only $(x+3, y+1)$ is occupied; $p_L = p_R = 1/2$ in all other cases.

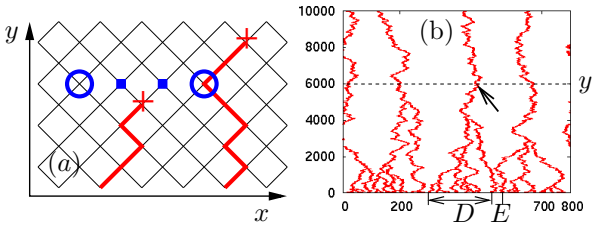


Figure 1: (*a*) Interacting directed random walks on a tilted square lattice. A random walker (+) represents a growth cone. For one walker, the possible future sites (□) and their nearest neighbors (○) are marked. The trail of a walker (line) models an axon shaft. (*b*) Typical late-time configuration ($t = 25T$) in a system with $L = 800$ and $N = 100$. For the fascicle identified at $y = 6000$ (arrow), D indicates its basin, i.e. the interval at the level $y = 0$ between the right-most and left-most axons belonging to the fascicle. The gap E is the inter-basin free space at $y = 0$. Note that the y-coordinate cannot be understood as equivalent to time.

To capture the effect of neuronal turnover, each random walker is assigned a lifetime from an exponential distribution of mean T. When the lifetime expires, the random walker and its entire trail is removed from the system. The time-averaged number of axons in the system therefore reaches the steady state value $N = \alpha/\beta$ (at $y = 0$), where $\beta = 1/T$ is the population death rate per axon. In the simulations reported here, $T = 10^5$ time steps and $y \leq T/10$. The birth rate α is chosen so as to obtain the desired axon density $\rho = N/L$, where L is the system size in x-direction.

A typical late-time configuration is shown in Fig. 1*b*. With increasing y, the axons are aggregated into a decreasing number of *fascicles*. Correspondingly, the mean fascicle size $\bar{n}(y, t)$, obtained by averaging over all existing fascicles at level y at time t, increases with y. At $y \simeq (L/2)^2$, complete fasciculation ($\bar{n} = N$) is expected.

Slow time scales: The measured mean fascicle size at a given fasciculation distance y (Fig. 2) grows with time as $\bar{n}(t) = n_\infty - p\exp(-\beta t) - q\exp(-t/\tau_{ap})$, where $\tau_{ap}(y)$ defines the time scale of approach to the steady state value $n_\infty(y)$. Asymptotically in y, we find $n_\infty = c + 2\rho y^b$, with $b = 0.48 \pm 0.02$ (Fig. 2 inset) – in good agreement with mean-field arguments [3]. The time scale τ_{ap} likewise increases with y, and can exceed the axon lifetime T by orders of magnitude (Figs. 2 and 3*b*).

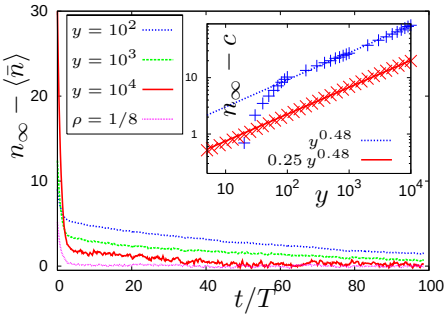


Figure 2: Approach to the steady state in the $L = 400$, $N = 200$ system at representative fasciculation distances y indicated in the legend. The mean fascicle size $\langle \bar{n}(t; y) \rangle$ [averaged over 10^3 initial conditions] approaches $n_\infty(y)$ as $t \to \infty$. The data set labeled as $\rho = 1/8$ is from the $L = 400$, $N = 50$ system, collected at $y = 5000$. Inset: Power-law growth of mean fascicle size $n_\infty - c = 2\rho y^b$ in the steady state, for system with density $\rho = 1/8$ ($\times$), and $\rho = 1/2$ ($+$).

The dynamics in the steady state is characterized by the auto-correlation function for the mean fascicle size $\bar{n}(t)$ at a fixed y-level: $c(t) = \langle \bar{n}(t)\bar{n}(0) \rangle$ which is well fit by the form $p + q\exp(-\beta t) + r\exp(-t/\tau_c)$. In Fig. 3*a* we plot the subtracted correlation function $g(t) = [c(t) - p]/(q + r)$. The correlation time τ_c increases with y and significantly exceeds the axon lifetime T (Fig. 3*b*). (Both $\tau_{ap}(y)$ and $\tau_c(y)$, however, drop to T at $y \simeq (L/2)^2$, where a single fascicle remains.) In addition, the time scales τ_{ap} and τ_c are found to be higher in systems with larger density ρ (Fig. 3*b*).

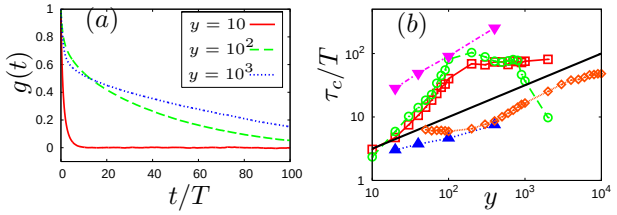


Figure 3: (*a*) Subtracted auto-correlation $g(t)$ at y-levels indicated in the legend for the $L = 100$, $N = 50$ system. The time series $\bar{n}(t)$ is collected over $t = 200T$ to $2 \times 10^4 T$; $g(t)$ is further averaged over 30 initial conditions. (*b*) The correlation time τ_c ($\Box$) and approach-to-steady-state time scale τ_{ap} ($\circ$) as a function of y. The theoretical time-scales τ (filled $\triangle$), τ_f (filled ∇) (see text) are evaluated from the values of a_+, b_+, c_+ in Table I. The solid line is y^b with $b = 1/2$. τ_c ($\diamond$) for the $L = 400$, $N = 50$ system is also shown.

Effective fascicle dynamics at fixed y: To understand the origin of the slow time scales, we next examine the dynamics of individual fascicles. At a given fasciculation distance y, the number $n(t)$ of axons in each fascicle may be viewed as given by a stochastic process specified by the rates $u_\pm(n, y)$ (for transitions $n \to n \pm 1$). The loss rate $u_-(n) = \beta n$, independent of y.

The gain rate $u_+(n, y)$ is governed by the properties of the fascicle *basin* (see Fig. 1*b*). Under the "always attach, never detach" rule, new axons initiated anywhere within the basin of size D cannot escape the fascicle at level y. In addition, some of the axons born in the two gaps (of size E) flanking the basin contribute. Therefore $u_+ = \alpha D/L + (\alpha E/L)[1 - \Pi(E, y)]$, where $\Pi(E, y)$ is the probability that an axon born within the gap of size E survives as a single axon at level y. At high y, $\Pi(E, y) \to 0$.

In Fig. 4*a*, we plot the number of axons $n(t)$ and the basin size $D(t)$ for a specific fascicle (from the full system simulation) followed over $200T$. It is seen that n and D tend to co-vary (cross correlation coefficient $c(D, n) = 0.74$). In the following effective model of fascicle dynamics, we treat the dynamics of D as slave to the dynamics of n, i.e. we assume that the average separation $S = D/(n - 1)$ between two neighboring axons within the basin is time-independent. This implies $u_+(n) = a + bn$ with $b = \beta\rho S$. The measured average gain rate $u_+(n)$ in the steady state deviates from linearity at high n, but is well fit by $u_+(n) = a_+ + b_+ n - c_+ n^2$ (Fig. 4*b*). The quadratic correction may be understood as a saturation effect which reflects that basins of size $D > 2y^{1/2}$ occur with low probability.

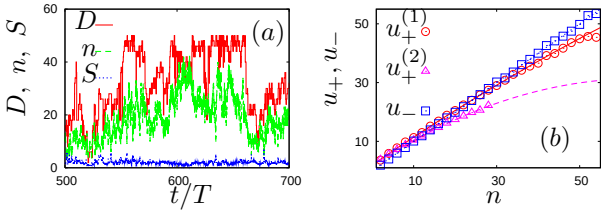


Figure 4: (*a*) Time series of number of axons n, basin size D and $S = D/(n - 1)$ for an individual fascicle in a system of $L = 100$ and $N = 50$ at $y = 400$. (*b*) Mean gain and loss rates (in units of β) [averaged over 10^3 initial conditions and the interval $100T \le t \le 150T$] as a function of fascicle size n. The rates are measured at $y = 400$ in a system with $L = 100$.

Two distinct time scales may be extracted from the effective birth-death process. The correlation time τ for the fascicle size n, near the macroscopic stationary point n_s [$u_+(n_s) = u_-(n_s)$] can be expressed as [4] $\tau = 1/(u'_-(n_s) - u'_+(n_s)) = 1/(\beta - b_+ + 2c_+ n_s)$. The time scale $\tau_a p$ for the approach of $\langle n \rangle(t)$ to its steady-state value is readily evaluated in the linear approximation $u_+(n) = a_+ + b_+ n$, yielding $\tau_{ap} = 1/(\beta - b_+)$.

It is seen that slow time scales ($\gg T$) are obtained when $\beta \simeq b_+$. This condition can be satisfied only as a consequence of the dynamics of the fascicle basins. To see that, imagine a fascicle with frozen boundary axons, for which $u_+ \approx (\alpha/L)D$ with D constant. In this case $u'_+(n_s) = 0$ and the correlation time $\tau \simeq T$. To obtain $\tau > T$, D must co-vary with n. At high y, $u'_+ \approx 1/T$, resulting in $\tau \gg T$.

Distribution of fascicle sizes: Further insight about the dynamics of the full system is obtained by studying the distribution of fascicle sizes $P_s(n, y)$, defined as the average number of fascicles of size n, at level y, in the steady state regime. As demonstrated

in Fig. 5, in the intermediate y-range $1 \ll y \ll L^2$ the distribution is well described by the scaling form

$$P_s(n,y) = \langle n(y)\rangle^{-\eta}\phi(n/\langle n(y)\rangle) \qquad (1)$$

where the exponent $\eta = 2.1 \pm 0.1$ and the scaling function $\phi(u) = \mathcal{N}u\exp(-\nu u - \lambda u^2)$.

Consistency with the effective single-fascicle description developed above requires that the birth-death process with rates $u_+(n) = a_+ + b_+n - c_+n^2$, $u_-(n) = \beta n$ has a similar stationary probability distribution $P(n)$ of fascicle sizes. Indeed, solving the master equation for the birth-death process one obtains (up to corrections of order 1/N) [3]

$$\beta P(n) \simeq J_+\ n^\gamma \exp[-\ell(n-1) - \kappa(n-1)^2], \qquad (2)$$

where the injection rate $J_+ \equiv \beta P(1)$, the exponent $\gamma = a_+/\beta - 1$, and $\ell = 1 - b_+/\beta$, $\kappa = c_+/2\beta$.

The knowledge of the fascicle size distribution allows us to evaluate an additional characteristic time scale τ_f, reflecting the turnover rate of *fascicles* in the full system. From the definition $\tau_f \equiv [\sum_1^\infty P_s(n,y)]/J_+(y)$ we directly obtain [3]

$$\tau_f = (T/2\kappa)\left[1 - \left(\sqrt{\pi}e^{\frac{\ell^2}{4\kappa}}(\ell - 2\kappa)\mathrm{erfc}(\ell/2\sqrt{\kappa})\right)/2\sqrt{\kappa}\right].$$

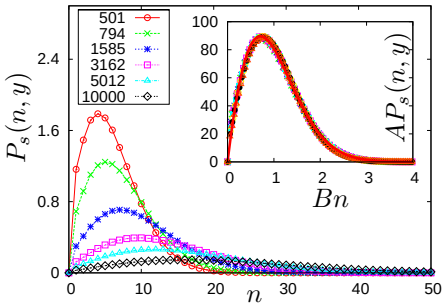


Figure 5: Steady state distribution of fascicle sizes $P_s(n,y)$ [averaged over 10^4 initial conditions and the time interval $10T \le t \le 25T$] for the $N = 100$, $L = 800$ system at y-levels indicated in the legend. Inset: Rescaling with $B = 1/\langle n\rangle$ and $A = \langle n\rangle^{2.1}$ collapses the data onto a single curve $\phi(u) = \mathcal{N}u\exp(-\nu u - \lambda u^2)$ with $u = n/\langle n\rangle$ and $\mathcal{N} = 274$, $\nu = 0.78$, $\lambda = 0.45$.

Scaling of y-dependent parameters: Full consistency of Eq. 2 with the scaling form Eq. 1 requires $J_+(y) \sim y^{-3.1\,b}$, $\kappa \sim y^{-2b}$ [i.e. $c_+ \sim y^{-2b}$], and $\ell \sim y^{-b}$ [i.e. $(\beta - b_+) \sim y^{-b}$]. This is in reasonable agreement with the simulation data in Table 1.

The gradual approach of $b_+ \approx \beta\rho S$ to β with increasing y (see Table 1) may be understood as follows. At low y, fascicles are formed preferentially by axons that started with small separation S at the $y = 0$ level, and the typical gap size E exceeds S. With increasing y, the smallest gaps are removed to become part of fascicles; consequently both E and S grow with y, and S approaches $1/\rho$ at high y. The time averaged S for selected fascicles is shown in the last two columns of Table I. A rather subtle feature of the system is the strong dependence (Fig. 3b) of the time scales on the density ρ, which can now be qualitatively understood as follows. In a system with lower axon density, the time scales are reduced as the increased inhomogeneity of axon separations at $y = 0$ leads to a stronger deviation of ρS from 1.

y	a_+/β	b_+/β	c_+/β	y	$\langle S\rangle$
20	1.96	0.862	0.0116	200	1.14
40	1.94	0.909	0.0082	400	1.60
100	1.96	0.947	0.0056	1000	2.02
400	1.92	0.974	0.0022	10000	2.21

Table 1: y-dependence of the fascicle parameters defined in the main text. System parameters are $L = 100$ and $N = 50$.

The y-dependence of the measured as well as the theoretically determined time scales is summarized in Fig. 3*b*. The measured correlation time τ_c falls in between the computed time scales τ and τ_f. It is seen that the three time scales show distinct y-dependence, notably: $\tau \sim y^b$ and $\tau_f \sim y^{2b}$.

Conclusion: To summarize, we have proposed a simple model for axon fasciculation that shows rich dynamical properties. We identified multiple time scales that grow distinctly with the fasciculation distance y and become $\gg T$, the average lifetime of individual axons. The slow time scales do not simply arise as a consequence of fascicles containing many axons, but are due to the dynamics of the fascicle basins. The model is readily generalized to include multiple axon types, type-specific interactions, and detachment of axons from fascicles [5]. We are currently applying our model to experimental studies of axon growth in neuronal cell culture [6]. Our theoretical results have wider relevance for existing related models (e.g. of river basin formation [7], insect pheromone trails [8] and pedestrian trail formation [9]), in which the slow maturation and turnover of the connectivity pattern have not been analyzed in detail.

[1] M. J. Katz, J. Neurosc. **5** (1985) 589.

[2] D.-J. Zou et al., Science **304** (2004) 1976.

[3] D. Chaudhuri, P. Borowski, P. K. Mohanty, and M. Zapotocky, arXiv:0808.1195.

[4] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry*, 2nd ed. (North Holland, Amsterdam, 1992).

[5] D. Chaudhuri, P. Borowski, and M. Zapotocky, in preparation.

[6] J. A. Hamlin, H. Fang, and J. E. Schwob, J. Comp. Neuro. **474** (2004) 438.

[7] A. E. Scheidegger, Bull. IASH **12(1)** (1967) 15.

[8] F. Schweitzer, K. Lao, and F. Family, Biosystems **41**, (1997) 153.

[9] D. Helbing, J. Keltsch, and P. Molnar, Nature **388** (1997) 47.

2.16 Diffusion of Active Particles

Benjamin Lindner

Classic Brownian motion and the Langevin equation. The erratic zig-zag trajectory of a micron-sized particle in a solution, known as Brownian motion looks at the first glance like a manifestation of live. However, as known to every student of physics, this motion entirely relies on the interaction of the particle with the many but finite smaller particles the solution consist of. Statistical mechanics provides a relation between the diffusion coefficient of this motion $D_{\rm eff}$, the friction coefficient γ of the particle, and the Boltzmann constant k_B of statistical mechanics

$$D_{\rm eff} = \lim_{t\to\infty} \frac{\langle (x(t)-x(0))^2\rangle}{2t} = \frac{k_B T}{\gamma} \qquad (1)$$

known as Einstein relation. It can be readily derived by means of the Langevin equation

$$\dot{x} = v, \quad \dot{v} = -\gamma v + \sqrt{2\gamma k_B T}\xi(t) \qquad (2)$$

where x and v are position and velocity of the Brownian particle which is subject to a Stokes drag (proportional to velocity) and a random force (modeled by a white Gaussian noise $\xi(t)$); the particle mass has been set to one. Many generalizations of the Langevin equation, taking into account memory damping and colored noise, the effect of hydrodynamic interactions and external force fields, to name but a few, have been studied to understand the stochastic dynamics of inanimate particles interacting with a heat bath.

Biological motility modeled by the Langevin equation. Soon after the pioneering studies of Brownian motion by Einstein, Langevin, and Planck, researchers started to use the framework of the Langevin equation to model biological motility phenomena which occur outside thermodynamic equilibrium [1]. While in the beginning the classic Langevin eq. 2 was used with effective friction coefficients and noise intensities, in the 1990s a more general approach was put forward by different groups: a Langevin equation with velocity-dependent friction and noise coefficients

$$\dot{x} = v, \quad \dot{v} = -\gamma(v)v + g(v)\xi(t). \qquad (3)$$

This *nonlinear* Brownian motion can describe an active motion in two special cases: (i) the friction function $\gamma(v)$ is negative for a restricted range of velocities and the noise is additive (active Brownian particle); (ii) only the noise intensity $g(v)$ depends nontrivially on the velocity. Both conditions imply that the system operates outside thermodynamic equilibrium.

Models of the form given in eq. 3 were fitted to experimental data of cell motility [2, 3]. Furthermore, such active motion models also emerged from phenomenological models of particles with energy depots [5, 6] and from biophysical models of coupled molecular motors [4].

For eq. 3 the diffusion coefficient and other characteristics of transport are not described by a simple Einstein relations like eq. 1. The analysis of the diffusive behavior of an active Brownian motion may help to understand how different motile objects like molecular motors or whole cells are adapted to their specific task.

Contributions of our group. We have recently studied the diffusion of active particles in various physical situations by means of a general quadrature expression for the diffusion coefficient in one spatial dimension [7–10]

$$D_{\rm eff} = \frac{\int_{-\infty}^{\infty} dz\, e^{U(z)} \left[\int_{-\infty}^{z} dy\, \frac{y-\langle v\rangle}{g^2(y)} e^{-U(y)}\right]^2}{\int_{-\infty}^{\infty} dv\, e^{-U(v)}/g^2(v)} \qquad (4)$$

where $\langle v\rangle$ is the mean velocity given by

$$\langle v\rangle = \frac{\int_{-\infty}^{\infty} dv\, v\, e^{-U(v)}/g^2(v)}{\int_{-\infty}^{\infty} d\tilde{v} e^{-U(\tilde{v})}/g^2(\tilde{v})} \qquad (5)$$

and $U(v)$ is an effective velocity potential

$$U(v) = \int^{v} dv' \frac{\gamma(v')v'}{g^2(v')}. \qquad (6)$$

For normal Brownian motion this potential would be just a parabola while for an active particle it is typically bistable.

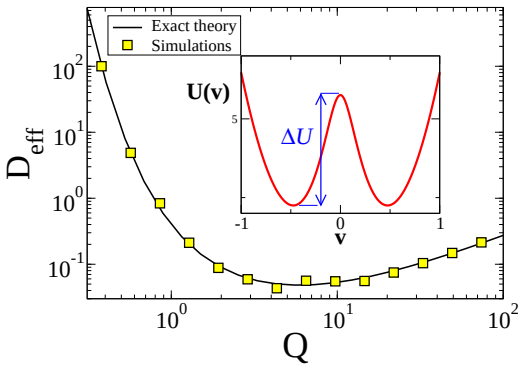


Figure 1: The diffusion coefficient of an active Brownian particle according to the Depot model [5] with additive noise ($g(v) \equiv \sqrt{2Q}$) as a function of the noise intensity Q; the inset shows the velocity potential eq.6. In contrast to normal Brownian motion, the diffusion coefficient of the active particle diverges for *both* vanishing and infinite noise intensity. Figure modified from [7].

Spatially symmetric case. For an even friction function ($\gamma(v) = \gamma(-v)$) corresponding to the Depot model [5] and an additive noise $g(v) \equiv \sqrt{2Q}$ with intensity Q, it has been shown that the diffusion coefficient may attain a minimal value at finite noise strength [7] (see Fig. 1), an effect reminiscent of stochastic resonance and other noise-induced phenomena. In contrast to Brownian motion (where we would have $D_{\text{eff}} = Q/\gamma$ according to eq. 1), there is a strong divergence of the diffusion coefficient for vanishing noise. This divergence can be understood by an ensemble of Brownian particles: in the steady state we have two subpopulations of particles with finite positive and negative velocities (corresponding to the minima of the potential). At vanishing noise these two populations drift apart with finite speed corresponding to a ballistic diffusion ($D_{\text{eff}} \to \infty$). The opposite limit of strong noise depends critically on the asymptotic form of the friction function; this asymptotic limit determines whether the diffusion coefficient shows a minimum or does not. The minimum is, for instance, absent for a Rayleigh friction function with dominating cubic nonlinearity [10] because for a pure cubic friction term (dominating in the strong noise limit), diffusion does not depend on the noise intensity [8].

Effect of an asymmetry on the diffusion. A problem for which the one-dimensional active Brownian motion is particularly relevant is the intracellular motion of assemblies of molecular motors along filaments [4]. The motility of such an assembly relies on the interplay of a Brownian ratchet mechanism for the single motor and collective effects due to the coupling among motors. The resulting motion is generally bidirectional (with two distinct velocities) but asymmetric (one velocity is usually preferred) and can be also subject to external forces in the cell. How the degree of asymmetry affects assembly diffusion appears to be vital for an understanding of the biological function of coupled motors.

It turns out that in a simple active Brownian motion model as well as in a biophysical model of coupled molecular motors, the diffusion coefficient depends critically on the asymmetry [9]. With a bias force F included (specifically, we use $\gamma(v) = v^2 - 1 - F/v$) and an additive noise of intensity Q, the diffusion coefficient diverges in the weak noise limit if the force is within a window $F \in [-F_{crit}, F_{crit}]$ (see Fig. 2). An asymmetry will naturally lead to two different potential barriers in the bistable potential. The analysis of eq. 4 reveals that the critical force is reached if the larger barrier is exactly *twice* the smaller barrier. This result does not depend on the specific friction function of the active particle.

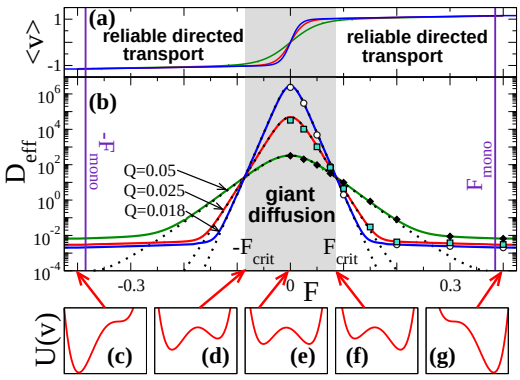


Figure 2: Mean velocity (a) and diffusion coefficient (b) of an active Brownian particle vs force for different values of the noise intensity Q. Panels (c-g) show the effective potentials at different values of the force as indicated by the arrows. Figure adopted from [9].

Conclusions. From a biological view point, maximizing or minimizing the diffusion may be essential for agents (animals, cells, intracellular transporters) for the performance in their task. By tuning the strength of intrinsic fluctuations or asymmetries, the transport characteristics of active Brownian motion can be switched between the regimes of regular transport (finite mean velocity with weak diffusion) and giant diffusion (strong but largely undirected transport). These regimes may serve different functionalities of biological motility in general and of intracellular transport in particular. How the level of intrinsic fluctuations could be controlled in these systems is an interesting but open question.

[1] D. Selmeczi et al. *Eur. Phys. J. ST*, 157(1):1, 2008.

[2] M. Schienbein and H. Gruler. *Bull. Math. Biol.*, 55:585, 1993.

[3] D. Selmeczi et al. *Biophys. J.*, 89:912, 2005.

[4] M. Badoual, F. Jülicher, and J. Prost. *Proc. Natl. Acad. Sci.*, 99:6696, 2002.

[5] F. Schweitzer et al. *Phys. Rev. Lett.*, 80:5044, 1998.

[6] U. Erdmann et al. *Eur. Phys. J. B*, 15:105, 2000.

[7] B. Lindner. *New J. Phys.*, 9:136, 2007.

[8] B. Lindner. *J. Stat. Phys.*, 130:523, 2008.

[9] B. Lindner and E. M. Nicola. *Phys. Rev. Lett.*, 101:190603, 2008.

[10] B. Lindner and E. M. Nicola. *Eur. Phys. J. ST.*, 157:43, 2008.

2.17 Enhancement of Sensitivity Gain and Frequency Tuning by Coupling of Active Hair Bundles

Kai Dierkes, Frank Jülicher, and Benjamin Lindner

The auditory amplifier. The performance of human hearing is truly remarkable. The ear is able to (i) resolve audible frequencies that differ by less than one percent; (ii) detect faint sounds; (iii) perceive sounds of a wide dynamic range (12 orders of magnitudes in sound intensity); and (iv) generate spontaneous and evoked opto-acoustic emissions. All of these features could be linked to an active amplifier residing in the cochlea [1].

Two cellular mechanisms have been proposed to be key components of the auditory amplifier in the mammalian cochlea [2]. On the one hand, there is the electromotile length change of outer hair cells in response to a modulation of their membrane potential (electromotility). On the other hand, hair bundles, which are the universal mechano-transducers in the auditory and vestibular system of all vertebrates, can also actively generate forces (hair-bundle motility).

Active hair bundle dynamics. The hair bundle is a tuft of stiff finger-like protrusions called stereocilia emanating from the surface of hair cells. By means of mechanically gated ion channels, the hair bundle can sense deflections of its tip and transduce this mechanical input into ionic currents entering the cell.

In vitro experiments with hair bundles from the bullfrog's sacculus have shown that it possesses many features pre-disposing it for a central role in sound amplification: spontaneous oscillations [3], amplification of applied sinusoidal stimuli in a frequency selective manner [4], and a region of non-linear compression for intermediate driving amplitudes [4].

Recently, a biophysical model for active hair bundle motility has been proposed [5] describing the interplay between deflections of the hair bundle, mechanical gating of ion channels, and calcium-dependent activity of molecular motors in the stereocilia. Mathematically, the hair bundle dynamics is given by stochastic differential equations for two variables X and X_a representing the stereociliary deflection and the position of molecular motors, respectively. Fluctuations stemming from Brownian motion, channel clatter, and stochastic activity of molecular motors is taken into account by means of noise terms. This stochastic model reproduces the statistics of spontaneous oscillations as well as frequency-tuning and nonlinear compression of the response to periodic stimuli as seen in experiments; some of its spectral statistics has been studied analytically [6].

Contributions of our group. The sensitivity of a single hair bundle is ultimately limited by noise. While the amplification gain of the cochlea is about 10^3, for a single hair bundle it is approximately 10. Single hair bundle dynamics thus cannot account quantitatively for the exquisite sensitivity of the cochlea.

In most hearing organs the tips of hair bundles are coupled via an overlying membranous structure (see Fig.1a). We investigate numerically, analytically, and experimentally which effects such a coupling could have on stochastic hair bundle dynamics.

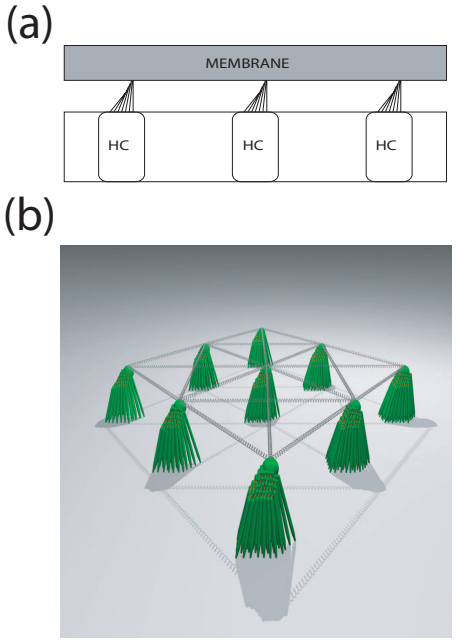


Figure 1: Coupled hair bundles. (a) Hair bundles in various inner ear organs are coupled via visco-elastic membranous structures. (b) Sketch of a group of hair bundles that is coupled by means of springs.

Coupled hair bundles. In a first approach we have focused on a purely elastic coupling. We have studied numerically regular arrangements of hair bundles on a square lattice with coupling between next nearest neighbors being implemented by means of linear springs of stiffness K (see Fig.1b). The governing equations read

$$\lambda \dot{X}^{i,j} = f_X(X^{i,j}, X_a^{i,j}) + \sum \frac{\partial U(X^{i,j}, X_a^{i,j})}{\partial X^{i,j}} + F_{\text{ext}}(t) + \eta^{i,j}(t) \quad (1)$$

$$\lambda_a \dot{X}_a^{i,j} = f_{X_a}(X^{i,j}, X_a^{i,j}) + \eta_a^{i,j}(t). \quad (2)$$

where U is the interaction potential due to the coupling and the sum extends over next nearest neighbors. Single hair bundle dynamics is described by $f_X(X^{i,j}, X_a^{i,j})$ and $f_a(X^{i,j}, X_a^{i,j})$; influences of noise are captured by $\eta^{i,j}(t)$ and $\eta_a^{i,j}(t)$ [5]. An external driving can be taken into account by means of the term $F_{\text{ext}}(t)$.

Response to periodic stimuli. When a hair bundle is driven by an external sinusoidal force $F_{\rm ext} = F\cos(2\pi f_s t)$ (see upper panel in Fig.2) its response is marked by two distinct properties. If the amplitude F of the external driving is small the predominant effect is an increase in the degree of phase-locking of the hair bundle's oscillation to the external signal (see Fig.2, red and green curves). However, for large driving amplitude also the amplitude of the hair bundle oscillation grows (see Fig.2, blue curve).

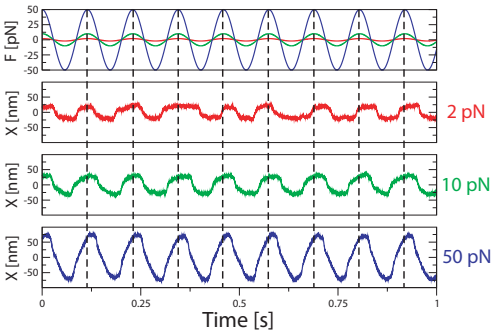


Figure 2: Driven oscillations of a single active hair bundle. In the upper panel we show three signals of differing amplitudes (2 pN (red), 10pN (green) and 50pN (blue)) and below the respective responses $X(t)$. Averaging for each amplitude over many of such noisy realizations, one obtains the time dependent mean value $\langle X(t)\rangle$ in eq. 3. Dashed lines indicated the maxima of the external force. Note how for increasing driving amplitude the degree of stochastic phase-locking increases (red and green curve). For even larger driving also the amplitude of the hair bundle oscillation grows (blue curve).

The time dependent mean response of the hair bundle reads

$$\langle X(t)\rangle = A_1\cos(2\pi f_s t - \phi_1) + A_2\cos(4\pi f_s t - \phi_2) + \dots \quad (3)$$

One measure of the quality of the hair bundle as a detector of an oscillatory signal with frequency f_s and amplitude F is its sensitivity $|\chi(f_s, F)| = A_1/F$, which is defined as the ratio of the amplitude A_1 of the first Fourier mode of the time dependent mean response and the driving amplitude F.

Enhancement of sensitivity. We have shown that coupling of active hair bundles can greatly enhance the sensitivity to weak driving (see Fig.3a) [7]. For instance, the sensitivity of a system of 9x9 hair bundles is increased by a factor of 40 when compared to a single hair bundle. Also, there is a pronounced extension of the region of nonlinear compression that characterizes the response to driving of intermediate amplitudes. The estimated value of -0.88 for the exponent of nonlinear compression is in accordance with measurements for the mammalian cochlea [1].

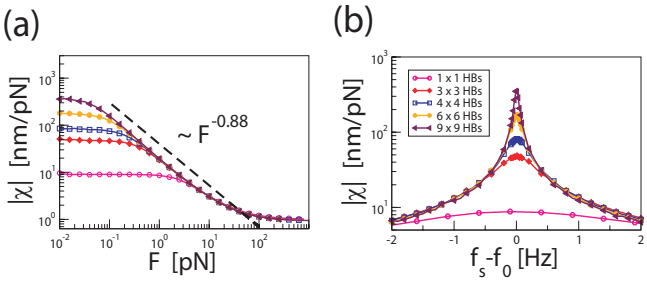


Figure 3: Sensitivity to external driving of the central hair bundle for groups of varying size as indicated. (a) Sensitivity $|\chi|$ as a function of driving amplitude F. Dashed line indicates a power law with exponent -0.88. (b) Sensitivity $|\chi|$ as a function of detuning $f_s - f_0$.

The sensitivity of a single hair bundle is largest at the frequency of spontaneous oscillations f_0. Sensitivity decreases along with increasing detuning $|f_s - f_0|$ (see Fig.3b, pink curve). We have found that this frequency tuning is drastically sharpened by coupling (see Fig.3b, for example purple curve for a 9x9 system) [7].

Conclusions. Our numerical investigation has shown that elastic coupling of active hair bundles could indeed play a beneficial role in sound detection and amplification. In order to further test the biophysical relevance of the observed effects, we have recently performed experiments on real hair bundles (collaboration with P. Martin, Paris). Also, we are working on analytical approaches to the amplification properties of groups of coupled hair bundles.

[1] L. Robles and M.A. Ruggero, Physiol. Rev. **81**, 1305 (2001).

[2] A.J. Hudspeth, Neuron **59**, 530 (2008).

[3] P. Martin, D. Bozovich, Y. Choe, and A.J. Hudspeth, J. Neurosci. **23**, 4533 (2003).

[4] P. Martin, and A.J. Hudspeth, Proc. Natl. Acad. Sci. **98**, 14386 (2001).

[5] B. Nadrowski, P. Martin, and F. Jülicher, Proc. Natl. Acad. Sci. **101**, 12195 (2004).

[6] D. Clausznitzer, B. Lindner, P. Martin, and F. Jülicher, Phys. Rev. E **77**, 041901 (2008).

[7] K. Dierkes, B. Lindner, and F. Jülicher, Proc. Natl. Acad. Sci. **105**, 18669 (2008).

2.18 Feedback Resonances and Intra-atomic Excitations in Heavy-fermion Superconductors

Ilya Eremin, Peter Thalmeier, and Peter Fulde

Magnetic resonances as a consequence of unconventional superconductivity are by now well established. So is the fact that not only phonons may be responsible for Cooper pair formation. To both research areas we have contributed during the last two years. A theory was developed for the occurrence of magnetic resonances in $CeCu_2Si_2$ as well as in $CeCoIn_5$ and it was shown that in the filled skutterudite $PrOs_4Sb_{12}$ Cooper paring is mainly due to intra-atomic excitations of the Pr $4f^2$ subshell.

An unconventional superconductivity shows a strong feedback on the magnetic spin excitations in these systems below the superconducting transition temperature T_c. One example is the famous resonance peak observed in various superconducting systems by means of inelastic neutron scattering(INS). Important to notice that the observation of a resonance at the AF wavevector $\mathbf{Q}$ puts a stringent condition on the gap symmetry by requiring a sign change $\Delta_{\mathbf{k}+\mathbf{Q}} = -\Delta_{\mathbf{k}}$ under translation by $\mathbf{Q}$ and shows that INS is a powerful technique to determine the superconducting gap symmetry. We show that the observation of the resonance peak in heavy-fermion superconductors $CeCu_2Si_2$ [1] and in $CeCoIn_5$ [2] at the incommensurate wave vector $\mathbf{Q}_{SDW}$ and at the antiferromagnetic wave vector $\mathbf{Q}_{AF}$, respectively, give a clear indication in favor of the $d_{x^2-y^2}$ superconducting state realized in these systems.

The resonance peak in the SC state of $CeCu_2Si_2$ as well as of $CeCoIn_5$ can be understood by considering the dynamical spin susceptibility within the random phase approximation (RPA), *i.e.*,

$$\chi_{RPA}(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{1 - g_{\mathbf{q}}\chi_0(\mathbf{q},\omega)}, \qquad (1)$$

where $g_{\mathbf{q}}$ is the fermionic four-point vertex and $\chi_0(\mathbf{q},\omega)$ is the heavy quasiparticle susceptibility. The latter is given by the sum of the bubble diagram consisting of either normal or anomalous ($T<T_c$) Green functions. For large momenta $\mathbf{q}$, $\mathrm{Im}\chi_0(\mathbf{q},\omega)$ is zero at low frequencies and can exhibit a discontinuous jump at the onset frequency of the p-h continuum $\Omega_c = \min(|\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{q}}|)$ where both $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ lie on the Fermi surface. Note, however, that the discontinuity in $\mathrm{Im}\chi_0$ occurs only if $\mathrm{sgn}(\Delta_{\mathbf{k}}) = -\mathrm{sgn}(\Delta_{\mathbf{k}+\mathbf{q}})$ which is not possible for isotropic s-wave order parameter. A discontinuity in $\mathrm{Im}\chi_0$ leads to a logarithmic singularity in $\mathrm{Re}\chi_0$. As a result, the resonance conditions (i) $g_{\mathbf{q}}\mathrm{Re}\chi_0(\mathbf{q},\omega_{res}) = 1$ and (ii) $\mathrm{Im}\chi_0(\mathbf{q},\omega_{res}) = 0$ can be both fulfilled at $\omega_{res} < \Omega_c$ for any $g_{\mathbf{q}} > 0$, leading to the occurrence of a resonance peak in form of a spin exciton below T_c as schematically depicted in Fig.1(a).

Since the symmetry of the superconducting gap has not yet been determined unambiguously in $CeCu_2Si_2$, we have analyzed all the spin singlet s- and d-wave functions allowed by the crystal-group symmetry of the lattice. We have found that the resonance-like feature, *i.e.*, the discontinuous jump in $\mathrm{Im}\chi_0$ and the corresponding logarithmic singularity in $\mathrm{Re}\chi_0$ occur at $\mathbf{Q}_{SDW}$ for the two-dimensional $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x a - \cos k_y a)$ belonging to the B_{1g} irreducible representation. In Fig.1(b) we show the RPA susceptibility in the normal and the SC state for the B_{1g} and for the B_{2g} channels, respectively. One finds that the susceptibility for the B_{1g} symmetry is larger in the SC state than it is in the normal state, while in the B_{2g} channel there is no enhancement of the normal state spin susceptibility. This definitely points towards a $d_{x^2-y^2}$-wave symmetry of the SC gap in $CeCu_2Si_2$.

Among possible superconducting symmetries in $CeCoIn_5$ a resonance peak forms only for the B_{1g} ($\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x a - \cos k_y a)$) symmetry. As in the case of $CeCu_2Si_2$ the antiferromagnetic wave vector connects states with opposite sign of the superconducting gap. This results in the formation of a resonance peak similar to the one in $CeCu_2Si_2$. The resonance peak forms near the particle-hole continuum, i.e., close to $\Omega_c = \min(|\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{q}}|)$ which is around Δ_0. This is because the points connected by $\mathbf{Q}_{AF}$ are lying relatively far from the part of the Fermi surface where the gap function has maximum value. Note, if the Cooper-pairing itself arises due to an exchange of AF spin fluctuations, the maximum of the SC gap occurs at points of the Fermi surface which are connected by $\mathbf{Q}_{AF}$. At the same time, the superconducting gap possesses still the $d_{x^2-y^2}$-wave symmetry, although with higher harmonics included. It is remarkable that like in $CeCu_2Si_2$ we find that only a gap function of $d_{x^2-y^2}$-wave (B_{1g}) type results in the formation of the resonance peak at $\mathbf{Q}_{AF}$. This unambiguously confirms the bulk symmetry of the superconducting gap in $CeCoIn_5$. The d_{xy}-wave (B_{2g}) symmetry discussed in the literature is clearly ruled out.

Our results shed light on the bulk symmetry of the superconducting gap in $CeCoIn_5$ and in $CeCu_2Si_2$. They show that the two heavy-fermion superconductors and the high-T_c cuprates possess the same symmetry of the superconducting order parameter suggesting that the same mechanism of the Cooper-pairing is probably involved.

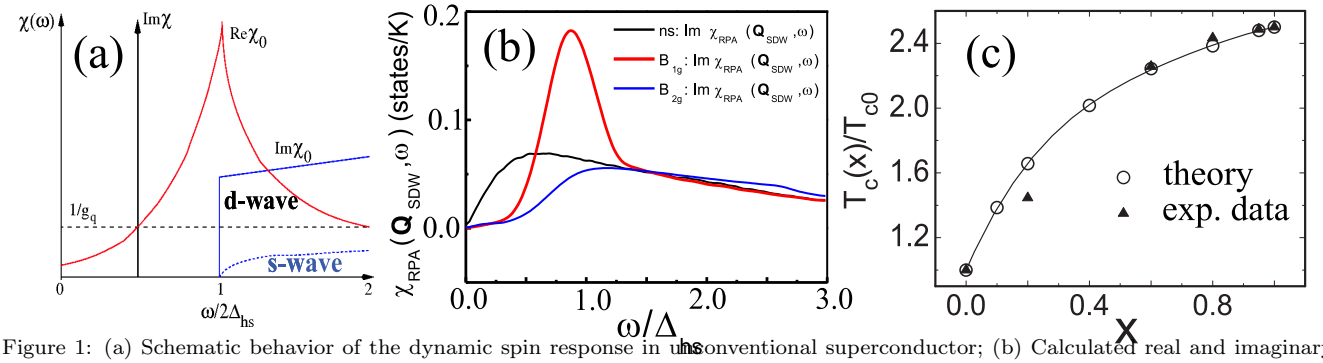


Figure 1: (a) Schematic behavior of the dynamic spin response in unconventional superconductor; (b) Calculated real and imaginary part of the RPA susceptibility at the $\mathbf{Q}_{AF}$ for $CeCu_2Si_2$ as a function of frequency in the normal (black) and superconducting, B_{1g} (red) and B_{2g} (blue) states; (c) Calculated superconducting transition temperature T_c for $La_{1-x}Pr_xOs_4Sb_{12}$ as a function of Pr concentration x.

The Pr-based filled-skutterudite compounds have attracted much attention because of their exotic properties like metal-insulator transition, or unusual heavy-fermion behavior. This also concerns $PrOs_4Sb_{12}$, the first Pr-based heavy-fermion superconductor with $T_c = 1.85$ K which possesses many exotic properties compared to that of the Ce- and U-based superconductors.

At present, the Cooper-pairing mechanism and the corresponding symmetry of the superconducting gap in $PrOs_4Sb_{12}$ is still under debate. However, an interesting experimental observation by means of dHvA effect was that $PrOs_4Sb_{12}$ has a very similar FS topology as the conventional s-wave superconductor $LaOs_4Sb_{12}$ ($T_c = 0.74$ K) which hints at a relatively weak hybridization of the conduction band with Pr^{3+} $4f^2$ electrons. Furthermore, the superconducting transition temperature in the alloy compound $La_{1-x}Pr_xOs_4Sb_{12}$ change smoothly upon changing x. These observations raise doubts on a purely unconventional nature of the Cooper-pairing in $PrOs_4Sb_{12}$. But the enhancement of T_c and the effective quasiparticle mass in this compound with respect to that of $LaOs_4Sb_{12}$ have to be understood.

It is well-known that scattering by magnetic impurities suppresses conventional s-wave superconductivity by destroying Cooper pairs in a singlet state. This situation, however, can change in the case of paramagnetic non-Kramers rare-earth impurities. For example for superconductors containing an impurity with crystal-field split energy levels the inelastic charge scattering of conduction electrons from the aspherical part of the $4f$ charge distribution may yield an increase of T_c. However, in most of the cases the usual magnetic exchange interaction is dominant, thus suppressing T_c.

To elucidate the origin of superconductivity in heavy-fermion skutterudite compounds, we have studied the influence of inelastic rare-earth impurity scattering on the superconductivity in $(La_{1-x}Pr_x)Os_4Sb_{12}$ systems [4]. The ground state in the crystalline electric field (CEF) for Pr^{3+} ion is a Γ_1 singlet, which is separated by the first excited state, a $\Gamma_4^{(2)}$ triplet by a gap of $\Delta_{CEF} \sim 8$ K. Because of the small Δ_{CEF}, the relation between the quadrupole fluctuations associated with the $\Gamma_4^{(2)}$ state and the superconductivity is of general interest. Solving the strong coupling Eliashberg equations we have found that the dominant quadrupolar component of the inelastic scattering on Pr impurities yields an enhancement of the superconducting transition temperature T_c in $LaOs_4Sb_{12}$ which is originally due to electron-phonon interaction. In agreement with experimental data [5] it increases monotonically as a function of Pr concentration as shown in Fig1(c). Our analysis suggests that both phonons and quadrupolar excitations cause the attractive electron interaction which results in the formation of Cooper pairs and singlet superconductivity in $PrOs_4Sb_{12}$.

[1] O. Stockert *et. al.*, Physica B **403**, 973 (2008).

[2] C. Stock *et al.*, Phys. Rev. Lett. **100**, 087001 (2008).

[3] I. Eremin, G. Zwicknagl, P. Thalmeier, and P. Fulde, Phys. Rev. Lett. **101**, 187001 (2008).

[4] J. Chang, I. Eremin, P. Thalmeier, and P. Fulde, Phys. Rev. B **76**, 220510(R) (2007).

[5] M. Yogi *et al.*, J. Phys. Soc. Jpn. **75**, 124702 (2006).

2.19 Correlated Electronic Structure of $3d$-metal Compounds with Wavefunction-based Quantum Chemical Methods

Liviu Hozoi and Peter Fulde

Wavefunction-based methods using quantum chemical approaches are an alternative to density-functional based calculations. They are more elaborate than the latter but have the advantage that all approximations are well controlled. We have applied these methods to the study of the electronic structure of correlated transition-metal compounds. Whereas the correlation treatment is performed in direct-space, a **k**-space representation can be obtained later on after accounting for the (strong) short-range correlations [1]. In some cases, a balanced treatment of the short-range interactions, on-site *and* inter-site, is essential for achieving even a qualitatively correct picture [2–4].

For the high-T_c cuprate superconductors, we found that the Fermi surface of the hole doped material evolves from small hole pockets in the deeply underdoped region to one with *both* hole- and electron-like sheets at slightly higher doping and to a large Fermi surface consistent with Luttinger's theorem at still higher doping concentrations [3]. Our results offer a route toward a resolution of the controversy generated by the apparent inconsistency between Shubnikov-deHaas measurements and the Luttinger sum rule for underdoped cuprates, as well as with recent Hall-effect data suggesting an *electron*-like Hall constant for *hole* doped cuprates at low temperatures [5, 6].

For the Co oxide perovskite $LaCoO_3$, we have provided new insight into the correlated multiorbital physics underlying the spin-state transition at 90 K, intensively debated for about 40 years, and the nature of charge carriers [2]. $LaCoO_3$ is quite unique because of the low-T nonmagnetic closed-shell ground state, which distinguishes it from a conventional Mott insulator. With respect to the lowest excited states, our results indicate that for an undistorted lattice the high-spin (HS), $S=2$ configuration is lower in energy than the intermediate-spin (IS), $S=1$ state. This agrees with recent x-ray absorption [7] and neutron scattering [8] experiments. Additionally, we explained the low-T paramagnetic phase in the lightly doped compound through the formation of Zhang-Rice-like [9] oxygen hole states and ferromagnetic clusters.

Quantum chemical calculations were also employed to unravel the nature of correlation effects in the pnictide superconductor LiFeAs. Our investigations [4] indicate a HS, $S=2$ configuration for the Fe ions, in contrast to density-functional calculations which predict lower magnetic moments [10] but in agreement with x-ray absorption data [11]. Further, we found that the ground state is degenerate: there is one hole associated with each pair of Fe (xz, yz) orbitals. So, although the intraorbital U is large enough to give a HS on-site configuration, the intersite charge fluctuations in the (xz, yz) sector are expected to be strong, due to the 3/4-filling of these levels. This is compatible with the "bad-metal" conductivity observed experimentally in the normal state. We also found that the lowest electron-removal states have As $4p$ character, in analogy to the ligand hole states in p-type cuprate superconductors [3].

[1] U. Birkenheuer, P. Fulde, H. Stoll, Theor. Chem. Acc. **116** (2006) 398; L. Hozoi, U. Birkenheuer, P. Fulde, A. Mitrushchenkov, H. Stoll, Phys. Rev. B **76** (2007) 085109.

[2] L. Hozoi, U. Birkenheuer, H. Stoll, P. Fulde, New J. Phys. **11** (2009) 023023.

[3] L. Hozoi, M. S. Laad, P. Fulde, Phys. Rev. B **78** (2008) 165107; L. Hozoi, M. S. Laad, Phys. Rev. Lett. **99** (2007) 256404.

[4] L. Hozoi, P. Fulde, Phys. Rev. Lett. **102** (2009) 136405.

[5] E. A. Yelland *et al.*, Phys. Rev. Lett. **100** (2008) 047003.

[6] D. LeBoeuf *et al.*, Nature **450** (2007) 533.

[7] M. W. Haverkort *et al.*, Phys. Rev. Lett. **97** (2006) 176405.

[8] A. Podlesnyak *et al.*, Phys. Rev. Lett. **97** (2006) 247208.

[9] F. C. Zhang, T. M. Rice, Phys. Rev. B **37** (1988) 3759.

[10] See, e.g., M. Johannes, Physics **1** (2008) 28.

[11] T. Kroll *et al.*, Phys. Rev. B **78** (2008) 220502.

2.20 Predictability of Extreme Events through Finite Size Effects in SOC Sandpiles

Anja Garber, Sarah Hallerberg, Holger Kantz

Extreme events are large deviations of a system with complex dynamics from its normal behaviour during short time intervals [1, 2]. One class of systems which generate such huge short time fluctuations are systems exhibiting self organized criticality (SOC). As suggested by Bak, Tang, & Wiesenfeld in 1987, a subtle balance of slow stress accumulation and fast stress release might drive a system into a self-generated scale-free, i.e., critical state. The presence of power laws for the distribution of typical observables implies that these can indeed assume arbitrarily large values.

One particular SOC model is the Abelian sand pile model [3] which mimics the dynamics of a sandpile where dropping sand grains on its top might cause avalanches. On a square lattice of size $L \times L$, random integer variables z_{ij} are defined. At each time step, a sand grain is added by randomly choosing a pair (i, j) and incrementing z_{ij} by 1. If any $z_{ij} > 3$, then sand grains are re-distributed:

$$z_{ij} \to z_{ij} - 4 \qquad z_{i'j'} \to z_{i'j'} + 1 \quad (1)$$
$$\text{for } (i', j') = (i, j \pm 1) \quad \text{and} \quad (i', j') = (i \pm 1, j)$$

This rule is applied repetitively until all $z_{ij} \leq 3$. Such a sequence of updates happens in one time step and is called *avalanche*. Its size s_i is measured as the number of topplings, i.e., as the total number of involved system sites with their multiplicity. It is commonly accepted [3] that in the thermodynamic limit $L \to \infty$, this system is critical. The magnitude-frequency distribution $p(s)$ of an avalanche of size s then follows a power law $p(s) \propto s^{-\alpha}$ with α around -1.2 [4]. In this limit, successive avalanches are independent of each other and the series of avalanche sizes s_i is uncorrelated. Consequently, the recurrence time distribution, i.e., the distribution of time intervals in between two successive avalanches, is an exponential.

In the finite-sized system, the largest possible avalanche has the size $s_{max} = 1/6 \cdot L(L+1)(L+2)$, and the power law has a cut-off already at sizes $L^2/2$ [5]. More importantly, the recurrence time distribution of very large avalanches is not exponential any more, but short return times are strongly suppressed. This is a finite-size effect [5]: An extremely large avalanche causes a relaxation of the system away from the critical state so that many added sand grains are needed until the system has rebuilt itself and can once again create avalanches of a similar or larger size. This weak repulsion can be used for their prediction.

To be realistic, we use as sole knowledge of the sandpile system a time series of avalanche sizes $\{s_i\}$, $i = 1, \ldots, N$, called the *observation series*, with $N = 2 \times 10^8$ time steps. From the observation series we construct an *event series*. As events, we consider avalanches which exceed a predefined magnitude η, i.e., the event series $\{X_i\}$, $i = 1, \ldots, N$ is defined as $X_i = 1$ if $s_i > \eta$ and $X_i = 0$ else. Only considering information from the past, we want to forecast whether the next avalanche exceeds the magnitude η. To do so, we construct a *decision variable*

$$y_i = \sum_{k=1}^{i} a^k s_{i-k}, \quad 0 < a < 1. \qquad (2)$$

Since y_i depends only on past values s_k, a prediction of the value of X_i based on y_i respects causality. The parameter a in eq.(2) is suitably chosen.

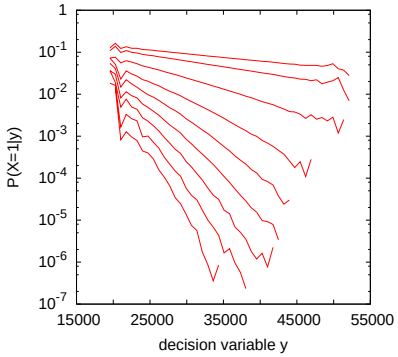


Figure 1: Conditional probability $P(X = 1|y)$ for the system size $L = 64$ as a function of the decision variable y, for events exceeding 1%, 2%, 5%, 10%, 15%, 20%, 25%, 30% and 35% of the maximal avalanche size s_{max} (from top to bottom).

A necessary condition for a decision variable to support predictability is that the conditional probability $P(X = 1|y)$ has at least one significant maximum in y. Numerical estimates of $P(X = 1|y)$ are shown in Fig. 1 on a semi-logarithmic scale for different values of the minimal event magnitude η and a system size $L = 64$. The conditional probabilities can be determined only on the observed range of y. All curves are approximately exponentials and have a maximum at the smallest observed y-value, i.e., when only small avalanches have occurred during the past period considered in the decision variable. This reflects the temporal repulsion of extreme events underlying our predictions. As expected, the smaller the minimal event magnitude η, the less pronounced the maximum is.

The actual prediction is made applying a threshold to predicted probabilities of an event to follow. A probabilistic predictor based on y_i is a map $y_i \mapsto \hat{p}_i$, $\hat{p}_i \in [0, 1]$. As a consequence of the Neyman-Pearson Lemma [6] and as discussed in [7], the optimal such predictor is $\hat{p}_i = P(X = 1|y_i)$, i.e., using the conditional probability of event and decision variable of the stochastic

process under study. A simple threshold converts this probabilistic prediction into a deterministic prediction $y_i \mapsto \hat{X}_i$ via

$$\hat{X}_i \quad = \quad \begin{cases} 1 & : \quad \text{if} \quad P(X=1|y_i) > p_c, \\ 0 & : \quad \text{else}, \end{cases} \qquad (3)$$

where $\hat{X}_i \in \{0,1\}$ is the prediction of the event variable. The value of p_c determines the total alarm rate. Comparing $\hat{X}_i$ and X_i allows one to verify or falsify one's prediction. This map optimizes the prediction for a given decision variable y with respect to the ROC analysis which will be discussed below. Since for our SOC model the probability distribution $P(X=1|y)$ is a priori unknown, we estimate it by construction of a histogram from the first half of the avalanche time series data (training set) (see Fig.1). The decision variable y_i is thereafter calculated at each time step of the second half of the avalanche time series (test set). This keeps the predictions strictly out-of-sample.

Since extreme events are rare, the scoring of the prediction skill should not depend explicitly on the rate of events. The prediction of binary events $\hat{X}_i \in \{0,1\}$ is a classification task, with two types of errors: missing an event, and giving a false alarm. We therefore choose the Receiver Operating Characteristics (ROC) [8] as a method to analyse prediction quality. This is a plot of the hit rate versus the false alarm rate, as a function of the total rate of alarms, which is tuned by the threshold p_c. For $p_c \to \max_y P(X=1|y)$, the condition for $\hat{X}_i = 1$ is almost never satisfied, so that both hit rate and false alarm rate are zero. For very small values of p_c, both rates tend to unity. Only if in between the hit rate exceeds the false alarm rate, the predictor is useful. A random prediction of $\hat{X}_i$ would generate equal hit and alarm rate, i.e., the diagonal in the ROC plot is the benchmark.

In Fig. 2 we report ROC curves for predictions using Eq.(3) on avalanche sequences for system sizes $L = 64$ and $L = 256$ and events exceeding different magnitudes η. The ROC plot shows two striking results: The larger the magnitude of the target events, limited by η from below, the better is the predictability. The predictability for given η does not depend on the system size L, if η is defined as a fraction of the maximal avalanche size $s_{max}(L)$. Each two curves for $L = 64$ and $L = 256$ are almost identical except for statistical fluctuations for large η.

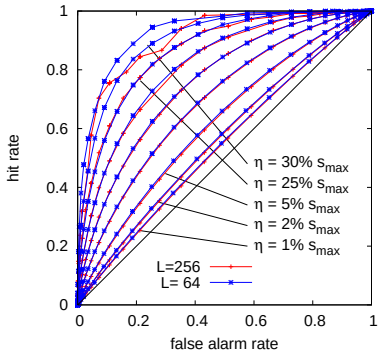


Figure 2: ROC plots for the prediction of extreme avalanches for different minimal event magnitudes η, comparing $L = 64$ and $L = 256$.

A quantitative comparison of our prediction skill with [9] shows that using information of the avalanche sequence alone is as successful as using as input data additional variables which reflect the internal state of the sandpile. Moreover, the predictive skill of [9] was thereby shown to be a finite-size effect as well. The remarkable outcome of this study is that as shown before for much simpler processes [10], the ROC-predictability of events is the better the larger their magnitude. Nonetheless, these predictions might be useless in practice: Due to the rareness of large events, the absolute number of false alarms is much larger than the number of hits, such that in between two successful hits there are thousands of false alarms. This is a simple consequence of the event rate. If false alarms cause costs, then not predicting at all might be the better strategy.

[1] A. Bunde, J. Kropp, H.J. Schellnhuber (Eds.), The Science of Disasters. Climate Disruptions, Heart Attacks, and Market Crashes. (Springer, Berlin, 2002)

[2] S.A. Albeverio, V. Jentsch, H. Kantz (Eds.), Extreme Events in Nature and Society (Springer, Berlin, 2006)

[3] P. Bak, C. Tang, K. Wiesenfeld, Phys. Rev. Lett. 59, 381 (1987); P. Bak, C. Tang, K. Wiesenfeld, Phys. Rev. A 38, 364 (1988)

[4] S. Lübeck, K.D. Usadel, Phys. Rev. E 55, 4095 (1997); L. Kadanoff, S. Nagel, L. Wu, S. Zhou, Phys. Rev. A 39, 6524 (1989); S. Manna, Physica A 179, 249 (1991); E. Milshtein, O. Biham, S. Solomon, Phys. Rev. E 58, 303 (1998).

[5] A. Garber, H. Kantz, Eur. Phys. Jour. B **67**, 437 (2009).

[6] J. Neyman, E. S. Pearson, Philosophical Transactions of the Royal Society of London 231, 289 (1933).

[7] S. Hallerberg, J. Bröcker, H. Kantz in Nonlinear Time Series Analysis in the Geosciences, Lecture Notes in Earth Sciences, Springer (2008).

[8] J. P. Egan, Signal detection theory and ROC analysis, Academic Press, New York, 1975

[9] A. B. Shapoval, M. G. Shnirman, Int. Jour. Mod. Phys. C 17, 1777 (2006)

[10] S. Hallerberg, H. Kantz, Phys. Rev. E **77**, 011108 (2008).

2.21 Asymptotic Continuous-time Random Walk Models for Deterministic Diffusion

Markus Niemann and Holger Kantz

An essential concept in the treatment of complex systems is the reduction of the number of degrees of freedom. In typical situations, the resulting reduced system is easier to handle, often simply because its phase space has less dimensions, or since by help of the reduction scheme essential properties are amplified. Brownian motion, e.g., results from the replacement of the action of many unspecified microscopic degrees of freedom on a heavy test mass by white noise. So through the reduction, the intrinsically stochastic character of such motion becomes visible. Depending on the properties of the original full system, different methods might be applied, most of them resulting in either fully deterministic reduced models or in models with a white noise stochastic driving.

White noise, i.e., noise without correlations and hence without time scale, is the result if the eliminated degrees of freedom possess an exponential decay of correlations. This reflects strongly chaotic mixing properties. However, quite often one observes intermittent dynamics, such as in turbulence or in Hamiltonian systems with mixed phase space, i.e., the dynamics is an alternation of laminar phases/regular behaviour and turbulent bursts/chaotic behaviour. If intermittency causes power laws for the autocorrelation function, Markov approximations which are usually employed in order to arrive at a white noise process are not justified: one expects that a reduced model is driven by non-gaussian non-white noises.

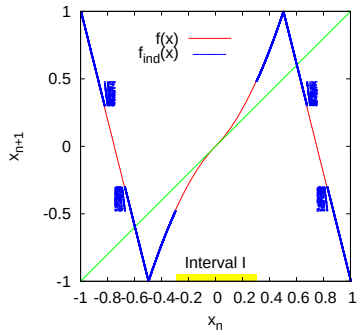


Figure 1: The intermittent map $f(x)$ of Pomeau-Manneville type (red graph) and the induced map (blue).

A specific example where one can rigorously calculate the asymptotic stochastic process for a fully deterministic system starts from a pseudo-Brownian path generated by the integration of the one-dimensional intermittent map $f(x)$ shown in Fig.1:

$$y_{n+1} = y_n + x_n \ , \ x_{n+1} = f(x_n) \qquad (1)$$

where $f(x)$ in the vicinity of $x = 0$ behaves like $x + x^z$. Hence $x = 0$ is a marginally stable fixed point. The map $f(x)$ possesses an indecomposable invariant measure with a singularity at the origin. This measure is normalizable for $z < 2$ only. Hence, the ergodic theorem is violated for $z \geq 2$: Time averages might not converge towards averages done with respect to the invariant measure. This property was called weak ergodicity breaking in [3].

In order to regularize the measure, we make use of the *induced map* [5]: One defines an interval I around the marginally stable fixed point $x_c = 0$ and defines a new map $f_{ind} : [0:1] \setminus I \to [0,1] \setminus I$ by $f_{ind}(x) := f^{k(x)}(x)$ with $k(x) = \min\{n \in \mathbb{N} : f^n(x) \notin I\}$. The invariant measure of f_{ind} lives on $[0,1] \setminus I$ and is there, apart from normalization, identical to the one of the map f, without the singularity at x_c. In the full system Eq.(1), one can account for that by introducing jumps of size Δ over time intervals of size δ:

$$y(t+\delta) = y(t) + \Delta \ , \ \Delta = \sum_{n=1}^{k} x_n \ ,$$
$$\delta = k = \min\{n \in \mathbb{N} : T^n(x) \notin I\} \qquad (2)$$

In the interpretation as a stochastic process, the dynamics is fully characterized by the joint probability $P(\Delta, \delta)$, the distribution of jump sizes and waiting times. Such a process has been named "continuous time random walk" (CTRW) [1].

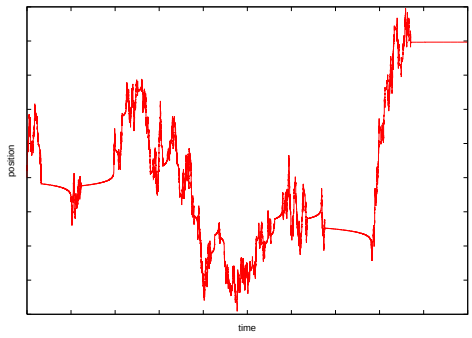


Figure 2: A typical trajectory $y(t)$ shows waiting times and rapid jumping, similar to a CTRW.

A typical trajectory shown in Fig.2 resembles this behaviour. It can be shown that asymptotically, on large spatial and temporal scales, the full system Eq.(1) over an ensemble of initial conditions is *identical* to a continuous-time random walk with a particular scaling behaviour [6]. To do this, we have set up a formalism which allows us to write down the multi-point joint probability distributions of a continuous-time random walk. A noteworthy characteristics of this construction is the separate treatment of the case of several points being in one waiting time interval. In contrast to the case of fast

decaying correlations these contributions do not vanish asymptotically when the waiting time has infinite mean. The continuous-time random walk is driven by iid noise, i.e., by independent, identically distributed increments. This means that the jump size/waiting time distribution, from which δ and Δ are taken, is not a function of x or y. This is of course different for the original system Eq.(1). Therefore, in analogy to the stochastic system, we have constructed the multi-point formalism for systems with coupling between successive steps. When the correlations of the induced map are decaying fast enough, we have shown with help of a coarse-graining procedure that all higher-order moments converge towards the moments of the asymptotic CTRW with iid noise. Using the results from [7] one can distinguish two different behaviors for the asymptotic CTRW: First, the joint distribution $P(\Delta, \delta)$ can factorise into the distribution for the waiting time and the jump size, i.e., Δ and δ are independent. This case can be associated with the spatial domination of the chaotic phase. Second, the joint distribution $P(\Delta, \delta)$ does not factorize, but the distribution of Δ scales with δ^β, where β is the scaling exponent $\langle x2(t)\rangle \sim t^{2\beta}$. This case can be associated with the spatial domination of the laminar phase.

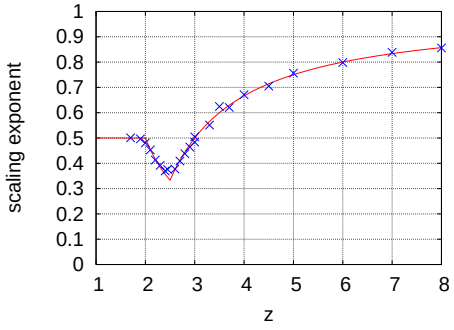


Figure 3: The spatial scaling exponent β of the CTRW as a function of the exponent z of the intermittent map.

By use of the renormalization group techniques for this type of intermittency [4] we have worked out the different domains in dependence on the control parameter z: The waiting time distribution has a power law tail with power $\alpha = 1/(z-1)$ $(z > 1)$ [5]. For $z < 2$, where the invariant measure of $f(x)$ is still normalizable, y exhibits normal diffusion, i.e., the scaling exponent is $\beta = 1/2$. For $2 < z < 2.5$, the chaotic bursts of f dominate the dynamics, and y is subdiffusive with an exponent $\beta = \frac{1}{2}\frac{1}{z-1}$. For $z > 2.5$ the laminar phases f dominate, and the behaviour of y ranges from subdiffusive to superdiffusive with $\beta = \frac{z-2}{z-1}$, the cross-over being at $z = 3$ (see Fig.3). These analytical results are well reproduced in numerical simulations (e.g., the scaling exponents: crosses in Fig.3, multipoint correlations see [8]).

A continuous time random walk with a waiting time exponent $\alpha > 2$ is non-ergodic: The largest waiting time is always of the same order of magnitude as the measurement interval or the duration of some numerical simulation. Hence, the value $y(t)$ during this longest time interval dominates every time average. Since it will be different in every different realization of the process, time averages will not agree and not converge. Hence, one potential dynamical mechanism for such a type of ergodicity breaking is strong intermittency of some microscopic degrees of freedom.

[1] E.W. Montroll and G.H. Weiss, *Random Walks on Lattices II*, Journal of Mathematical Physics **6**, 167 (1965).
R. Balescu, Statistical Dynamics - Matter out of Equilibrium, Imperial College Press (1997).

[2] R. Metzler and J. Klafter, *The random walk's guide to anomalous diffusion: a fractional dynamics approach*, Physics Reports **339** 1 (2000).

[3] J.P. Bouchaud, *Weak ergodicity breaking and aging in disordered systems*, Journal de Physique I **2**, 1705 (1992).

[4] J.E. Hirsch, M. Nauenberg and D.J. Scalapino, *Intermittency in the presence of noise: A renormalization group formulation* Physics Letters A **87**, 391 (1982); B. Hu and J. Rudnick, *Exact Solutions to the Feigenbaum Renormalization-Group Equations for Intermittency*, Phys. Rev. Lett. **48**, 1645 (1982).

[5] M. Thaler, *Infinite Ergodic Theory*, `http://www.sbg.ac.at/mat/staff/thaler/paper.pdf`.

[6] M. Niemann and H. Kantz, *Asymptotic continuous-time random walk models for deterministic diffusion* in preparation.

[7] P. Becker-Kern, M.M. Meerschaert and H. Scheffler, Ann. Prob. **32**, 730 (2004).

[8] Markus Niemann and Holger Kantz, *Joint probability distributions and multipoint correlations of the continuous-time random walk*, PRE **78**, 051104 (2008).

2.22 The Origin of Short Transcriptional Pauses

Martin Depken, Eric A. Galburt, Stephan W. Grill

The ability of cells to adapt to environmental conditions, to reproduce, and to serve varying roles within an organism critically depends on the control of gene expression. A major part of this regulation occurs at the level of transcription, where the RNA polymerase (RNAP) molecule moves along the DNA template creating an RNA copy of the genetic information. This motion is typically interspersed by pauses. Pauses can be classified into pause states where the enzyme forms an inactive configuration without appearing to displace along the DNA template, or pauses where the enzyme forms an inactive configuration by displacing in the rearward direction along the DNA template. Examples of the first type of pauses include the ubiquitous pause [1], which is thought to correspond to an internal structural rearrangement of the enzyme. The second type of pause is referred to as a backtrack, manifesting itself through a displacement of the RNAP molecule in the upstream direction opposite to normal transcriptional elongation [2]. While non-translocating pauses simply act to reduce the overall rate of transcription during elongation, backtracking is also implicated as a prerequisite for removing copy errors by transcript cleavage and contributes significantly to transcriptional fidelity. Upon backtracking the polymerase moves rearwards (Fig. 1a), and the polymerization reaction ceases until the enzyme is realigned with the polymerizing 3' end of the RNA molecule. However, the enzyme can reside in different translocation states while backtracked [2]; and since no chemical energy is consumed, the associated motion can be described as a one-dimensional random walk along the DNA strand. While this mechanism provides an attractive explanation for the experimentally measured broad distribution of return times [3], it is not clear that this simple mechanism alone will generate the two distinct populations of pauses that are observed. Here we show that a random-walk pause scheme will naturally do this, and is able to account for characteristics of the short-time ubiquitous and long-time backtracked pauses.

We model backtracking as diffusion in a one-dimensional free-energy landscape, focussing on general characteristics that survive averaging over different template sequences (see Fig. 1 b). Because the energy landscape of the backtracking polymerase is strictly bounded by the possible states of the nine basepair hybrid, the enzyme will undergo normal diffusion [4]. We ignore sequence dependence, and in the absence of an overall forcing we take the free-energy landscape to be periodic. The application of a force f tilts the free-energy landscape by adding the energy fa per step, with $a \simeq 0.34\,\mathrm{nm}$

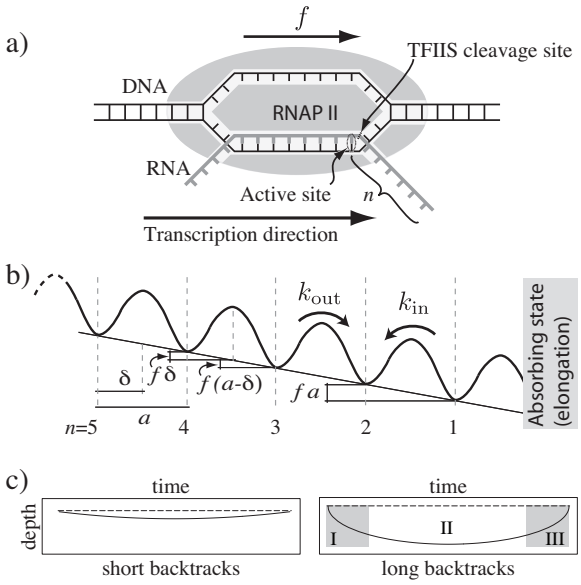


Figure 1: (a) Schematic drawing of RNAP with an applied assisting force f. The integer n corresponds to the number of RNA bases that protrude past the active site. (b) Corresponding schematic free-energy landscape. (c) An illustration of the average trajectory in the two regimes. Short trajectories remain shallow throughout the backtrack (left hand panel), while long trajectories display the three regimes reported in [2] (right hand panel).

being the physical extent of a basepair. The landscape is bounded on one side by an absorbing state corresponding to the active elongation pathway. The hopping rates between the free-energy minima are given by Kramers rates [5] with $k_{\mathrm{out}} = k_0 \exp(f\delta/k_BT)$ and $k_{\mathrm{in}} = k_0 \exp(-f(a-\delta)/k_BT)$. Here, k_0 is the bias-free hopping rate and δ describes the physical distance along the force coordinate from a free-energy minimum to a putative transition state (see Fig. 1 b). The duration of a backtrack corresponds to a first-passage time, the calculation of which is extensively discussed in the literature. The particular problem considered here is that of a discrete random walk with an absorbing boundary and is easily solved for the conditional probability of being at site n at time t, given that we were at site m at time 0,

$$P(n,t|m,0) = \left(\frac{k_{\mathrm{in}}}{k_{\mathrm{out}}}\right)^{\frac{n-m}{2}} \exp\left\{-(k_{\mathrm{out}}+k_{\mathrm{in}})t\right\} \left[I_{n-m}(2t/t_0) - I_{n+m}(2t/t_0)\right].$$

Here the characteristic stepping time $t_0 = 1/\sqrt{k_{\mathrm{out}}k_{\mathrm{in}}} = \exp\{(a/2-\delta)f/k_BT\}/k_0$ has been introduced, and I_n are the modified Bessel functions. To allow for a comparison to experiments [1, 3], we use the theoretical

return time distribution to identify two characteristic times and discuss the effect of an externally applied force. Since the system always enters at and exits from the backtrack position $n = 1$, the probability distribution of first passage return times t is given by $\Psi(t) = k_{\rm out} e^{-(k_{\rm out}+k_{\rm in})t} I_1(2t/t_0)(t/t_0)^{-1}$. This distribution has two characteristic times $t_1 = t_0$ and $t_2 = 1/(\sqrt{k_{\rm out}} - \sqrt{k_{\rm in}})^2$ which gives three asymptotic return time regimes. For pause durations $t \ll t_1$ the probability density falls off exponentially with the rate $k_{\rm out}+k_{\rm in}$. For intermediate pause durations $t_1 \ll t \ll t_2$ the decay is algebraic with exponent $-3/2$. For larger t the algebraic region gets cut off by an exponential with characteristic time t_2. It should also be noted that for opposing forces only the finite fraction $\exp(f/f_0)$ of the pauses is able to exit, with the rest embarking on non-returning excursions. This demonstrates that backtracking offers a simple explanation for the broad distributions observed.

In what follows, we demonstrate that long and short backtracks are very different in terms of the average backtracking path traversed. This effect originates from the discreteness of the lattice: while the short-time backtracks are strongly dependent on the lattice spacing a, this spacing can be absorbed into an effective diffusion constant for the long-time backtracks. Consider the probability $\Pi_T(n,t)$ of being at position n at time t, given an exit at time T, $\Pi_T(n,t) = \frac{Tt_0}{t(T-t)} \frac{n^2 I_n(2(T-t)/t_0) I_n(2t/t_0)}{I_1(2T/t_0)}$, which is invariant with respect to $t \to T-t$ and depends on force only through a possible rescaling of the characteristic stepping time t_0. With a transition state located half way between two adjacent backtracked positions also this force dependence vanishes (see above). The asymptotic forms of the average trajectory in the short- (S) and long- (L) time regimes separate into a penetration depth $\lambda_{\rm S,L}$ and a shape function $\Lambda_{\rm S,L}$ according to

$$\langle n(t)\rangle_T \sim \begin{cases} 1 + \lambda_{\rm S}(T/t_0)\Lambda_{\rm S}(t/T), & t,T \ll t_0 \\ \lambda_{\rm L}(T/t_0)\Lambda_{\rm L}(t/T), & t,T \gg t_0, \end{cases} \tag{1}$$

with the asymptotic forms given by (Fig. 1 c)

$$\lambda_{\rm S}(x) = (x/2)^2, \quad \Lambda_{\rm S}(y) = 4y(1-y),$$
$$\lambda_{\rm L}(x) = 2\sqrt{x/\pi}, \quad \Lambda_{\rm L}(y) = \sqrt{4y(1-y)}.$$

The shape function $\Lambda_{\rm L}$ can be split into three distinct phases (see Fig. 1 c, right hand panel). This is in good agreement with experimental observations where long backtracks can be split into three qualitatively different regimes [2], a rapid entry into the backtrack (phase I), followed by a longer and flatter region (phase II), and a rapid exit (phase III).

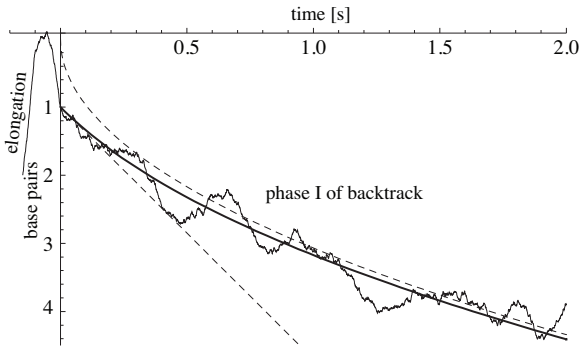


Figure 2: Single parameter fit of the asymptotic long-pause shape function for regime I to data from [2], giving a characteristic time $t_0 = 0.54$ s (solid line). Also shown are the corresponding asymptotic curves of Eq. 2 (dashed lines).

From the above one can show that the backtracking path becomes independent of the pause length T in region I of the long pauses,

$$\langle n(t)\rangle_{\rm L} \sim \begin{cases} 1 + 2t/t_0, & t \ll t_0 \\ 4\sqrt{\frac{t}{\pi t_0}}, & t_0 \ll t \ll T. \end{cases} \tag{2}$$

The absence of a T dependence enables us to make a least square fit of t_0 to the experimental data of [2] over the time interval from the first entrance into the backtrack up to some suitable time $t_{\rm max}$ by utilizing a numerical approximation of the asymptotic form for $T \gg t$. The estimated value of t_0 and the mean-square residue is insensitive to $t_{\rm max}$ within the rage of 0.5 to 2 s, and is best fit by $t_0 = 0.54$ s (using a force of $f \approx -8$pN as applied in the experiments; see Fig. 2). This time constant sets the lower corner time t_1 ($t_1 = t_0$) for short-time backtracks, and is of the same order as the short characteristic time constant of ubiquitous pauses (1.2 ± 0.1 s, see [1]). In conclusion, the bacterial polymerase appears to step about twice per second while backtracked, which will naturally generates two classes of pauses: long-time pauses with the expected behavior of diffusive backtracks, and a novel class of short-time backtracks with characteristics similar to those ascribed to the ubiquitous pause.

[1] Neuman K. C. *et al.* 2003. *Cell*, 115(4):437–447.

[2] Shaevitz J. W., E. A. Abbondanzieri, R. Landick, and S. M. Block. 2003. *Nature*, 426(6967):684–687.

[3] Galburt E. A. *et al.* 2007. *Nature*, 446(7137):820–823.

[4] Harms T. and R. Lipowsky. 1997. *Physical Review Letters*, 79:2895–2898

[5] Hänggi P., P. Talkner, and M. Borkovec. 1990. *Rev. Mod. Phys.*, 62(2):251–341.

2.23 Cortical Flows in the One-cell Embryo of *Caenorhabditis elegans*

Justin S. Bois, Mirjam Mayer, Frank Jülicher, and Stephan W. Grill

Cellular polarity, mechanical and biochemical spatial asymmetry, is an essential feature of myriad cell types. For developing embryos in particular, polarity is required for asymmetric divisions giving rise to cellular differentiation. While a diverse set of cells are polarized, the core mechanisms for polarity establishment, which involve differentiation of regions of the cortex, a thin mesh-work consisting primarily of actin and myosin lying immediately below the cell membrane, are largely conserved [1, 8]. In an effort to understand this central phenomenon in developmental biology, we investigate cortical dynamics in the one-cell embryo of the model organism *C. elegans*.

Prior to polarizing, the cortex of the one-cell *C. elegans* embryo features uniformly-distributed dense flocks of myosin (called foci) connected by F-actin. Myosin consumes energy through ATP hydrolysis and exerts force on the actin filaments, giving an essentially uniform active stress throughout the cortex. Polarization is marked with a biochemical cue from the sperm-donated pronucleus at the posterior of the embryo, which serves to downregulate myosin [3, 6, 7], thereby locally reducing the active stress. After this cue, the cortex flows toward the anterior pole, creating a a region of high myosin density in the anterior and low density in the posterior (see Figure 1a). The flow serves to segregate specific proteins to the anterior pole, establishing polarity in protein composition. That physical mechanisms are central to cortical flow has long been recognized [2], but general conclusions about driving forces remain elusive.

Here, we present experimental measurements of cortical flow velocity and myosin density and a simple theory for cortical dynamics. We show that a gradient in active stress alone is sufficient to drive cortical flow. The microscopic details of the cortex are very difficult to access experimentally, so we make bulk measurements and use a hydrodynamic theory, which considers only long length and time scale behavior.

To measure myosin dynamics, we image embryos with GFP-labeled myosin, enabling easy measurement of myosin density, which is proportional to GFP intensity and assumed proportional to active stress. We track the motion of the labeled myosin through time and determine bulk cortical velocity using particle image velocimetry (PIV). To obtain density and velocity profiles, we bin the measurements along the posterior-anterior axis, as depicted in Figure 1b. These measurements are then averaged over many embryos to get representative profiles.

In developing a theoretical basis for understanding cortical flows, we employ a hydrodynamic description in the spirit of the active polar gel theories of Jülicher and coworkers [4, 5], though much simplified. Because the time scale of the cortical flow is about eight minutes, far longer than the elastic relaxation time of the cortex, which is approximately five seconds (determined by laser ablation experiments in our lab), we take the the cortex to behave viscously, ignoring elasticity. Furthermore, we neglect the polarity of actin filaments in our simple treatment. Finally, the cortex is constantly kept out of equilibrium by energy consumption through ATP hydrolysis through myosin motor activity. Thus, we consider the cortex to be a thin sheet of an active, isotropic, viscous fluid. The constitutive relation and equation of motion describing the cortex are, respectively,

$$\sigma = \zeta\Delta\mu + \xi\,\partial_x\, v \tag{1}$$

$$\partial_x\,\sigma = \gamma\, v \tag{2}$$

where σ is the total deviatoric stress, v is the velocity of cortical flow, and $\zeta\Delta\mu$ is the active stress, which is proportional to the (constant) change in chemical potential for ATP hydrolysis, $\Delta\mu$. The parameter ξ is an effective viscosity which includes both the shear and expansion viscosity, as the cortex is compressible in a one dimensional description, with compression and expansion necessarily coinciding with a velocity gradient. The left-hand side of Eq. 2 is related to the friction associated with contact with the cytosol and cell membrane. Combining Eq. 2 and Eq. 1 and nondimensionalizing gives the equation of motion

$$\ell^{-2}\, v - \partial_x^2\, v = \partial_x\, \zeta\Delta\mu, \tag{3}$$

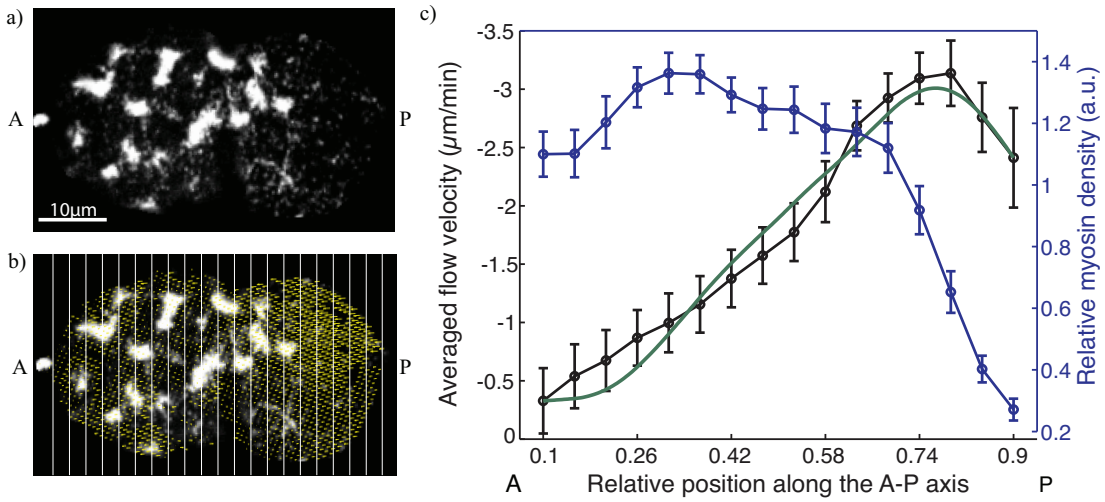


Figure 1: a) The one-cell *C. elegans* embryo with GFP-labeled myosin. The cortex is in the focal plane, and the posterior (P) is to the right and anterior (A) to the left. Cortical symmetry has been broken and the cortex is flowing giving a region of higher myosin density in the anterior. b) Schematic of experimental measurement of myosin density and cortical flow velocity. The rectangular boxes indicate the binning in the quantification and the arrows represent the P-A component of the cortical velocity as determined by PIV. c) Measured myosin density (blue curve) and P-A velocity (black curve) for each bin averaged over 144 embryos. The green curve is a curve fit of the solution of Eq. 3 to the experimental velocity profile given an active stress profile proportional to the myosin density. Error bars are standard error of the mean with a 95% confidence interval.

where all variables are now dimensionless. The parameter $\ell \equiv L^{-1}\sqrt{\xi/\gamma}$, where L is length of the embryo, is the decay length of the velocity in response to the active stress gradient appearing on the right-hand side, which is clearly the driving force for flow.

To assess the efficacy of our theoretical description to describe observed cortical dynamics, we use the experimentally measured myosin density profile as $\zeta\Delta\mu(x)$, solve Eq. 3 for $v(x)$, and then vary ℓ to fit the solution to the experimental velocity profile. We calculate $\ell \approx 0.5$ and the theoretical curve agrees well with the experimental measurements, as shown in Figure 1c. The fact that ℓ is close to unity indicates that the effect of a local gradient in active stress is felt over length scales commensurate with the size of the entire embryo. Thus, a local downregulation in myosin activity gives rise to the large-scale flows essential for sorting proteins to distinct regions to establish cellular polarity.

[1] J. Betschinger and J. A. Knoblich. 2004. *Curr. Biol.*, 14:R674–R685.

[2] D. Bray and J. G. White. 1988. *Science*, 239:883–888.

[3] C. R. Cowan and A. A. Hyman. 2007. *Development*, 134:1035–1043.

[4] J. F. Joanny, et al. 2007. *New J. Phys.*, 9:422.

[5] K. Kruse, et al. 2005. *Eur. Phys. J. E*, 16:5–16.

[6] E. M. Munro, J. Nance, and J. R. Priess. 2004. *Developmental Cell*, 7:413–424.

[7] E. M. Munro. 2006. *Curr. Op. in Cell Biol.*, 18:86–94.

[8] W. J. Nelson. 2003. *Nature*, 422:766-774.

2.24 Cooperation in Adaptive Networks

Thilo Gross and Anne-Ly Do

Over the recent years it has become apparent that networks–ensembles of discrete *nodes* connected by *links*–offer a useful metaphor to describe the structure and dynamics of a large variety of complex systems from different disciplines. At present, *dynamical networks* appear in two distinct contexts giving rise to two different lines of research. On the one hand the notion of a dynamical network can refer to a network that is a dynamical system in itself. In these networks the topology of the network evolves in time as the result of the addition and deletion of nodes or links (dynamics OF networks). On the other hand the notion of a dynamical network can refer to a system in which the topology is fixed but the nodes represent individual dynamical systems. Here internal variables of the nodes evolve in time while coupled according to the network topology (dynamics ON networks).

In almost all real world networks the dynamics of the network and the dynamics on the network take place simultaneously; they are so-called *adaptive* or *coevolutionary* networks [1]. It is therefore the next logical step to bring the two strands of research back together to understand the intricate interplay between topological evolution and local dynamics. Already, the investigation of conceptual models has revealed several fundamental mechanisms leading to new phenomena, such as robust self-organization to critical states, self-assembly of complex topologies, and the spontaneous appearance of distinct classes of nodes from an initially homogeneous population [2]. As a result of recent progress the dynamics of a certain class of adaptive networks is now quite well understood. This class is characterized by a small number of possible states of nodes and links. By contrast, the investigation of the larger class of weighted networks, in which the states of links an nodes are continuous variables, is currently hampered by the lack of analytically tractable models.

The group "Dynamics of Biological Networks" at mpi**pks** presently explores different approximation schemes that allow for the analytical treatment of adaptive networks, such as moment closure approximations [3]. An important part of this work is to come up with simple models that are sufficiently complex to show interesting behavior, sufficiently realistic to hold relevance for real world systems, and sufficiently simple to allow for a systematic analysis. In the work reported here we propose a simple game-theoretical model describing a population of N rational players engaged in cooperative interactions. Cooperation is ubiquitous in biology and is now frequently studied in the context of adaptive networks. However, in contrast to other models, which focus on boolean players (cooperator and defectors), our model allows players to maintain different levels of cooperation with different self-chosen partners.

Consider a population of players. Every player can invest time/money/effort into each of the $N-1$ potential interactions with other players. The actual amount invested by player i into the collaboration with player j is denoted as e_{ij}. We write the payoff received by i as $P_i = B_i - C_i$, where B_i is the total benefit gained from collaborating and C_i is the cost incurred by collaborative investments. Furthermore we assume that $B_i = \sum_j B_{ij}$, where B_{ij} is the benefit generated by the specific collaboration between i and j. The benefit B_{ij} is assumed to be a function of the sum the resources invested into the collaboration, i.e., $B_{ij} = B(e_{ij} + e_{ji})$, while the cost C_i is a function of all investments made by player i, so that $C_i = C(\sum_j e_{ij})$. Finally let us assume that B is sigmoid and C is superlinear.

We consider rational self-interested players trying to maximize their payoff by adapting their investments dynamically in time. The players are assumed to continuously change their investment in the direction of the steepest ascent of their respective payoff. This simultaneous downhill-gradient optimization of individual payoffs constitutes a $N(N-1)$-dimensional system of ordinary differential equations of the form

$$\frac{\mathrm{d}}{\mathrm{dt}} e_{ij} = \frac{\partial}{\partial e_{ij}} P_i \tag{1}$$

Even for a low number of players an explicit analytical solution of the system is prohibitively difficult. Nevertheless analytical reasoning can be used to prove certain properties of stationary states in systems with an arbitrary number of players. Let us focus on a bidirectional link, i.e., a collaboration receiving nonzero investments $e_{ij}, e_{ji} > 0$. By considering the stationarity conditions $\partial P_i/\partial e_{ij} = 0 = \partial P_j/\partial e_{ji}$ we can show that in every stationary state the players i, j must be perceiving the same slope of the cost function, such that $\partial C_i/\partial e_{ij} = \partial C_j/\partial e_{ji}$. Since we assumed the cost C to be a superlinear function, the total amount invested by the players (into all of their collaborations) must be identical. Iterating this argument along sequences of links proves the following: In every stationary state all players that are in the same bidirectionally connected community (BCC) make the same total investment.

By considering the stationarity condition for multiple links connecting to single player i one finds that the derivatives of the link benefit $\partial B_{ij}/\partial e_{ij}$ must be identical for all partners j. For sigmoid B this implies that in a stationary state the benefit generated by all collaborations of a given player can take, at most, two dif-

ferent values, one of which is above the inflection point (IP) of B while the other is below the IP. Again this argument can be iterated along sequences of links to show that all collaborations within a BCC produce, at most, two different levels of benefit. This can be further narrowed down by demanding that the steady state under consideration is dynamically stable. Using certain symmetries of the systems Jacobian matrix and applying Jacobi's signature criterion we can show that every player can have at most one link producing the lower of the two possible levels of benefit. Furthermore, we can show that, for realistic benefit functions, stability requires that all links produce a benefit above the IP. In this case in every stable equilibrium all collaborations in a BCC produce the same benefit.

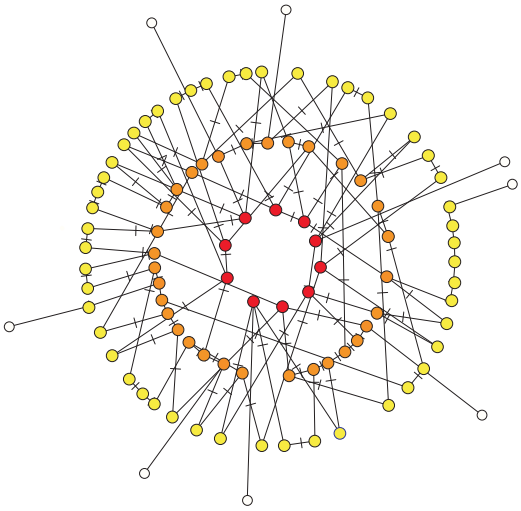


Figure 1: Self-organized network of collaborations. Collaborations are shown as links between players (circles). The asymmetry of investments into a given collaboration is shown by a fairness indicator (small dash), the closer the indicator is to a player, the smaller is the players proportional investment into the collaboration. Players extracting high payoffs are color coded darker and placed toward the center of the figure. In the evolved state all players make an identical collaborative investment and all collaborations convey the same benefit. Nevertheless the investments in a given collaboration are in general asymmetric and some players manage to secure privileged topological positions in which higher payoffs can be extracted.

The coordination of benefits and investments is remarkable as no player has sufficient information to infer the the total investment of any other player and markedly different levels of investment are found in different communities. Note furthermore, that the coordination does *not* imply that all players receive the same benefit. As the benefit per link is identical, the total benefit extracted by a player is proportional to the number of collaborations the player maintains. Players occupying a position of high connectivity thus profit from a significantly higher payoff than average players (see Fig. 1). Also, two connected players generally do not contribute identical investments to the collaboration connecting them. Instead, highly connected make in average smaller contributions as they have to divide their investment among more collaborations. Further investigations show that this asymmetry of investment does not hinder coordination on the network, but in fact is needed to enable an effective flux of resources toward regions of high connectivity where large payoffs are extracted.

For numerical studies coordination of the investment per link is advantageous as it allows us to characterize the evolved network structures by the tools of graph theory for unweighted graphs. This property survives in certain extensions of the basic model. For instance we can allow collaboration with more than two participants or reduce the cost of investments for successful players. The latter modification enables successful players to start new collaborations leading to broader payoff distributions in the population.

Apart from social coordination, a precursor for social norms, and the appearance of distinguished players from an initially homogeneous population, the model reproduces certain other phenomena. One of these is the observation of different responses to withdrawal of one partner from a collaboration, which are well known in pair-psychology. In our model these responses can be linked to the relative position of the IP of B thus providing a simple rationale for the observation.

In summary, we have proposed a simple model of cooperation between selfish players that reproduces well known phenomena from sociology and psychology. However, more importantly, the model constitutes a much-needed example of a weighted adaptive network in which at least some properties can be computed analytically. This model can thus serve as a simple test bed for approximations schemes that are presently being developed to deal with the more complicated adaptive networks encountered in many biological systems. In a wider context the ongoing work on conceptual models and approximation schemes complements a different line of research in which we aim to assess the importance of adaptive network phenomena in real world systems by the numerical investigation of realistic models.

[1] T. Gross and B. Blasius, JRS Interface **5** (2008) 259.

[2] T. Gross and H. Sayama, eds., Adaptive Networks, Springer, Heidelberg, 2009.

[3] T. Gross et al., Phys. Rev. Lett. **96** (2006) 208701.

2.25 Generalized Models of Food Web Stability

Thilo Gross and Lars Rudolf

As a result of the ongoing revolution in experimental biology the structure of important systems, such as metabolic pathways and gene regulatory networks are presently being revealed. However, the functioning and failure of these systems is often linked to their dynamics, which is difficult to observe in biological experiments. An important challenge in theoretical biology is therefore to predict dynamical properties of a system based on the known or purported interaction topology of system components. In addition to the schematic representation of interactions, further information is typically not available or costly to acquire. Therefore mathematical methods are needed that can extract some insights from the very limited information available. Even if these insights do not paint a complete picture of the system, they can lead to the formulation of working hypothesis and feed into the design of future experiments.

In the past members of the group "Dynamics of Biological Networks" at mpi**pks** have proposed the approach of generalized modeling [1]. Starting from a system of differential equations, which defines the topology of interactions but leaves the functional form of the interactions undetermined, generalized modeling identifies a set of parameters (the GM parameters) that together determine the local dynamical stability of all stationary states in the system. In contrast to conventional modeling where one would start by parameterizing the unknown functions in the system, GM is based on a direct parameterization of the system's Jacobian matrix. This parameterization can in general be done such that the individual parameters are interpretable quantities, which have a well-defined meaning in the context of the application. To do justice to the complexity of the system under consideration a large number of GM parameters may be necessary. But, since the numerical performance of GM is very favorable, large parameter spaces can be explored by statistical sampling.

In the past generalized modeling has been applied to questions from different areas of research such as cell biology, ecology, laser physics, and economy [1, 2]. While we presently use GM mainly to study the dynamics of systems from cell biology, the work reported here focuses on the stability of ecological food webs. Food webs are networks of predative interactions between populations. In nature large densely-connected food webs form the backbones of most natural ecosystems. Ever since Robert May [3] pointed out that, on theoretical grounds, large strongly connected webs are likely to be unstable, the questions, what lends natural food webs their stability, has been a topic of intense research and hot debate [4]. Another reason to focus on food webs is that only little information of the interactions of populations is available and food web models are difficult to handle with conventional modeling techniques. They thus provide a challenge that is well suited to demonstrate the advantages of GM.

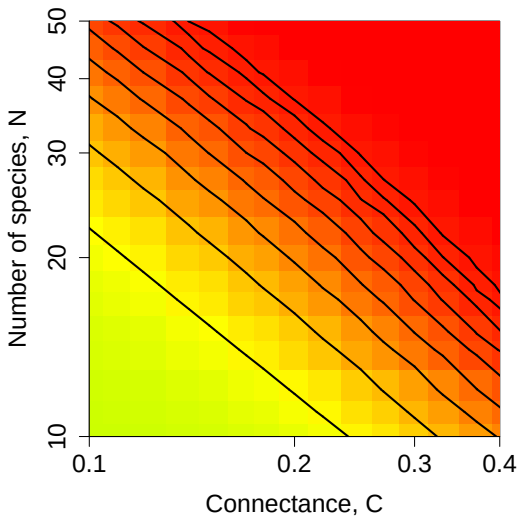


Figure 1: Impact of web size and connectance (links per species squared) on food web stability. Color-coded is the probability of randomly drawing a stable web. This probability is approximately 70 percent for small, spare webs and decreases with increasing size and connectance. Every level line (black) marks a decrease of the density of stable webs by a factor of $\sqrt{10}$. Note that the level lines in the double-logarithmic plot are almost straight, indicating a power-law-like relationship.

Food webs are typically modeled by systems of ordinary differential equations in which every dynamical variable describes the abundance (i.e., population size) of a population of individuals of a certain species. The investigation of these systems is complicated by the strongly nonlinear interactions between the different populations and the large range of different timescales in the system (easily 7 orders of magnitude in nature). Because of the stiffness of the corresponding systems of equations, numerical studies of food web stability are typically limited to the investigation of few (e.g., some thousand) replicates of small (e.g., 10-species) food webs.

Previously a GM for food webs was derived [1]. In this model the abundance X_n of a population n is assumed to follow a differential equation of the form

$$\frac{\mathrm{d}}{\mathrm{dt}}X_n = S_n(X_n) + F_n(\mathbf{X}) - M_n(X_n) - \sum_m G_{mn}(\mathbf{X})$$

where S_n, F_n, M_n, G_{mn} are nonlinear functions describing the gain due to primary production, the gain due to predation, the loss due to natural mortality, and the loss due to predation by another species m, respectively. We

do not restrict these functions to any specific functional form, but rather consider the whole class of ecologically feasible models. An ecologically consistent relation between the predative gain of a predator and the predative loss of the predator's prey is assumed, while who-eats-who is determined by a given food web topology.

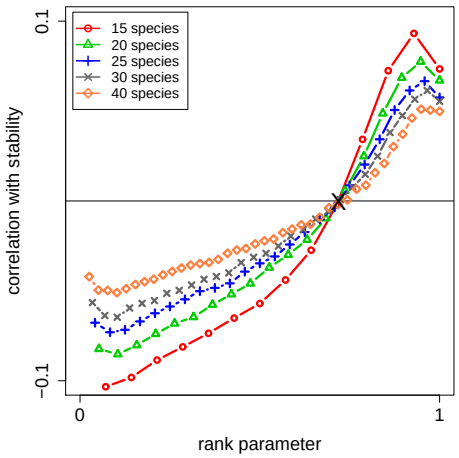


Figure 2: Dependence of food web stability on the distribution of links within the food web. Shown is the correlation of the probability of randomly drawing a stable web with the number of prey species predated upon by a focal species. This property is plotted depending on the normalized trophic position of the focal species. Stability is enhanced if apical predators are generalists, while intermediate predators are specialists. The lines corresponding to webs with different numbers of species all cross in one point at which the correlation vanishes.

In order to explore the impact of food web size N and the number of links L on the dynamical stability, we generate random food web topologies, using the so-called niche model [5]. For every single topology GM is then used to determine the dynamical stability for a random parameter set. In this way we generate sample webs that differ in the number of species N and the connectance $C = L/N^2$. Specifically, the size and connectance of the sample webs is generated to lie on the vertices of a double-logarithmic grid. At every vertex, we then compute the proportion of stable webs (PSW), i.e., the probability of randomly drawing a stable food web. Results from 35 billion random food webs with 10 to 50 species are shown in Fig. 1. As expected, the PSW decreases as N and C increase. Note furthermore, that the iso-stability lines in the figure are almost perfectly straight corresponding to a power-law-like relationship.

In principle, the GM approach can be used for a systematic search for stabilizing network properties. We have for instance investigated the effect of having links of different strength in the web, which was implicated as stabilizing by previous studies, using conventional models. Our investigation confirmed that variation in link strength has a stabilizing influence in small webs. However, in larger webs ($N > 30$) this effect is reversed so that variability in link strength exerts a destabilizing influence.

Another factor for food web stability, revealed by our investigations, is the distribution of links within the web. To see this we assign a trophic rank index z to every species. In a given web this index enumerates the trophic position equidistantly from the lowest to the highest. We normalize the index to the interval $[0, 1]$, so that the most basal species in a web is always characterized by $z = 0$ and the most apical species by $z = 1$. In a large ensemble of food webs of a fixed size, we then compute the correlation between the PSW and the number of prey species on which a species is feeding. In Fig. 2 this correlation is shown as a function of the index z of the focal species. For most species, the PSW correlates negatively with the number of prey species. However a positive correlation is found for species in high trophic positions ($z > 0.719$). Given a fixed number of links, the stability of a food web is thus enhanced if top-predators are generalists that feed on a large number of prey species.

The example of food web stability shows that GMs can efficiently extract certain insights based on limited information. In particular GMs can be used to identify important factors determining local stability, locate the transitions in which stability is lost, and reveal some information on global dynamics. It is therefore promising to use GMs as a high-throughput screening tool for classes of potential models before conventional modeling of a given phenomenon is attempted. In this context it is advantageous that all information needed for GM can be captured in a diagrammatic representation. Thus diagrams can be used as a means of communication with collaborators. Using GMs the analysis of the class of models corresponding to a given diagram can be automated, so that basic insights can be gained within hours or days. Present activities aim to establish an iterative collaboration with experimental biologists in which hypothesis in the form of diagrams and predictions are exchanged on a short timescale.

[1] T. Gross and U. Feudel, Phys. Rev. E **73** (2006) 016205.
[2] R. Steuer et al., PNAS **103** (2006) 11868.
[3] R.M. May Nature **238** (1972) 413.
[4] K.S. McCann, Nature **405** (2000) 228.
[5] R.J. Williams and N.D. Martinez, Nature **404** (2000) 180.

2.26 Time: Quantum and Statistical Mechanics Aspects

Lawrence S. Schulman

Within physics, *time* raises several well-defined problems. Venturing beyond physics, things get murkier and the definitions of the problems themselves may be unclear. The "advanced study group," *Time: quantum and statistical mechanics aspects* (ASG), focused on physical problems, but occasionally took up some of the other issues. The principal areas studied were the following:

Arrows of time. There is a growing consensus that the thermodynamic arrow of time follows that of cosmology, as first suggested by T. Gold. But then there are the details! What emerged from our ASG was a simple statement—less ambitious than that sought by some cosmologists—but covering the essential *observed* phenomena. As established by Boltzmann, what you need for entropy increase today is low entropy in the past. The problem is that in the past, as today, entropy increases, not decreases; his solution was to postulate an enormous fluctuation, an idea that is no longer given much credence. (Not to show anything but respect for Boltzmann, but he had no inkling of the now accepted history of the universe.) Our statement makes use of a single known phenomenon: the near uniformity of the distribution of visible matter at the time of "decoupling" (of matter and radiation, at about 380000 years). Proof of this feature is the 1 part in 10^5 constancy of temperature in the cosmic background radiation. This uniformity was the natural outcome of the fact that prior to decoupling the dominant forces were short range (electromagnetic with shielding within the plasma). Once electrons and protons combined, photons decoupled, and gravity became the dominant force. A basic fact about gravity is that under its influence uniformity is the *least* likely of states, no longer the most likely. Gravity makes things clump. Thus low entropy is achieved not by a fluctuation, but by the ordinary evolution of the universe under expansion with its built-in change in the nature of the dominant force. Many cosmologists worry about much earlier times and our argument does not settle those issues. The point, however, is that with only very little theorizing we go from an observed phenomenon—uniformity at decoupling—to another observed phenomenon—the present day thermodynamic arrow.

Another issue was a search for experimental indications of "opposite arrow" regions in the universe, as suggested by a feasibility demonstration some years ago. Because of temporal paradoxes it is not clear that such a region would be noticed. A number of model systems were considered with emphasis on the issue of signaling. This is work in progress.

Quantum operators for time and arrival time. Every physicist has encountered the time-energy uncertainty relation $\Delta t \Delta E \geq \hbar/2$—along with an apology, that this differs from the corresponding position-momentum relation, since a time operator does not exist. Physically, the problem is that if you had a bona fide pair of conjugate operators, exponentiating the time operator should allow you to perform unlimited translations on energy. But energy is bounded from below. By contrast, *time* is the most precisely measured of physical quantities. How can one reconcile this with the mantra that measurements give the eigenvalues of observables?

The approach taken is to look at what the experimentalist does. Typically, it is *arrival time* that is measured. This suggests that for traversing a particular distance, an operator for arrival time could be mx/p (symmetrized). One can take care of the p^{-1} singularity by considering a generalization of standard operators, so-called POVM's (Positive Operator Valued Measure). Other approaches use the operators of the measurement apparatus, which *de facto* become the time operators. The group explored these and other approaches, both in previous publications and in those associated with the ASG (see below). A central concept is the *distribution* of arrival times, with one of the prominent candidates the "Kijowski distribution" (related to the POVM approach). An interesting synergy occurred when this same distribution appeared in what seemed at first totally unrelated work. One of our speakers, Y. Strauss, whose main interest was the unstable particle issues discussed below, defined what he calls Lyapunov operators. They are monotonic functions of time for any evolving wave function. (Since Schrödinger evolution is time-symmetric there must be an asymmetry in the definition—realized by an astutely placed i.) A week after his departure from the MPI, Hegerfeldt arrived and was told of Strauss's work. Hegerfeldt took off with this and introduced extensive generalization. Next came Muga who recognized that emerging from the time operator defined by Strauss/Hegerfeldt was the Kijowski distribution mentioned above in connection with POVM's and time of arrival.

Unstable "fundamental" particles. What is an *unstable* particle? More poignantly, what is the 2s state of hydrogen? At the level of elementary quantum mechanics the outgoing wave boundary condition solution (which you want for "2^{nd} sheet" solutions) for a particle confined by a barrier yields an exponentially growing

state, much worse than the continuum states of scattering theory. So even for non-relativistic quantum mechanics, a transient state presents problems.

ASG members have looked at *semigroup* representations—following Wigner's beautiful work on the representations of the Poincaré group—as a way to define unstable particles. (The "semi" refers to the absence of translation to negative time—before the particle was created.) But announcing a representation is not the same as identifying the space on which it is defined. This challenge has been met by defining generalizations of Hilbert Space. It has been found that a particular extension, the Hardy Space, is the appropriate construct. Moreover, once you have this, the concepts of resonance and decay can coexist in a well-defined mathematical framework.

Non-equilibrium thermodynamics. There is no time in traditional thermodynamics. Nevertheless, one would like to bring thermodynamic reasoning to time-dependent phenomena. This is a currently active field. One question considered by the ASG was what level of dissipation is required to achieve a given level of power. (Carnot ratio efficiency requires infinite slowness, hence yields no power.) Our approach focused on the use of stochastic dynamics. A closely related inquiry probes the nature of the *currents* that exist in a non-equilibrium system. Stochastic dynamics is used in many applications and implicitly assumes certain rules for transition rates between states. But this is guesswork, or better, a theoretical construct. What one generally observes are *currents*, i.e., *net* transition rates. Our question was, given the currents, what can be said about the underlying stochastic dynamics. It turns out that given a set of currents a transition matrix can be constructed having those currents; moreover the remaining ambiguity can be fully characterized. Another result was to prove something "obvious": increasing the transition probability between a pair of states increases their current. OK, this will not shock anyone, but proving it is surprisingly subtle. In a sense this is like proving the GHS inequalities, also "obvious" and also difficult to establish. Of course I am not claiming that our result will have the same impact as GHS.

[1] Generalized Clausius relation and power dissipation in non equilibrium stochastic systems, B. Gaveau, M. Moreau and L. S. Schulman, Phys. Rev. E (Rap. Comm.) **79**, 010102(R) (2009).

[2] Currents in nonequilibrium statistical mechanics, B. Gaveau and L. S. Schulman, Phys. Rev. E **79**, 021112 (2009).

[3] Source of the observed thermodynamic arrow, L. S. Schulman, J. Phys.: Conf. Series, to appear.

[4] We know why coffee cools, L. S. Schulman, Physica E, to appear.

[5] Energetic consequences of decoherence at small times for coupled systems, B. Gaveau and L. S. Schulman, preprint.

[6] Arrival Times, Complex Potentials and Decoherent Histories, Jonathan Halliwell and J. Yearsley, sub. to Phys. Rev. A.

[7] Time in Quantum Mechanics-Resonances and Decay, A. Bohm, H. Kaldass, S. Komy, and W.P. Schleich,and H. Uncu, in preparation.

[8] Quantum jumps, state trajectories and Gamow vectors, A. Bohm, P. Bryant, H. Kaldass, S. Komy, W.P. Schleich, H. Uncu, and S. Wickramasekara.

[9] A Brief Survey of the Mathematics of Quantum Physics, Arno Bohm, David McGhan and Haydar Uncu, sub. to Rep. Math. Phys.

[10] Time Asymmetry in Quantum Mechanics and spectrally invariant decay properties of Resonances, H. Baumgärtel.

[11] Semigroup Integrability of Point form Dynamics, S. Wickramasekara and N. Harshman, sub. Rep. Math. Phys.

[12] Relativistic Dynamics of Quasistable States I: Perturbation Theory for the Poincaré Group; Relativistic Dynamics of Quasistable States II: Differential Representations of the Causal Poincaré Group, S. Wickramasekara, preprints.

[13] Detector models for the quantum time of arrival, A. Ruschhaupt, J. G. Muga, G. C. Hegerfeldt, for *Time in Quantum Mechanics, Vol. 2*, ed. by J. G. Muga, A. Ruschhaupt and A. del Campo (Springer, 2009).

[14] Quantum post-exponential decay, J. Martorell, J. G. Muga, D. W. L. Sprung, for *Time in Quantum Mechanics, Vol. 2*, ed. by J. G. Muga, A. Ruschhaupt and A. del Campo (Springer, 2009).

[15] Momentum-space interferometry with trapped ultracold atoms, A. Ruschhaupt, A. del Campo, and J. G. Muga, to appear, Phys. Rev. A.

2.27 Three Ways to Achieve Directional Emission from Optical Microcavities and Microlasers

Martina Hentschel

From Quantum Chaos to Microlasers. Optical microcavities with various cross sections are important model systems in the field of quantum chaos as these systems are realizations of open billiards. They are well suited to test ray-wave correspondence in open systems not only from the basic-research point-of-view but also in connection with experiments and applications. Light confinement by total internal reflection in such two-dimensional microresonators is important for a wide range of applications and research areas. The particular practical relevance of deformed microdisks is that they can provide directed light emission which is essential, e.g., for many applications such as microlasers or single-photon sources.

In this overview we present three approaches how to achieve such a directional emission. All were investigated in the mesoscopic physics group (with Tae-Yoon Kwon), partly in collaboration with Jan Wiersig (University of Magdeburg). The mechanisms that provide the directional emission are very different: (i) Mode hybridization at an avoided resonance crossing, tuned by modifying the resonator geometry, was employed to achieve directed emission from whispering-gallery modes (WGMs) in annular cavities [1], (ii) manipulation and customization of the pumping scheme is used in the case of microlasers of spiral shape [2], and, eventually, (iii) the intimate relation between the far-field characteristics and the so-called unstable manifold leads to robust and mode-independent, universal directional emission from cavities of Limaçon shape [3]. All approaches, even the first one which seems to be the experimentally most demanding one [4], have been verified in experiments. We now focus on the last two and the case of TM (transverse-magnetic) light polarization.

Spiral microlasers. Spiral microcavities have been considered a suitable path to directional emission for a couple of years. The simple idea behind is that the symmetry breaking by the so-called notch (the off-set in the cavity boundary, cf. Fig. 1) will make WGMs to leave the cavity in a directional manner, namely from this notch. We now understand to what extent this picture holds [2]. and that is has to be modified considerably in the details. Directional emission from the notch is indeed possible, but requires an intricate mode-beating-type interaction between clockwise and counterclockwise propagating WGMs (where the latter do not hit the notch), see Ref. [2] for details.

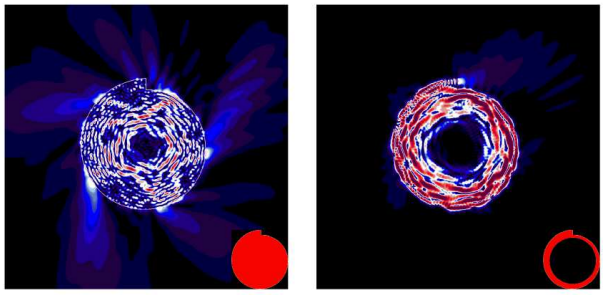


Figure 1: Characteristic mode pattern and emission profiles from uniformly (left) and boundary pumped (right) spiral microresonators. The notch is on top.

This interaction is facilitated by pumping of the microlaser along its boundary (the smaller the pumped ring the better) and a notch size corresponding to about two wavelengths (i.e., sufficient, but not too strong deviation from the circular geometry). The importance of the mode interaction is clearly visible when comparing the boundary-pumping scheme (Fig. 1 right) with a uniformly pumped spiral cavity (Fig. 1 left): Counterclockwise traveling WGMs dominate in the uniformly pumped case and determine the far-field pattern that visibly carries this sense of rotation. It is dominated by a number of sharp spikes. Their position sensitively depends on the excited resonance and on the notch size and reflects the chaotic classical dynamics in spiral billiards. Such a characteristics was recently observed by the Capasso group (Harvard) with quantum cascade microlasers, where boundary pumping is not possible technically.

Limaçon cavities. Another way to customize microlasers towards a directional output characteristics employs the understanding gained from the quantum-chaos approach to optical microcavities. After the theoretical prediction by Wiersig and Hentschel in Ref. [3], the idea was verified in experiments by three different groups within one year.

The basic idea is that the light output is due to rays that cross the critical line in phase-space, i.e., violate the condition of confinement by total internal reflection. This occurs when the (modulus of the) sine of the angle of incidence is smaller than the critical angle given by the inverse refractive index (we assume air outside).

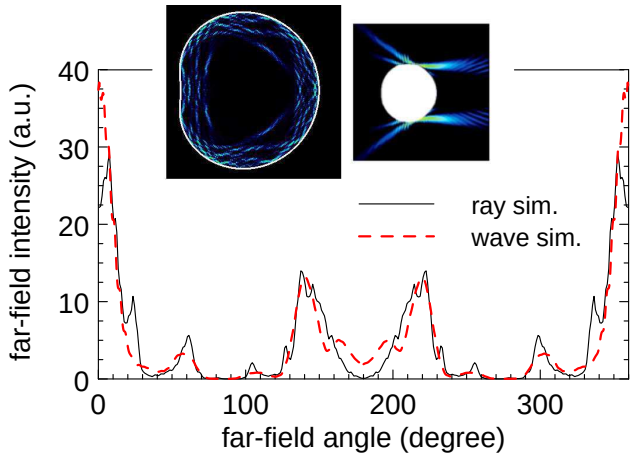


Figure 2: Far-field emission from a Limaçon cavity in the ray and wave picture. Inset: Resonator geometry with a sample resonance and the far-field in real space. A far-field angle of zero corresponds to horizontal emission to the right. Note that experimental results very nicely agree with these simulations [5].

This set of rays is characterized by the unstable manifold in phase space, that, for the open, optical cavities considered here, has to be weighted by the Fresnel reflection coefficient. For the Limaçon cavity, this yields the highly directional far-field emission characteristics shown in Fig. 2. Slight changes in the resonator geometry modify the emission profile and can be used to optimize, and customize, the light output [5]. The most important advantage of this approach is, however, its robustness: The far-field properties are universal and do *not* depend on the specific resonance that is lasing. That clearly is an advantage for all applications.

To summarize, we have presented three successful approaches to the quest for directed emission from microlasers. Whereas there is certainly room for improvement (emission into smaller solid angles), the application potential of the spiral and Limaçon cavities is at hand. From the theoretical point of view, the next challenge is a deeper understanding of the surprisingly nice agreement between ray/wave simulations and experiments even deep in the wave regime (where corrections to the ray model become important [6]) and even for lasing microcavities.

[1] J. Wiersig and M. Hentschel, Phys. Rev. A **73**, 031802(R) (2006).

[2] M. Hentschel and T.-Y. Kwon, Opt. Lett. **34**, 163 (2009).

[3] J. Wiersig and M. Hentschel, Phys. Rev. Lett. **100**, 033901 (2008).

[4] F. Wilde, PhD Thesis, University of Hamburg (2008).

[5] C. Yan, Q. J. Wang, L. Diehl, M. Hentschel, J. Wiersig *et al.*, submitted to Optics Express (2009).

[6] E. G. Altmann, G. D. Magno, and M. Hentschel, Europhys. Lett. **84**, 10008 (2008).

2.28 Dirac Fermions on Graphene Edges: Parity Violation and Quantum Hall Physics

Grigory Tkachov and Martina Hentschel

Introduction. Due to the close connection between their topological and physical properties, two-dimensional (2D) electron systems have traditionally been in the focus of fundamental research. From the practical side, device functionalities in the 2D geometry are of great importance for applications and particularly suitable for lateral electronic architecture. The interest in these general aspects of 2D electron systems has recently revived in the light of the experimental success in isolating individual layers of graphite, preserving the honeycomb crystal structure (see, Fig. 1). Such a system - graphene - exhibits elementary excitations that behave at low energies and long distances as massless Dirac fermions. Due to this formal analogy with ultrarelativistic electrons, graphene stands out among other 2D electron systems, which opens hitherto unexplored research directions.

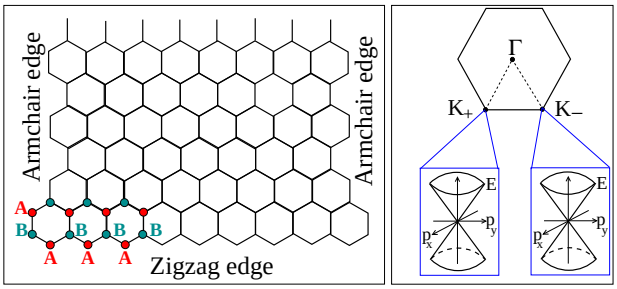


Figure 1: Left: Honeycomb crystal structure of graphene. It consists of two triangular sublattices whose sites are marked by A and B. The figure also shows two basic types of graphene edges commonly referred to as "zigzag" and "armchair" according to their geometrical profile. Right: Near the corner points of graphene's Brillouin zone the quasiparticle spectrum $\varepsilon(p_x, p_y)$ has a conical form reminiscent of the ultrarelativistic electron.

In particular, understanding boundary effects in graphene and the need for their characterization are among the outstanding current challenges in the field,

arising from potentially promising electronic applications of graphene ribbons and quantum dots.

We have been studying electronic properties of graphene in the presence of extended defects, such as linear edges [1–4]. There are two basic types of graphene edges commonly referred to as "zigzag" and "armchair" which are schematically shown in Fig. 1. The zigzag edge is a type of the honeycomb lattice termination where the outermost lattice sites all belong to one of the two triangular sublattices (e.g. A in Fig. 1), while the armchair boundary has exactly equal numbers of the A and B sublattice sites.

Due to the sublattice asymmetry, the zigzag edge exhibits a remarkable property: it can bind massless Dirac fermions, leaving only the freedom of a quasi-1D motion along the edge. Such a quasi-1D Dirac fermion system is formed on the scale of a few nanometers and displays various broken symmetries, which have implications for its electronic properties.

Violation of Dirac fermion parity on graphene edges. As an example of rather unusual electronic properties of the zigzag-type edges, in Fig. 2 we plot the local density of states (LDOS) [1], a directly measurable quantity that provides the most complete information on the quasiparticle spectrum of the material.

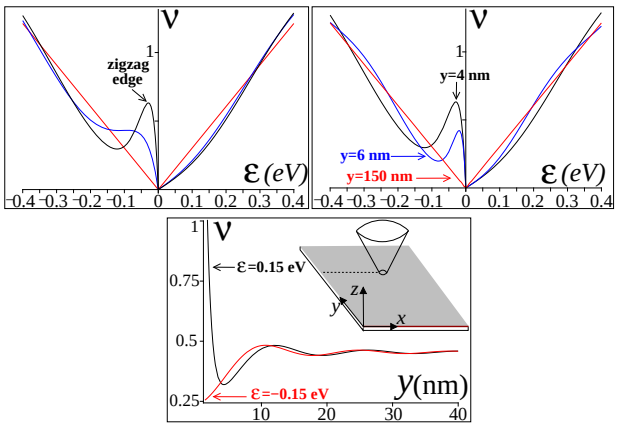


Figure 2: Left: Local density of states (LDOS), ν vs. energy, ε for the zigzag edge. The peak at $\varepsilon \approx -25$ meV is due to the branch of states localized at the edge. The linear LDOS (red) corresponds to the Berry-Mondragon mass confinement that does not support edge states. Right: Suppression of the LDOS peak with distance from the edge, y. Bottom: LDOS vs. distance from the edge, y. Inset: Scheme of the setup used to measure the LDOS in scanning tunneling experiments.

The LDOS peak at ≈ -25 meV corresponds to the branch of states localized at the edge. It appears asymmetric with respect to the energy inversion $\varepsilon \to -\varepsilon$. The asymmetry is inherent to the zigzag-type edges as they turn out to spontaneously violate one of the Dirac fermion internal symmetries - parity [1]. This finding provides an adequate and quite general interpretation for recent scanning tunneling measurements of the LDOS in graphene.

Graphene as a model quantum spin Hall system. The electronic properties of zigzag-type graphene edges are also of interest in view of the fact that in 2D systems the existence of gapless edge states is intimately related to the quantum Hall topological order. There is however an important difference compared to the conventional quantum Hall effect: the zigzag graphene edge states occur in the absence of any external magnetic field. For this reason, zigzag-terminated graphene is reminiscent of the quantum spin Hall (QSH) systems [2,3]. We have shown that, if realized in graphene, the QSH state could be identified by the particle-hole symmetry of the LDOS [see, Fig. 3d]. That contrasts the particle-hole asymmetric LDOS of the usual zigzag-terminated graphene [see, Fig. 3a]. Such a drastic contrast results from the modification of the edge-state spectrum due to a spin-orbit coupling mechanism specific to the QSH state and originating from broken inversion symmetry with respect to coordinate reflection along the edge [2].

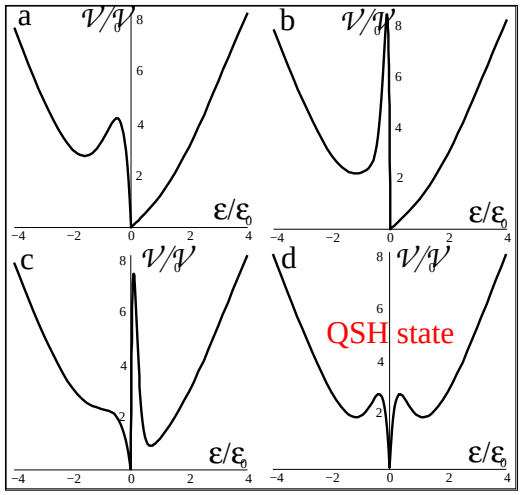


Figure 3: Local density of states (LDOS): (a) for usual zigzag-terminated graphene, (b) and (c) near the quantum spin Hall phase transition, and (d) in the quantum spin Hall phase. The crossover from (a) to (d) occurs as a function of the parameter breaking inversion symmetry with respect to coordinate reflection along the edge [2].

[1] G. Tkachov and M. Hentschel, submitted to Phys. Rev. Lett.; arXiv: 0810.0632.

[2] G. Tkachov and M. Hentschel, submitted to Europhys. Lett.; arXiv: 0803.0713.

[3] G. Tkachov, Phys. Rev. B **79** (2009) 045429.

[4] G. Tkachov, Phys. Rev. B **76** (2007) 235409.

2.29 Temporal Self-restoration of Compressed Optical Filaments

Stefan Skupin, Luc Bergé, and Günter Steinmeyer

The physics of ultrashort optical filaments has recently received increased attention as it enables self-compression of intense laser pulses into the few-cycle regime [1, 2]. Femtosecond pulses with input powers close to the self-focusing threshold, $P_{\rm cr}$, indeed produce a single filament in which the spectrum broadens and the pulse duration decreases during propagation. For evidencing self-compression, experiments currently employ Brewster-windowed cells filled with noble gas at pressures controlling the ratio of input power over critical. Diagnostics are furthermore placed several tens of cm beyond the sample, making the pulse undergo a last stage of atmospheric propagation. In this context, a crucial question is whether the main characteristics of the compressed pulse are preserved when it exits the output window. First, the pulse entering the glass sample undergoes a nonlinear index being three decades higher than in the gas. This renders the robustness of the exiting optical structure questionable as a light beam with several thousands of critical powers is expected to immediately break up by modulational instability [3]. Second, the much stronger dispersion of glass should severely alter the temporal compression. In the following we will show that despite these apparent sources of instability, filamentary propagation holds a hidden self-healing mechanism for ultrashort pulses. We report on simultaneous spatio-temporal self-restoration of light bullets having experienced a perturbation that should have immediately caused spatial and temporal decay of the filament.

Propagation equations model the forward component of the pulse envelope, $\mathcal{E}(x,y,z,t)$, coupled with the free electron density, $\rho(x,y,z,t)$ [4]

$$\begin{aligned}\partial_z\mathcal{E} = {}& \frac{i}{2k_0}T^{-1}\nabla_\perp^2\mathcal{E} + i\mathcal{D}\mathcal{E} - i\frac{k_0}{2n_0^2\rho_c}T^{-1}\rho\mathcal{E} \\ & - \frac{\sigma}{2}\rho\mathcal{E} - \frac{U_i W(I)(\rho_{\rm nt}-\rho)}{2I}\mathcal{E} \\ & + i\frac{\omega_0}{c}n_2 T\int\mathcal{R}(t-t')|\mathcal{E}(t')|^2dt'\mathcal{E}, \qquad (1)\end{aligned}$$

$$\partial_t\rho = W(I)(\rho_{\rm nt}-\rho) + \sigma\rho I/U_i - \rho/\tau_{\rm rec}, \qquad (2)$$

where $I = |\mathcal{E}|^2$, z is the propagation variable and t the retarded time in a reference frame moving with group velocity at laser mid-frequency ω_0. The operator $T = 1 + (i/\omega_0)\partial_t$ accounts for higher order corrections to the usual slowly varying envelope approximation [5]. For more details of the model see also Refs. [6, 7]. Simulations have been performed in full 3D and radially-symmetric ($r = \sqrt{x^2+y^2}$) geometries, yielding analogous results. The starting pulse, being Gaussian with duration 30 fs, is focused by a lens ($f = 50$ cm) into an argon cell (uniform pressure of 0.5 bar) with a 1.5 m maximum length. The following analysis is divided into three steps devoted to pulse propagation in argon, inside the silica window, and in air.

1. Filamentation in argon. With one critical power, the pulse develops a light bullet dynamics [6], characterized by a primary focusing sequence, followed by a second, limited refocusing [Fig. 1(a)]. Minimum FWHM duration is attained when the plasma relaxes, and the filament is compressed to about 6 fs at $z \simeq 0.7$ m [Fig. 1(b)]. The three subplots of Fig. 1(c) show intensity distributions at distances $z = 0.5$, 1 and 1.5 m where the on-axis fluence ($\mathcal{F} \equiv \int |\mathcal{E}|^2 dt$) reaches 1.7 J/cm^2, 0.2 J/cm^2, and 0.05 J/cm^2, respectively. These distances define the position of the exit glass window.

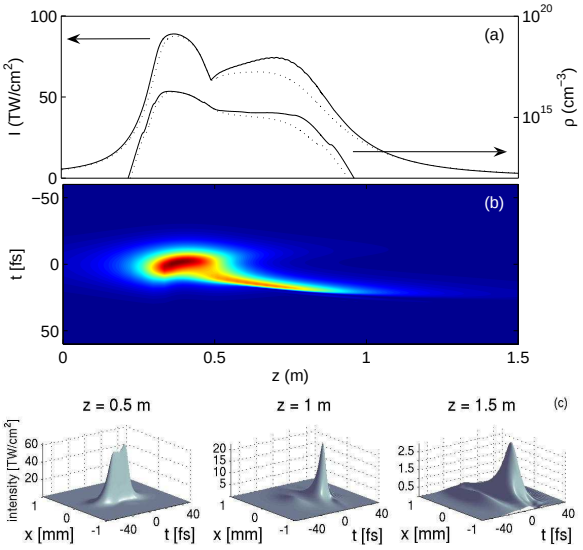


Figure 1: (a) Peak intensity (measured on left axis) and electron density (resp. right axis) for a 500 μm-waisted, 30 fs Gaussian pulse focused with $f = 50$ cm inside a 1.5 m long cell of argon computed in 3D geometry (solid curves) and in radial symmetry (dotted curves). 3D simulations involve a 5 % noise in the input. (b) Temporal on-axis dynamics. (c) Intensity profiles in the (x,t) plane at the three positions selected for the exit glass window.

2. Crossing the silica window. At high enough fluences > 0.1 J/cm^2, only a fraction of the forward pulse can be transmitted through a silica surface. Output profiles of Fig. 1(c) multiplied by appropriate transmission rates are used as initial conditions of Eqs. (1)-(2) solved for silica [7]. Figure 2(a) summarizes our results. 3D and radially-symmetric simulation results almost superimpose; hence, no severe azimuthal distortions affect the intensity profiles in the (x,y) plane. The pulse captured at $z = 0.5$ m (pulse I) begins to diffract over 1 mm, but it refocuses and collapses just afterwards. Although

experimentally irrelevant, this extreme configuration already points out the importance of the first few mm of propagation dominated by pulse dispersion. When the window is positioned at $z = 1$ m (pulse II), again dispersion first prevails, but does not prevent beam collapse over 5 mm long paths. In contrast, the low-intensity pulse III disperses rather slowly over the same distance and beyond. Rows (II) and (III) of Fig. 2 depict the evolution of pulses II and III in the (x, t) plane ($y = 0$). Pulse II enters the dielectric with time extent of ~ 8 fs. After 0.5 mm in silica, this pulse decays into a broader structure of ~ 33 fs, forming a pedestal that extends deep into the trailing region. Pulse III first exhibits a duration of 13 fs, which then broadens to 28 fs over 0.5 mm in glass and more afterwards.

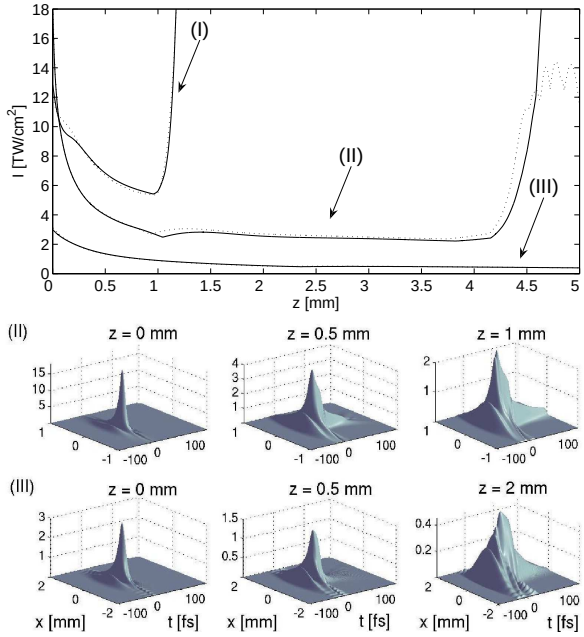


Figure 2: (Top) Peak intensity of the filament exiting the argon cell at (I) $z = 0.5$ m, (II) $z = 1$ m and (III) $z = 1.5$ m, and propagating into the silica window over mm distances. Solid (dotted) curves refer to 3D (radial) computations. (Middle and bottom) Rows (II) and (III) detail the (x, t) evolution of the pulse intensity profiles II and III, expressed in TW/cm^2, inside the exit window.

It is important to note the complete absence of multi-filamentation (MF) in our simulations. Estimates from modulational instability theory predict MF and subsequent collapse over short distances ~ 0.1 mm. In fact, as group velocity dispersion (GVD) rapidly damps the peak intensity, the amplification of periodic spatial modulations leading to MF is practically prevented. Besides, it turns out that both GVD and the Kerr response are responsible for the strong increase of the pulse duration that highly exceeds predictions by linear estimates for Gaussian pulses [7].

3. Air propagation. Because diagnostics are usually positioned tens of cm away from the cell, the beam finally propagates in atmosphere. Figures 3(a,b) show the temporal evolution of pulses II and III as they exit a 0.5 mm thick window and are fully transmitted in air. These pulses contain time slices with maximum powers of $\sim 3.5\ P_{\rm cr}$ in air. This fact contributes to make them refocus and thus recompress. Besides the local Kerr response, self-healing also proceeds from the spatial phase curvature imprinted by the silica window. This phase modification is a key process, which causes a focusing lens effect in air. Finally, Figs. 3(c,d) detail temporal profiles with FWHM durations of ~ 10 and ~ 18 fs for pulse II and pulse III, respectively. These durations are comparable to those reported in experiments [2].

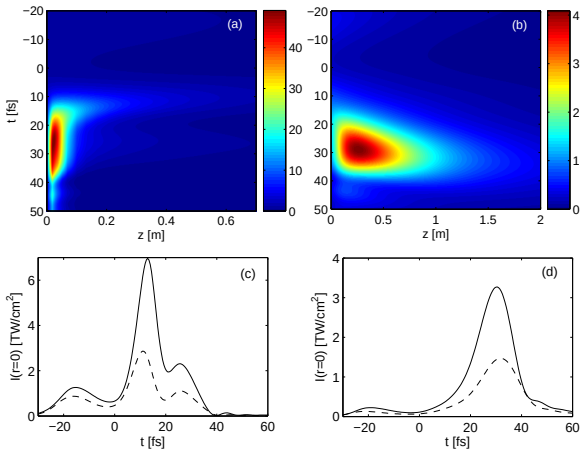


Figure 3: On-axis temporal evolution of (a) pulse II and (b) pulse III in the atmosphere, after exiting a 0.5 mm thick window. (c) Recompressed profiles in air at the distances $z = 0.25$ m (solid line) and 0.5 m (dashed line) for pulse II. (d) Same for pulse III at $z = 0.5$ m (solid line) and $z = 1$ m (dashed line).

[1] C. P. Hauri *et al.*, Appl. Phys. B: Lasers & Optics **79**, 673 (2004).

[2] G. Stibenz, N. Zhavoronkov, and G. Steinmeyer, Opt. Lett. **31**, 274 (2006).

[3] V. I. Bespalov and V. I. Talanov, JETP Lett. **3**, 307 (1966).

[4] L. Bergé, S. Skupin, R. Nuter, J. Kasparian, and J.-P. Wolf, Rep. Prog. Phys. **70**, 1633 (2007).

[5] T. Brabec and F. Krausz, Phys. Rev. Lett. **78**, 3282 (1997).

[6] L. Bergé and S. Skupin, Phys. Rev. Lett. **100**, 113902 (2008).

[7] L. Bergé, S. Skupin, and G. Steinmeyer, Phys. Rev. Lett. **101**, 213901 (2008).

2.30 Control of Randomized Laser Beam Propagation in Inertial Confinement Fusion Plasmas

Mickael Grech, G. Riazuelo, D. Pesme, S. Weber, and V.T. Tikhonchuk

Controlling the propagation of randomized laser beams through large scale plasmas is a problem of ongoing concern in inertial confinement fusion (ICF). Optical smoothing techniques are used to limit the effect of self-focusing, to reduce reflectivities of backscattering instabilities and to improve laser irradiation uniformity onto the target. The resulting intensity distribution is made of many spikes, the so-called speckles, randomly distributed in space and time. The statistical properties of such laser beams are known in vacuum [1], but can be modified by the interaction with plasma. This phenomenon, referred to as plasma induced smoothing, arises from forward scattering of the laser light on the laser induced density perturbations in the plasma [2].

Several processes of forward scattering on such perturbations like self-focusing (SF), filament instability (FI), forward stimulated Brillouin scattering (FSBS) and multiple scattering (MS) have been considered. It is commonly assumed that the beam spray mainly follows from the SF in speckles carrying a power above the critical power $P_c \propto T_e/(n_0/n_c)$, where T_e is the electron temperature and n_0/n_c is the ratio of the electron density to the critical density. However, recent studies [2,3] provide growing evidences of the effect of FSBS in beam spraying and a comprehension of this phenomenon is of a great importance for design of future ICF experiments.

In this work, it is demonstrated that coherent excitation of FSBS outside the incident laser cone, and hence strong beam spray, is to be expected when the average power in a speckle $\langle P\rangle > (\nu_s/\omega)P_c$ and that the instability cannot be prevented by smoothing of the incident beam [4]. Here, ν_s/ω is the normalized ion-acoustic damping rate. For ICF conditions $\nu_s/\omega \ll 1$ and beam spray is expected well below the SF threshold.

A correct understanding of FSBS driven by a monochromatic, spatially incoherent pump wave requires a statistical model of the laser beam propagation. The pump $a^{(p)}_{\mathbf{k}}$ and scattered $a^{(d)}_{\mathbf{k}}$ electromagnetic waves (both described within the paraxial approximation) are coupled to the ion acoustic wave $a^{(s)}_{\mathbf{k}}$ with frequency $\Omega^{(s)}_{\mathbf{k}}$:

$$\left(c\,\partial_z + i\,\Omega^{(d)}_{\mathbf{k}}\right) a^{(d)}_{\mathbf{k}} \;=\; \gamma_0 \int d\mathbf{k}_p\, a^{(p)}_{\mathbf{k}_p} a^{(s)*}_{\mathbf{k}_p-\mathbf{k}}\,, \quad (1)$$

$$\left(\partial_t + \nu_s + i\,\Omega^{(s)}_{\mathbf{k}}\right) a^{(s)}_{\mathbf{k}} \;=\; \gamma_0 \int d\mathbf{k}_p\, a^{(p)}_{\mathbf{k}_p} a^{(d)*}_{\mathbf{k}_p-\mathbf{k}}\,, \quad (2)$$

where the FSBS coupling constant is $\gamma_0^2 = \Omega^{(s)}_{\mathbf{k}_s}\,\omega_0\,(n_0/n_c)\,\langle I\rangle/(8c\,n_c\,T_e)$, with ω_0 the laser frequency and $\langle I\rangle$ the average incident laser intensity. Statistical properties of the spatially incoherent, monochromatic, pump can be prescribed. For usual spatial smoothing techniques, they follow Gaussian statistics with a zero mean value:

$$\langle a^{(p)}_{\mathbf{k}_p}\rangle = \langle a^{(p)}_{\mathbf{k}_p}\, a^{(p)}_{\mathbf{k}'_p}\rangle = 0\,,\ \langle a^{(p)}_{\mathbf{k}_p}\, a^{(p)*}_{\mathbf{k}'_p}\rangle = n^{(p)}_{\mathbf{k}_p}\,\delta(\mathbf{k}_p-\mathbf{k}'_p), \quad (3)$$

where $n^{(p)}_{\mathbf{k}_p} = (\rho_0^2/2\pi)\,\exp\!\big(-\rho_0^2\,\mathbf{k}_p^2/2\big)$ is the Gaussian pump spatial spectrum normalized to one. The statistical properties of the scattered and acoustic fields are considered using an iterative method [5]. It allows to calculate average values for successive momenta of $a^{(d,s)}_{\mathbf{k}}$. From Eqs. (1)-(3) follows:

$$c\,q\;\langle\hat a^{(d)}_{\mathbf{k}_d}\rangle = \Big[\frac{\gamma_0^2}{\gamma+\nu_s+\Delta\omega_s} + \mathcal{O}(\gamma_0^4)\Big]\,\langle\hat a^{(d)}_{\mathbf{k}_d}\rangle, \quad (4)$$

$$\big(\gamma+\nu_s\big)\;\langle\hat a^{(s)}_{\mathbf{k}_s}\rangle = \Big[\frac{\gamma_0^2}{c\,q+\Delta\omega_d} + \mathcal{O}(\gamma_0^4)\Big]\,\langle\hat a^{(s)}_{\mathbf{k}_s}\rangle, \quad (5)$$

where $\langle a^{(d,s)}_{\mathbf{k}}\rangle = (2\pi)^{-2}\int dq\,d\gamma\,\langle\hat a^{(d,s)}_{\mathbf{k}}\rangle\,\mathrm{e}^{q\,z+\gamma\,t}$. The frequency widths $\Delta\omega_s \sim \Omega^{(s)}_{\mathbf{k}_s}\,\theta_p/\theta_s$ and $\Delta\omega_d \sim \omega_0\,\theta_p\,\theta_s$ depend only on the scattering angle $\theta_s = |\mathbf{k}_s|/k_0$ and the pump angular aperture $\theta_p \sim (k_0\,\rho_0)^{-1}$.

Under suitable assumptions (that are verified in our case) the iterative procedure converges and the following results can be extracted. Concerning the scattered wave: for long times, $t > t^{(d)}_{sat} \equiv (\gamma_0/\Delta\omega_s)^2\,z/c$, one finds a spatial amplification, $\langle a^{(d)}_{\mathbf{k}_d}\rangle \simeq \exp q^{(d)}_{incoh}\,z$, with the spatial growth rate $q^{(d)}_{incoh} \equiv \gamma_0^2/(c\,\Delta\omega_s)$. This result suggests that spatial growth of the average amplitude $\langle a^{(d)}_{\mathbf{k}_d}\rangle$ is limited by the pump incoherence. For shorter times $t < t^{(d)}_{sat}$, the scattered wave behaves asymptotically in time and z as: $\langle a^{(d)}_{\mathbf{k}_d}\rangle \simeq \exp\big(2\,\gamma_0\,\sqrt{t\,z/c} - \Delta\omega_s\,t\big)$. In this transient regime, the spatial growth rate is smaller than $q^{(d)}_{incoh}$. The growth of $\langle a^{(d)}_{\mathbf{k}_d}\rangle$ is thus reduced by spatial smoothing for all times, and this regime is referred to as the incoherent amplification of FSBS.

Similarly, one obtains the evolution of the ion acoustic wave average amplitude $\langle a^{(s)}_{\mathbf{k}_s}\rangle$. For times $t > t^{(s)}_{sat} \equiv (\gamma_0^2/\nu_s)^2\,z/c$, the ion acoustic wave grows spatially: $\langle a^{(s)}_{\mathbf{k}_s}\rangle \simeq \exp(q^{(s)}_{coh} - \Delta\omega_d/c)\,z$, where $q^{(s)}_{coh} = \gamma_0^2/(c\,\nu_s)$ is the spatial growth rate of FSBS driven by a coherent pump. For shorter times $t < t^{(s)}_{sat}$, the ion acoustic wave is in a transient regime $\langle a^{(s)}_{\mathbf{k}_s}\rangle \simeq \exp\big(2\,\gamma_0\,\sqrt{t\,z/c} - \Delta\omega_d\,z - \nu_s\,t\big)$. In this regime, Eq. (5) is valid only for times $t > t^{(s)}_{val} \equiv (\gamma_0^2/\Delta\omega_s)^2\,z/c$ that does not exceed a few picoseconds for a millimetric plasma.

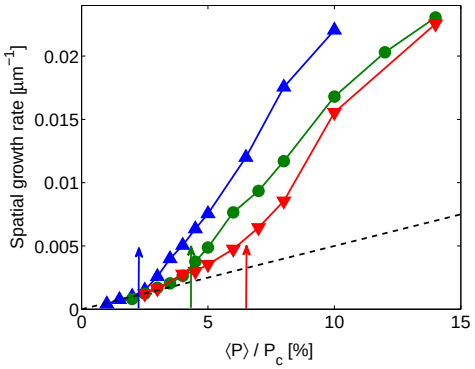


Figure 1: Dependence of the spatial growth rate of the scattered wave intensity after 2 ns on the normalized average power $\langle P\rangle/P_c$. Ion acoustic damping rates are 2.75% (blue), 5.5% (green) and 8.25% (red). The dashed curve shows the incoherent growth rate.

The condition for spatial growth of $\langle a_{\mathbf{k}_s}^{(s)}\rangle$ reads: $c\,q_{coh}^{(s)} > \Delta\omega_d$. It defines a threshold for the average power in a speckle: $\langle P\rangle/P_c > \sqrt{2/\pi}\,(\nu_s/\Omega_{\mathbf{k}_s}^{(s)})\,(\theta_d/\theta_p)$. Above this threshold, one observes the coherent spatial amplification $\langle a_{\mathbf{k}_s}^{(s)}\rangle \simeq \exp q_{coh}^{(s)}\,z$, that is not reduced by the pump incoherence. This result is so far valid only for times $t > t_{sat}^{(s)}$. However, defining the effective spatial growth rate in the transient regime as $q_{eff}^{(d)} \equiv \left(\gamma_0^2\,ct/z\right)^{1/2} - \Delta\omega_d$, one obtains that the pump incoherence does not affect the spatial amplification of $\langle a_{\mathbf{k}_s}^{(s)}\rangle$ for times $t \gg (\Delta\omega_d/\gamma_0)^2\,z/c$. For a millimetric plasma, this time ranges between a few tenth to a few hundreds picoseconds, much shorter than the characteristic durations of ICF laser pulses. This leads us to the following figure of merit (FOM) for beam spray:

$$C \equiv \sqrt{\frac{\pi}{2}}\,\gamma_T\,\frac{\langle P\rangle/P_c}{\nu_s/\Omega_{\mathbf{k}_s}^{(s)}}\,, \qquad (6)$$

where $\gamma_T = 1 + 1.76\,Z^{5/7}(\rho_0/\lambda_{ei})^{4/7}$ accounts for thermally enhanced density perturbations [6].

This FOM has a straightforward physical meaning. The light scattered outside the cone with aperture $C\,\theta_p$ is amplified in the incoherent regime. On the contrary, the light scattered inside this cone demonstrates a strong, coherent amplification. Thus, for $C < 1$, coherent excitation of FSBS occurs only for scattering angles $\theta_d < \theta_p$, *i.e.* in the cone of the incident wave. Enhanced FSBS in the incident aperture enhances plasma induced smoothing and in turn reduces the reflectivity of backward instability. Conversely for $C > 1$, coherent excitation of FSBS can occur outside the incident cone. In this regime $C > 1$, beam spray is thus expected. Because the ion acoustic damping rate $\nu_s/\Omega_{\mathbf{k}_s}^{(s)} \ll 1$, the threshold is well below P_c, usually considered as the threshold for beam spray.

The above FOM can be rewritten in particle units:

$$0.1\,\gamma_T\,\frac{\Omega_{\mathbf{k}_s}^{(s)}}{\nu_s}\,\lambda_0^2[\mu\mathrm{m}]\,I_{13}\,\frac{n_0}{n_c}\,\frac{3}{T_e\,[\mathrm{keV}]}\left(\frac{f_\sharp}{8}\right)^2 > 1\,. \qquad (7)$$

All the above given analytical considerations were confirmed using three-dimensional paraxial simulations. We considered a Helium plasma with an electron density $0.03\,n_c$, and the electron and ion temperatures 500 and 50 eV, respectively. The ion acoustic damping rate, $\nu_s/\Omega_{\mathbf{k}_s}^{(s)} = 2.75$, 5.5 or 8.25 %, is chosen independently. A Gaussian laser beam is focused through a random phase plate providing a speckle pattern with coherence width $\rho_0 \simeq 4.3\,\mu$m. The average intensity is varied in the range $(1.1-16)\times10^{13}\,\mathrm{W/cm^2}$, corresponding to variation of the average power in a speckle $\langle P\rangle = \pi\,\rho_0^2\,\langle I\rangle$ from 1 to 14 % of P_c.

The spatial growth rate of light scattered at the frequency $\omega_0 - 2\,c_s/\rho_0$ is plotted as a function of $\langle P\rangle/P_c$ in Fig. 1. In the low power regime, the spatial growth rate is less than $0.5\times10^{-2}\,\mu\mathrm{m}^{-1}$. It evolves almost linearly with $\langle P\rangle/P_c$ and agrees rather well with predictions in the incoherent regime (dashed line). These numerical results confirm that, below the threshold power (6), the growth of FSBS is limited by the pump incoherence. On the contrary, when the power in a speckle is above the threshold power (see vertical arrows), much higher growth rates are observed. These results are consistent with expectations for the coherent regime.

In conclusion, it has been shown that FSBS is not always suppressed by pump incoherence. The instability even leads to a strong deterioration of the beam propagation when the average power exceeds a threshold power. This threshold power is shown to depend on the ion acoustic wave damping rate. This provides an important insight on the control of beam spray in future ICF experiments.

[1] H. Rose and D. Dubois, Phys. Fluids B **5**, 590 (1992).

[2] M. Grech et al., Phys. Plasmas **13**, 093104 (2006) and references therein.

[3] P. Lushnikov and H. Rose, Plasma Phys. Control. Fusion **48**, 1501 (2006).

[4] M. Grech et al., *Coherent forward stimulated Brillouin scattering of a spatially incoherent laser beam in a plasma and its effect on beam spray*, accepted for publication in Phys. Rev. Lett.

[5] P. Kubo, J. Math. Phys. **4**, 174 (1963); R. L. Stratonovitch, *Topics in the Theory of Random Noise* (Gordon and Breach, New York, 1967), vol. 2, Chap. 10; A. Brissaud and U. Frisch, J. Math. Phys. **15**, 524 (1974).

[6] A. Brantov et al., Phys. Plasmas **6**, 3002 (1999).

2.31 Absence of Energy Diffusion in Disordered Nonlinear Systems

G. Kopidakis, S. Komineas, S. Flach and S. Aubry

Introduction It is well-known that Anderson localization occurs for a one-dimensional linear system with random potential. Since all the linear eigenmodes – Anderson modes (AMs) – are localized, any wavepacket which is initially localized remains localized for all time which implies no energy diffusion [1]. When nonlinearities are added to such models, AMs interact with each other, giving rise to more complex situations. Numerical studies of wavepacket propagation in several models suggested that the second moment of the norm distribution may grow subdiffusively in time as t^α [2], with α in the range $0.3 - 0.4$.

Discrete Breathers A corresponding situation has been studied in the simpler case of spatially periodic nonlinear systems which sustain discrete breathers (DBs), which are spatially localized time periodic solutions [3] with frequencies outside the frequency spectrum of the linear system. The temporal evolution of a localized wavepacket leads to the formation of a DB, while a part of the energy of the wavepacket is radiated ballistically to infinity (in the form of weakly nonlinear plane waves) [4]. In that case, the second moment of the energy density distribution diverges as t^2. The participation number P of the norm/energy distribution is a well-known measure of the degree of localization. In the case of a periodic nonlinear lattice, P will saturate at a finite value, correctly indicating the formation of a DB.

For nonlinear random systems it was proven rigorously that AMs survive in the presence of nonlinearities as spatially localized and time-periodic solutions [5] with frequencies which depend on the amplitude of the mode. The allowed frequencies form a fat Cantor set (with finite measure) whose density becomes unity for weak nonlinearity. They are located inside the frequency spectrum of the linear system. Numerical techniques for obtaining these (dynamically stable) intraband DB solutions at computer accuracy were developed [6]. When they are chosen as an initial wavepacket, they persist for infinite time and there is no diffusion at all.

Investigated Models We investigated the evolution of the participation number of wavepackets as a function of time [7], in situations where subdiffusion was claimed to exist [2]. Two models with similar behavior were studied. The first one is the disordered discrete nonlinear Schrödinger equation (DDNLS) with Hamiltonian

$$\mathcal{H}_D = \sum_n \left(\epsilon_n |\psi_n|^2 - \frac{1}{2}\beta |\psi_n|^4 - V(\psi_{n+1}\psi_n^\star + \psi_{n+1}^\star \psi_n) \right) \quad (1)$$

with complex variables ψ_n. The random on-site energies ϵ_n are chosen uniformly from the interval $\left[-\frac{W}{2}, \frac{W}{2}\right]$. The equations of motion are generated by $\dot{\psi}_n = \partial \mathcal{H}_D / \partial(i\psi_n^\star)$. We choose $\beta = 1$ and $V = -1$ here [2] and note that varying the norm of the initial wavepacket is strictly equivalent to varying β. The second model is the disordered quartic Klein-Gordon chain (DQKG) (see [7] for details).

Rigorous Result for Norm Conserving Models Hamiltonian DDNLS (unlike DQKG), in addition to conserving the energy, also conserves the total norm $S \equiv \sum_n |\psi_n|^2 = \langle \psi | \psi \rangle$. We use this norm conservation for proving rigorously that initially localized wavepackets with a large enough amplitude cannot spread to arbitrarily small amplitudes. The consequence is that a part of the initial energy must remain well-focused at all times.

For proving this result, we split the total energy $\mathcal{H}_D = \langle \psi | \mathbf{L} | \psi \rangle + H_{NL}$ into the sum of its quadratic term of order 2 and its nonlinear terms of order strictly higher than 2. Then, $\mathbf{L}$ is a linear operator which is bounded from below (and above). In our specific example, we have $\langle \psi | \mathbf{L} | \psi \rangle \geq \omega_m \langle \psi | \psi \rangle = \omega_m S$ where $\omega_m \geq -2 - \frac{W}{2}$ is the lowest eigenvalue of $\mathbf{L}$. Otherwise, the higher order nonlinear terms have to be strictly negative.

If we assume that the wavepacket amplitudes spread to zero at infinite time, we have $\lim_{t\to+\infty}(\sup_n |\psi_n|) = 0$. Then $\lim_{t\to+\infty}(\sum_n |\psi_n|^4) < \lim_{t\to+\infty}(\sup_n |\psi_n^2|)(\sum_n |\psi_n|^2) = 0$ since $S = \sum_n |\psi_n|^2$ is time invariant. Consequently , for $t \to +\infty$ we have $\mathcal{H}_{NL} = 0$ and $\mathcal{H}_D \geq \omega_m \sum_n |\psi_n|^2 = \omega_m S$. Since $\mathcal{H}_D$ and S are both time invariant, this inequality should be fulfilled at all times. However when the initial amplitude A of the wavepacket is large enough, it cannot be initially fulfilled because the nonlinear energy diverges as $-A^4$ while the total norm diverges as A^2 only. For example, a wavepacket initially at a site 0 ($\psi_n = 0$ for $n \neq 0$ and $\psi_0 = \sqrt{A}$) has energy $\mathcal{H}_D = \epsilon_0 A^2 - \frac{1}{2}A^4$. Consequently, the above inequality is not fulfilled when $A^2 > -2(\omega_m - \epsilon_0) > 0$. Thus such an initial wavepacket cannot spread to zero amplitudes at infinite time.

Numerical Observation We performed extensive numerical simulations, and characterized the wavepacket spreading both in real space for DDNLS and normal mode space (Anderson space or AS) for DQKG. We used relatively large amplitude initial wavepackets localized on a single site n_0, or single AM, or combinations, close to n_0 so that in the DDNLS model, our theorem holds. Nonlinearity induces some diffusion in Anderson space, where each AM is characterized by a

amplitude a_ν and momentum $\dot{a}_\nu$. We analyze distributions $z_l \geq 0$ using the second moment $m_2 = \sum_l (l-l_0)^2 z_l$ and the participation number $P = (\sum_l z_l)^2 / \sum_l z_l^2$, which measures the number of the strongest excited sites in z_l. In the results presented here, for the DDNLS $z_n = |\psi_n|^2$ is the norm density in real space, and for the KG $z_\nu = \dot{a}_\nu^2/2 + \omega_\nu^2 a_\nu^2/2$ is the (harmonic) energy density in AS. The system size was $N = 1000$ for KG, and $N = 2000$ for DDNLS.

In both models, the second moment m_2 and participation number $P(t)$ are plotted in Fig.1

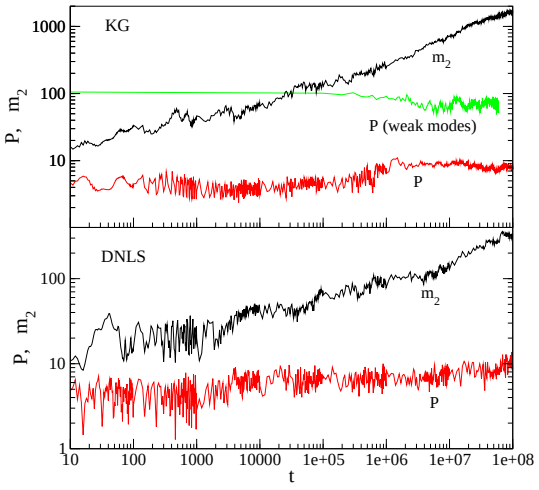


Figure 1: P and m_2 versus time, on logarithmic scale. Top panel: KG, AS. Bottom panel: DNLS, real space.

for the same runs. $m_2(t)$ grows as a function of time while $P(t)$ fluctuates around a value of 7-10 but does not seem to grow. Thus, the observed growth of the second moment $m_2 \sim t^{0.3...0.4}$ is not related to a complete delocalization process.

The Fourier transform [7] of the system coordinates indicates that the solution becomes quasiperiodic and thus stationary without anymore spreading. Thus, this limit state is not a DB as we might have expected (by analogy with spatially periodic systems), but is more reminiscent of a KAM torus [8]. Actually such solutions (which could be better called Quasiperiodic Discrete Breathers) were predicted to exist not only as exceptional solutions but with full probability approaching probability 1 in the small amplitude limit in a wide class of random nonlinear models similar to ours (though they were slightly modified).

At weaker disorder further numerical simulations [9] show that the participation number grows over the whole computing time and perhaps forever which would indicate in that case the wavepacket spreads to zero and thus we would have complete diffusion. However, there are also weak amplitude initial conditions but at strong disorder which seem to remain stationary forever and will not spread as expected from theorems [8] (though they were only proven on modified models).

Conclusion In contradiction with early beliefs, we obtained the rigorous proof (for the large class of random nonlinear models with norm conservation) that when the initial amplitude of the wavepacket is large enough, the spreading of a wave packet cannot be complete . Our numerical observations confirm this prediction not only as expected in models with norm conservation (DDNLS) but also in models without norm conservation (DQKG) which actually behave very similarly though our theorem does not hold. However, there are also situations where complete diffusion seems to be observed at least during the computing time.

In summary, the answer to the problem of diffusion of wavepacket remains unclear because the results obtained up today as well by us than early by other authors seems to be inconsistent one with each other. It remains to understand which initial conditions could produce complete diffusion (if any?) and what is the limit state when there is no diffusion (or incomplete) diffusion?

[1] P. W. Anderson, Phys. Rev. **109** 1492 (1958).

[2] D. L. Shepelyansky, Phys. Rev. Lett. **70** 1787 (1993); M. I. Molina, Phys. Rev. B **58** 12547 (1998); A. S. Pikovsky and D.L. Shepelyansky, Phys. Rev. Lett. **100** 094101 (2008)..

[3] A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61** 970 (1988); R. S. MacKay and S. Aubry, Nonlinearity **7** 1623 (1994); S. Flach and C. R. Willis, Phys. Rep. **295** 181 (1998); S. Flach and A. V. Gorbach, Phys. Rep. **467** 1 (2008).

[4] S. Flach and C. R. Willis, Phys. Lett. A **181** 232 (1993); S. Flach, C. R. Willis and E. Olbrich, Phys. Rev. E **49** 836 (1994); S. Flach, K. Kladko and C. R. Willis, Phys. Rev. E **50** 2293 (1994); M. Johansson, M. Hörnquist and R. Riklund, Phys. Rev. B **52** 231 (1995).

[5] C. Albanese and J. Fröhlich, Comm. Math. Phys. **138** 193 (1991).

[6] G. Kopidakis and S. Aubry, Phys. Rev. Lett. **84** 3236 (2000);

[7] G. Kopidakis,S. Komineas, S. Flach and S. Aubry, Phys. Rev. Lett. 100, 084103 (2008)

[8] J. Fröhlich, T. Spencer and C. E. Wayne, J. Stat. Phys. **42** 247 (1986).

[9] S. Flach, D. O. Krimer, and Ch. Skokos, Phys. Rev. Lett. **102** 024101 (2009)

2.32 Self-organization of Dynein Motors Generates Meiotic Nuclear Oscillations

Sven K.Vogel, Nenad Pavin, Nicola Maghelli
Frank Jülicher, and Iva M.Tolić-Nørrelykke

At the onset of meiosis in the fission yeast Schizosaccharomyces pombe, 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 [1]. These oscillations have a period of about ten minutes and last for several hours [1]. The oscillations are crucial for proper chromosome pairing, recombination, and spore viability [2]. Similar chromosome movements have been observed in meiotic prophase in a variety of model organisms, from budding yeast to mouse, and the role of these movements in chromosome pairing and recombination has been demonstrated [3]. The oscillations of the nucleus follow the oscillatory movement of the spindle pole body [1] (SPB, a centrosome equivalent in yeast). The movement depends on microtubules and the cortically anchored minus end-directed motor protein dynein [2].

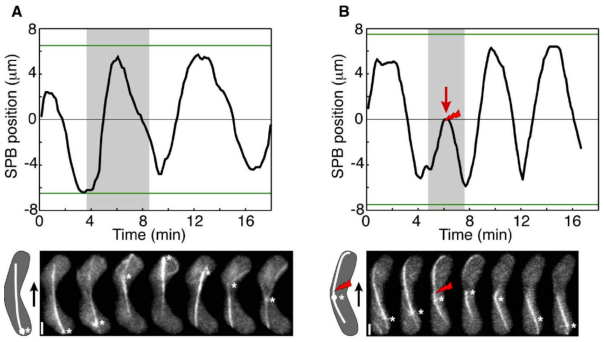


Figure 1: Spindle pole body (SPB) movement is driven by pulling via the leading microtubules. (A) Control cell without laser ablation. (B) Laser ablation (marked by a lightning sign) of the leading microtubules induced a change of direction of the SPB movement (red arrow). Scale bars represent 2 μm. Figure from [6].

The microtubules extend from the SPB in opposite directions, with the minus ends at the SPB and the plus ends pointing towards the cell periphery, while dynein motors accumulate on the SPB and microtubules [2]. Although the key proteins involved in the oscillations have been identified and localized, the underlying physical mechanism is unknown. We perturbed the force balance in the cell in order to directly test the contribution of microtubule pulling and pushing to the SPB movement. Here, we used laser cutting of specific microtubules [4,5]. The microtubules extending from the SPB in the direction of the SPB movement and in the opposite direction are called the leading and trailing microtubules, respectively. As the SPB moves, the leading microtubules typically shrink, while the trailing ones grow. Our experiments showed that after a selective cutting of the leading microtubules the SPB rapidly changed the direction of motion (within ∼25 seconds, compared to the oscillation period of 4-7 minutes; see Figure 1). To the contrary, cutting of trailing microtubules did not affect the movement. These data provide direct evidence that the SPB movement is driven by pulling via the leading microtubules, while the contribution of pushing is negligible.

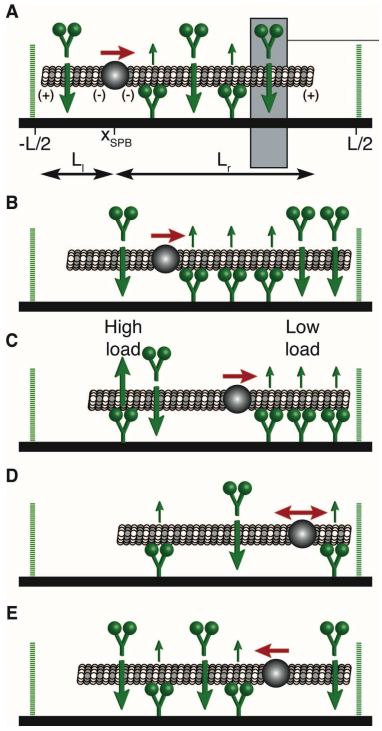


Figure 2: (A-D) Schematic drawing of events during oscillations. (A) The position of the SPB along the cell longitudinal axis is denoted x_{SPB}. Two microtubules grow from the SPB. There are more motors attached to the microtubule on the right, thus the SPB moves to the right. As the SPB moves, the motors on the left microtubule are under high load, which stimulates their detachment. The asymmetry in the number of motors on the two microtubules grows, resulting in a faster SPB movement. (B) The faster movement further increases the asymmetry in the load on the motors. (C) However, because of the finite size of the cell, the right microtubule shrinks and thus loses motors. (D) When the number of motors on the left and the right microtubule is equal, the SPB does not move. Since the left microtubule is longer than the right one, it accumulates more motors. (E) Thus, the SPB changes direction and the oscillation cycle continues.

The next question was whether the pulling force is generated at the interaction site between the leading microtubule tip and the cell end, or largely along the whole length of the leading microtubules. To distinguish

between these scenarios, we ablated the leading microtubules ∼2 μm away from the microtubule tip. After the selective cutting of the microtubule tip region, the SPB continued to move forward, indicating that the force generated along the lateral microtubule-cortex interactions is large enough to move the SPB.

In order to identify the key mechanisms necessary to account for the observed SPB movement, we developed a minimal one-dimensional description. The geometry of the minimal model is represented in Figure 2. Two microtubules extend from the SPB in opposite directions. Microtubule dynamics is described by

$$\frac{\mathrm{d}L}{\mathrm{d}t} = v_{mt} \tag{1}$$

where $v_{mt} = v_g$ if the microtubule grows and $v_{mt} = v_s$ when it shrinks. Here, v_g and v_s are the growth and shrinkage velocity, respectively. Equation 1 describes the dynamics of the microtubule growing to the left and to the right if one replaces L by L_l and L_r, respectively. The transition from growing to shrinking occurs when the plus end of a microtubule reaches the cell end. Subsequently, the microtubule shrinks until its length vanishes; this is followed by nucleation of a growing microtubule. The viscous friction force and the forces F_l and F_r acting on the left and the right microtubule, are balanced,

$$\xi \frac{\mathrm{d}x_{SPB}}{\mathrm{d}t} = F_l + F_r \tag{2}$$

where x_{SPB} is the position of the SPB along the long axis of the cell, and ξ the friction coefficient of the system consisting of the nucleus, SPB, and microtubules. The forces F_l and F_r are exerted by attached motors, $F_l = N_l f_l$ and $F_r = N_r f_r$. Here, N_l and N_r are the total number of motors attached to each microtubule and linked to the cortex, and f_l and f_r the forces generated by a single motor on the left and the right microtubule, respectively. The forces f_l and f_r are described by linear force-velocity relationships, $v = v_0(1 + f_l/f_0)$ and $v = v_0(-1 + f_r/f_0)$, respectively [7]. The velocity of the motor with respect to the microtubule is $v = -v_{SPB} = -\mathrm{d}x_{SPB}/\mathrm{d}t$, where v_{SPB} is the SPB velocity. The velocity in the absence of force is denoted v_0, and f_0 is the stall force of the motor. The linear densities, $n_l = N_l/L_l$ and $n_r = N_r/L_r$, of the motors attached to the left and the right microtubule, respectively, obey kinetic equations which describe attachment and detachment of motors. For the right microtubule this equation reads:

$$\frac{\mathrm{d}n_r}{\mathrm{d}t} = k_{on}c - k_{off}(f_r)n_r \tag{3}$$

with $n_r = 0$ at microtubule nucleation. Here, c is the cytoplasmic concentration of motors, k_{on} characterizes the rate of attachment of motors to microtubules. The load-dependent motor detachment rate, k_{off}, is described by

$$k_{off}(f) = k_0 \exp(f/f_c) \tag{4}$$

Here, f_r is the load force acting on individual motors, k_0 is the detachment rate in the absence of a load, and f_c a characteristic force. The equations that describe the kinetics of motors on the left microtubule are obtained by substituting the subscript r by l in Eqs. 3 and 4, and changing the sign of the exponent in Eq. 4.

The model accounts for the experimentally observed end-to-end SPB oscillations with a triangular waveform and the key features of the dynein dynamics: positive feedback of the SPB movement on the number of dynein at the leading microtubules and the absence of dynein at the fast-moving trailing microtubules. According to the measured force-velocity curve of dynein [7], a reverse motion corresponds to a high load on the motors, leading us to interpret the above observation as a consequence of the load-dependent dynein detachment.

[1] Y. Chikashige, D. Ding, H. Funabiki, T. Haraguchi, S. Mashiko, M. Yanagida, and Y. Hiraoka, "Telomere-led premeiotic chromosome movement in fission yeast," *Science*, vol. 264, pp. 270–3, Apr 1994.

[2] A. Yamamoto, R. West, J. McIntosh, and Y. Hiraoka, "A cytoplasmic dynein heavy chain is required for oscillatory nuclear movement of meiotic prophase and efficient meiotic recombination in fission yeast," *J Cell Biol*, vol. 145, pp. 1233–49, Jun 1999.

[3] H. Scherthan, H. Wang, C. Adelfalk, E. White, C. Cowan, W. Cande, and D. Kaback, "Chromosome mobility during meiotic prophase in saccharomyces cerevisiae," *Proc Natl Acad Sci U S A*, vol. 104, pp. 16934–9, Oct 2007.

[4] I. Raabe, S. K. Vogel, J. Peychl, and I. Tolić-Nørrelykke, "Intracellular microsurgery and cell anucleation using a picosecond laser," *J Microsc*, in press, 2009.

[5] N. Maghelli and I. Tolić-Nørrelykke, "Versatile laser-based cell manipulator," *J Bioph*, vol. 1, pp. 299–309, Jul 2008.

[6] S. K. Vogel, N. Pavin, N. Maghelli, F. Jülicher, and I. Tolić-Nørrelykke, "Self-organization of dynein motors generates meiotic nuclear oscillations," *PLoS Biol*, in press, 2009.

[7] A. Gennerich, A. Carter, S. Reck-Peterson, and R. Vale, "Force-induced bidirectional stepping of cytoplasmic dynein," *Cell*, vol. 131, pp. 952–65, Nov 2007.

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 2007 we had a total of 62 PhD students at mpi**pks**, including 31 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 2008 were a total of 72 PhD students at mpi**pks**, including 36 students from abroad. We counted 7 successful final PhD exams for the year 2007 and 8 exams for the year 2008.

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* started its operation in January 2005. It belongs to the 4th round of approved research schools of the Max Planck society. In 2008 the school was evaluated by the Max Planck Society.

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)

The IMPRS was founded to attract talented students, seeking to obtain a PhD in atomic, molecular or solid state physics, to Dresden. The research focus is on dynamical processes and comprises theoretical and experimental work. Since the last report 2006 the IMPRS has established a collaboration with institutes of the Czech Academy of Sciences in Prague.

PhD students

The IMPRS has admitted so far 68 PhD students, 16 of which have obtained their doctoral degree by the end of 2008. While about 40 % of the students are Germans, the other 60 % come from all over the world. The predominant countries of origin are China (5 students), Poland (4), Czech Republic (4), Ukraine (4), and India (4). The affiliation to the participating partners is as follows, TUD: 20, FZD: 1, IFW: 9, MPI-CPfS: 3, mpi**pks**: 10, ILTSR: 5, IOCB: 4. The four Polish students are enrolled in Wrocław universities and are financed by grants of the Klaus-Tschira foundation. All of them spent about one year of their PhD studies in Dresden at the IFW and the MPI-CPfS, respectively, with financial support 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.

We organize soft-skill seminars with the focus on presentation skills on a regular basis. These seminars start with a general introduction by an external expert. Most importantly, presentations by the students are analyzed and discussed. In February 2006 the presentation skill seminar was led by Kerstin Kathy Meyer-Ross (Max-Planck-Institut Informatik, Saarbrücken), the one in February 2008 by Dr. Claus Ascheron (Springer Science + Business Media, Heidelberg).

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 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.

IMPRS *meeting in Schöna (Sächsiche Schweiz) in October 2007.*

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. Bernd Büchner (IFW)
Prof. Gotthard Seifert (TUD)	Prof. Pavel Jungwirth (IOCB Prague)
Prof. Yuri Grin (MPI-CPfS)	Prof. Jozef Sznajd (ILTSR Wrocław)
Prof. Helmut Eschrig (IFW)	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. Loewenhaupt (until Aug 2008), Prof. Büchner (since Sept 2008) 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**.

Evaluation by the Max-Planck-Society

The Max-Planck-Society has appointed a committee — consisting of Prof. Brenig (Braunschweig), Prof. Cederbaum (Heidelberg), Prof. Müller (Erlangen), Prof. Oleś (Cracow/Poland) and Prof. Richter (Regensburg) — for a scientific evaluation of the IMPRS. The committee visited mpi**pks** on July 4, 2008. Beside scientific presentations (talks by five students and a poster by every student) there were discussion rounds with the students and faculty of the IMPRS. The final report attests the IMPRS a very successful work for the period under evaluation (Jan 2005 – May 2008). It emphasizes that the "IMPRS under review has been able to recruit excellent doctoral students",

"interaction and collaboration between the partner institutes (especially Poland and Czech Republic) is excellent", "there is definitely a high degree of satisfaction of the students with the research school" and "the resources of the school are spent on its principal purpose, to enable the students to carry out their PhD research programme". (All quotations from the report by the evaluation committee.)

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 Seminar and Workshop "Bio-inspired Complex Networks in Science and Technology - from Topology to Structure and Dynamics", April 14 - May 09, 2008

During 2007 the mpi**pks** hosted 183 guest scientists with contracts for at least three months, and 185 during the year 2008, 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 2008 two new *Advanced Study Groups* started their activities, with one reaching into the year 2009.

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 *Bose-Einstein condensation*. 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. 132).

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. Masudul Haque* on *Quantum Many-Body Phenomena in Condensed Matter*, *Dr. Balasz Dora* on *Magnetic Impurities in d-Density Waves*, and *Dr. Vitali Averbukh* on *Interatomic Decay Processes*, see report on p. 124. One PKS fellow has left the institute: *Dr. Kay Hamacher* (*Computational Methods for Investigating Structures and Functions of Molecular Systems*) took a faculty position with the Biology Department at the Technische Universität Darmstadt. Another former PKS fellow *Dr. Benjamin Lindner* (*Stochastic Processes in Biophysics*) is now heading a research group at mpi**pks**.

Together with the TU Braunschweig the institute supports a junior professorship (*Prof. Ilya Eremin*, see report on p. 126). *Prof. Eremin* is teaching at the TU Braunschweig, and is conducting research work at mpi**pks**.

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 2007 and 2008 fellows were *Prof. M. S. Hussein* and *Prof. J. M. R. Parrondo* (see report on p. 129).

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 new levels, 255 during the year 2007 and 314 during the year 2008.

3.3.1 PKS-Fellowship

Report by *Dr. Masud Haque*: Collective phenomena in many-particle systems

I study various aspects of condensed matter theory, *i.e.*, collective phenomena in many-particle quantum systems. One major research focus is the use of concepts from quan-

tum information theory, such as measures and classifications of entanglement, to characterize many-particle phases, phase transitions, and non-equilibrium dynamics.

Projects at the mpipks

I have worked on several collaborations with mpi**pks** members. A selection is listed below. My mpi**pks** collaborators are current or past postdocs (Guest Scientists) except those noted otherwise.

(1) With *Weibin Li* and *Stavros Komineas*, I am studying the dynamics of a few vortices in a trapped Bose-Einstein condensate. We focus on mean-field dynamics described by the Gross-Pitaevskii equation, which supports a rich range of dynamical phenomena.

(2) With *Ricardo Pinto* and *Sergej Flach* (Head of Visitor's Program), I found and studied edge-localized states in one-dimensional quantum lattices. We showed that edge-localized eigenstates can be found in both bosonic and fermionic systems (the Bose-Hubbard model and the interacting spinless fermion model).

(3) With *Emil Bergholtz* and *Andreas Läuchli* (Group Leader), I am exploring entanglement measures in fractional quantum Hall states on torus geometries, with the aim of developing entanglement calculations as a tool for addressing topological order in quantum Hall states.

(4) With *Andreas Läuchli*, I am studying new entanglement quantifiers such as the 'entanglement spectrum' and the 'single-copy entanglement' in spin chain models.

(5) With *V. Ravi Chandra* and *Jayendra Bandyopadhyay*, I characterized the physics of a spin model (the frustrated ferromagnetic chain) using entanglement measures.

Cooperations

With *Kareljan Schoutens* and *Oleksandr Zozulya* at the University of Amsterdam (the Netherlands), I explored the physical meanings of entanglement measures in various many-particle states. For example, we analyzed the entanglement between two sets of particles making up an itinerant many-particle system.

Together with *Ed Rezayi* of the California State University at L.A. (U.S.A.) and *Nicolas Regnault* at the École Normale Supérieure [ENS] Paris (France), I and my Amsterdam collaborators (named above) also studied entanglement in fractional quantum Hall states, and used entanglement calculations to characterize topological order in these states and quantum phase transitions involving these states.

With *Jorge Quintanilla* of the Rutherford Appleton Laboratory (U.K.) and *Andrew Schofield* of Birmingham University (U.K.), I developed a description of the Fermi surface shape deformation instabilities (known as Pomeranchuk instabilities) in a two-dimensional continuum fermion system.

With *Henk Stoof* of Utrecht University (the Netherlands), I worked on the theory of fermionic pairing in atom traps, when the two spin states are unequally populated.

Articles completed and written at the mpipks

- O. Zozulya, M. Haque and N. Regnault: *Entanglement signatures of Quantum Hall phase transitions*; Phys. Rev. B **79** 045409 (2009).
- O. Zozulya, M. Haque, and K. Schoutens: *Particle partitioning entanglement in itinerant many-particle systems*; Phys. Rev. A **78**, 042326 (2008).
- W. Li, M. Haque and S. Komineas: *A vortex dipole in a trapped two-dimensional Bose condensate*; Phys. Rev. A **77**, 053610 (2008).

- J. Quintanilla, M. Haque and A. J. Schofield: *Symmetry-breaking Fermi surface deformations from central interaction in two dimensions*; Phys. Rev. B **78**, 035131 (2008).
- M. Haque: *Probing topological order in quantum Hall states using entanglement calculations*; AMS Contemp. Math. (CONM Proceedings) series (2009).
- J. Quintanilla, C. Hooley, B. J. Powell, A. J. Schofield, and M. Haque: *Pomeranchuk instability: symmetry breaking and experimental signatures*; Physica B **403**, 1279 (2008).
- O. Zozulya, M. Haque, K. Schoutens, and E. H. Rezayi: *Bipartite entanglement entropy in fractional quantum Hall states*; Phys. Rev. B **76**, 125310 (2007).
- M. Haque & H. T. C. Stoof: *Trapped fermionic clouds distorted from the trap shape due to many-body effects*; Phys. Rev. Lett. **98**, 260406 (2007).
- A. Mikaberidze and M. Haque: *Survival benefits in mimicry: a quantitative framework*; arxiv:0809.0391, Journ. Theor. Biol., accepted (2009).
- M. Haque, V. Ravi Chandra and J. N. Bandyopadhyay: *Entanglement and level crossings in finite frustrated ferromagnetic chains.* arxiv:0811.3419, Phys. Rev. A, accepted (2009).
- R. Pinto, M. Haque, and S. Flach: *Edge-localized states in quantum one-dimensional lattices*; arxiv:0902.3249; submitted (2009).

3.3.2 Junior Professorship

Report by *Prof. Ilya Eremin*:
Unconventional superconductivity and magnetism in strongly correlated electronic systems

The physics of strongly correlated fermion systems is at the center of theoretical activities in condensed-matter physics over the last decade. 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 superconductors. The major discovery of the last year is the observation of high temperature superconductivity in iron based materials. 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.

Projects at the mpipks Together with J.-P. Ismer (Ph. D. student at the mpipks who is currently finishing his thesis) I work on the understanding the behavior of the spin excitations in the normal and superconducting state of hole- and electron-doped cuprates and their evolution with doping. Together with Peter Fulde and Jun Chang, I have also studied the properties of the heavy-fermion superconductors. For example, we have analyzed the influence of inelastic rare-earth impurity scattering on electron-phonon-mediated superconductivity and mass renormalization in $La_{1-x}Pr_xOs_4Sb_{12}$ compounds. In addition, our analysis of the magnetic excitations in superconducting $CeCoIn_5$ and $CeCu_2Si_2$ reveals the similar origin of the resonance peaks in these two heavy-fermion

superconductors and in layered cuprates (see also contribution on the page 91). In collaboration with M. Korshunov, A. Donkov, and J. Knolle (internship student from TU Dresden) we have studied the itinerant magnetism on the triangular lattices in application to the lamellar cobaltates. Most recently, together with M. Korshunov we have developed the theoretical model for understanding the superconductivity and magnetism in novel iron-based superconductors. Our results were used by the neutron scattering experiments to confirm unambiguously the symmetry of the superconducting order parameter in these systems. Finally, together with Bin Liu we have analyzed the local density of the states around the non-magnetic impurity in non-centrosymmetric superconductors.

External collaborations With A. Chubukov from University of Wisconsin at Madison (USA) we have studied theoretically within the renormalization-group technique the properties of high-temperature superconductors such as cuprates and ferropnictides (see also contribution on page 60). Our collaboration has been supported by the DFG grant that allowed Prof. Chubukov to spend three months at TU Braunschweig. Together with Dirk Morr from UIC at Chicago we are working on the understanding of the evolution of unconventional superconductivity in d-wave superconductors. This project is supported through the bilateral DAAD grant. Another project in collaboration with the experimental groups of Prof. Büchner and H.-H. Klauß from IFW and TU Dresden applies to the study of unconventional superconductors with various spectroscopic techniques such as muon spin relaxation or photoemission. Together with the groups of P. Lemmens and W. Brenig from TU Braunschweig we have analyzed various response functions such as optical Raman and magnetic response in application to sodium cobaltates both theoretically and experimentally. We further collaborated with the experimental group of D. Reznik (FZ Karlsruhe) and analyzed their experimental data on inelastic neutron scattering in layered cuprates. Together with J. Sichelschmidt (MPI CPFS, Dresden) and B.I. Kochelaev (Kazan State University, Russian Federation) we have performed a combined theoretical and experimental study of the electron spin-resonance in the heavy-fermion Kondo compound $YbRh_2Si_2$ supported through the Volkswagen foundation. Finally together with G. Zwicknagl (TU Braunschweig) and P. Thalmeier (MPI CPFS) we are working on the understanding of physics of heavy-fermion compounds.

Further activities My duties as a junior-professor include not only scientific research which is done at the mpi**pks** but also teaching at the Physics Department of the Technical University of Braunschweig. During the last two years I have given the following courses at the Bachelor and the Master levels: Visualization of Physics (Summer Term 2008), Theory of Phase Transitions , Crash-Course on Mathematics for Physicists (Winter Term 2007/2008), Computational Physics II (Summer Term 2007) and Quantum Electrodynamics (Winter Term 2006/2007). Together with Prof. Peter Lemmens from TU Braunschweig I have organized the Internal Symposium of Division Low Temperature Physics of the German Physical Society Spring Meeting in 2007 on Superconductivity and Magnetism of lamellar cobaltates. In 2008, I have run (together with Profs. James F. Annett and Dirk K. Morr) the workshop and seminar on Competing Orders, Pairing Fluctuations, and Spin Orbit Effects in Novel Unconventional Superconductors at mpi**pks**, and (with W. Brenig, J. Litterst, and R.K. Kremer) the International Conference on Highly Frustrated Magnetism that took place at TU

Braunschweig.

Articles completed and written at the mpipks for the last two years

- A.V. Chubukov, D. Efremov, and I. Eremin, - Magnetism, superconductivity, and pairing symmetry in Fe-based superconductors, Phys. Rev. B 78, 134512 (2008) (editor's choice)
- I. Eremin, G. Zwicknagl, P. Thalmeier, and P. Fulde, - Feedback spin resonance in superconducting $CeCu_2Si_2$ and $CeCoIn_5$, Phys. Rev. Lett. 101, 187001 (2008).
- M. M. Korshunov, and I. Eremin, - Theory for magnetic excitations in novel superconductors with Fe-based layered structure, Phys. Rev. B 78, 140509(R) (2008).
- Andrey Chubukov and Ilya Eremin, - Temperature dependence of the nodal Fermi velocity in layered cuprates, Phys. Rev. B 78, 060509(R) (2008) (editor's choice).
- D. Reznik, J.-P. Ismer, I. Eremin, L. Pintschovius, M. Arai, Y. Endoh, T. Masui, S. Tajima, - Short-range antiferromagnetism in an optimally-doped high T_c superconductor, Phys. Rev. B 78, 132503 (2008).
- A.S. Kutuzov, A.M. Skvortsova, S.I Belov, J. Sichelschmidt, J. Wykhoff, I Eremin, C Krellner, C. Geibel, and B.I. Kochelaev, - Magnetic susceptibility of $YbRh_2Si_2$ and $YbIr_2Si_2$ on the basis of a localized 4f electron approach, J. Phys.: Cond. Matter 20, 455208 (2008).
- M. Korshunov and I. Eremin, - Doping evolution of itinerant magnetic excitations in Fe-based oxypnictides, Europhys. Lett. 83, 67003 (2008).
- H.-H. Klauss, H. Luetkens, R. Klingeler, C. Hess, F.J. Litterst, M. Kraken, M. M. Korshunov, I. Eremin, S.-L. Drechsler, R. Khasanov, A. Amato, J. Hamann-Borreo, N. Leps, A. Kondrat, G. Behr, J. Werner, B. Bchner, - Commensurate Spin Density Wave in LaFeAsO: A Local Probe Study, Phys. Rev. Lett. 101, 077005 (2008).
- Bin Liu and Ilya Eremin, - Impurity resonance states in non-centrosymmetric superconductor $CePt_3Si$: A probe for Cooper-pairing symmetry, Phys. Rev. B 78, 014518 (2008).
- A.A. Donkov, M. Korshinov, I. Eremin, P. Lemmens, V. Gnezdilov, F.C. Chou, and C. T. Lin, - Electron-phonon interaction in the lamellar cobaltate Na_xCoO_2, Phys. Rev. B 77, 100504(R) (2008).
- M.M. Korshunov and I. Eremin, - Dynamical magnetic susceptibility in the lamellar cobaltate superconductor $Na_xCoO_2{\cdot}yH_2O$, Phys. Rev. B 77, 064510 (2008)
- Ilya Eremin, Evelina Tsoncheva, Andrey V. Chubukov, - Signatures of non-monotonic d-wave gap in electron-doped cuprates, Phys. Rev. B 77, 024508 (2008).
- P. Thalmeier, T. Takimoto, J. Chang, and I. Eremin, - Multipolar Order and Superconductivity in f-Electron Compounds, J. Phys. Soc. Jpn. 77, 43(2008) Suppl. A.
- Jun Chang, Ilya Eremin, Peter Thalmeier, and Peter Fulde, - Eliashberg theory of superconductivity and inelastic rare-earth impurity scattering in filled skutterudite $La_{1-x}Pr_xOs_4Sb_{12}$, Phys. Rev. B 76, 220510(R) (2007).
- J.-P. Ismer, I. Eremin, E. Rossi, and D.K. Morr, - Resonance peak in electron-doped cuprates, Phys. Rev. Lett. 99, 047005 (2007).
- Ilya Eremin, Dirk K. Morr, Andrey V. Chubukov, Karl Bennemann, - Spin susceptibility in bilayered cuprates: resonant magnetic excitations, Phys. Rev. B 75, 184534 (2007).
- D.S. Inosov, S.V. Borisenko, I. Eremin, A.A. Kordyuk, V.B. Zabolotnyy, J. Geck, A. Koitzsch, J. Fink, M. Knupfer, B. Buechner, H. Berger, and R. Follath, - Relation between the one-particle spectral function and dynamic spin susceptibility in superconducting $Bi_2Sr_2CaCu_2O_8$, Phys. Rev. B 75, 172505 (2007).
- M.M. Korshunov, I. Eremin, A. Shorikov, V.I. Anisimov, M. Renner, and W. Brenig, - Itinerant magnetic fluctuations and many-body correlations in Na_xCoO_2, Phys. Rev. B 75, 094511 (2007).
- J. Chang, I. Eremin, P. Thalmeier, and P. Fulde, - Theory of magnetic excitations in the heavy-fermion superconductor UPd_2Al_3, Phys. Rev. B 75, 024503 (2007).

3.3.3 Gutzwiller-Fellowship

Report by *Prof. J. M. R. Parrondo*:
Information in Biophysics and Statistical Mechanics

The role of information in Statistical Mechanics has a long and controversial history [1], but it has revived in the light of recently developed fluctuations and work theorems [2–5]. I have found at the mpi**pks** several opportunities to discuss these issues with people from different groups, in particular, from the Division of Biological Physics. One of the results of these discussions is the development of a tool to estimate the dissipation along a process by analyzing the time-reversal asymmetry of a single stationary trajectory. Such a tool could be useful, for instance, to determine whether a given biological process is active or passive. A second main project during my stay at the Institute has been the study of the proofreading mechanism in transcription, based on experimental data of the RNA-polymerase motion obtained by Stephan Grill and Eric Galburt [6].

In one of the group meetings of the Division of Biological Physics, I presented a recent paper written in collaboration with Ryoichi Kawai and C. Van den Broeck [5]. In this paper we derive an exact relationship between the entropy production and the distinguishability of a process from its time-reverse. The precise formulation of this relationship is as follows: we prepare a system in a Gibbs canonical state at temperature T and manipulate it by modifying a parameter λ of the Hamiltonian, following an arbitrary protocol $\lambda(t)$, $t \in [0, \tau]$. The system is isolated except for the change in λ, which eventually introduces some energy. The process can be as far from equilibrium as we wish. After it is completed, we drive the system to equilibrium, by coupling with a thermal bath at temperature T. We then consider the time reversal of this process, starting at equilibrium with the corresponding value of the parameter $\lambda(\tau)$ and reversing the protocol followed by λ. If $\rho(q, p, t)$ and $\tilde{\rho}(q, p, t)$ are the probability distributions of the system along the forward and backward process, respectively, one can show that the entropy production in the forward process is given by [7]:

$$\Delta S = kD(\rho(q, p; t)||\tilde{\rho}(q, -p; t)) \tag{1}$$

where k is the Boltzmann constant and

$$D(\rho(q, p)\|\tilde{\rho}(q, -p)) = \int dq\, dp\, \rho(q, p, t) \ln \frac{\rho(q, p, t)}{\tilde{\rho}(q, -p, t)} \tag{2}$$

is the relative entropy between ρ and $\tilde{\rho}$. Moreover, the relative entropy between probability densities is expressing the difficulty of distinguishing samplings from these densities [8]. In the present case, it measures the difficulty of distinguishing whether observed data of the micro-state correspond to those from a forward or backward experiment. Therefore, the relative entropy (2) can be considered as a quantitative measure of the arrow of time. Due to the mathematical properties of the relative entropy, the above equality (1) becomes an inequality when one uses probability distributions of some magnitudes, instead of the whole statistical information of the micro-state of the system, which is usually unavailable.

In my seminar, Frank Jülicher and Benjamin Lindner suggested to apply this result to stationary trajectories. An estimation of the relative entropy between the trajectory

and its time reversal would provide an estimation of the dissipation and, in particular, would determine if the trajectory is produced by a system at equilibrium or not. Such determination has been carried out before for the motion of ear cells, but using fluctuation dissipation relations which require two types of experiment: one recording the stationary free motion to calculate stationary time correlations and a second one forcing the system to obtain the response [9]. On the other hand, our new approach will be able to determine dissipation only from the trajectories obtained in the first experiment, without the need of the forcing (which is usually harder to implement).

This project was started at the Institute and continued along the fall of 2008 and 2009 in Madrid, with the collaboration of the PhD. student Edgar Roldán. The problem of estimating relative entropy between stationary trajectories is almost straightforward for Markov processes, and we have already good estimations of entropy production for some toy models, such as a simple Markov chain and a flashing ratchet. However, the estimation is much harder for non Markovian systems and requires the use of different techniques that we are now developing and expect to have ready for my second stay at the Institute, in the summer of 2009. Then we could apply the technique to other sources of data, in particular from biological experiments, in collaboration with Frank Jülicher and Benjamin Lindner.

The second main project that I started in the Institute is done in collaboration with the group of Stephan Grill. Single molecule experiments with the RNA polymerase indicate that this molecular motor responsible of transcription from DNA to RNA undergoes pauses of different durations. The statistical analysis of these pauses revealed a diffusive backtracking state, in which the RNAp moves back a small number of nucleotides before resuming transcription [6]. We propose that this backtracking is in fact a proofreading mechanism which allows the removal of incorrectly incorporated nucleotides in the nascent RNA. To support this idea we have performed an exhaustive analysis of the correction probability using techniques from Markov chain theory and specially from continuous time random walks. We started this project in 2008 and it will be completed in 2009.

[1] H. S. Leff. and A. F. Rex, *Maxwell's Demon 2*, (Institute of Physics Philadelphia, 2nd ed., 2003).

[2] G. Gallavotti and E. G. D. Cohen, Phys. Rev. Lett. **74**, 2694 (1995).

[3] C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997); Phys. Rev. E **56**, 5018 (1997).

[4] G. E. Crooks, J. Stat. Phys. **90**, 1481 (1998); Phys. Rev. E **60**, 2721 (1999).

[5] R. Kawai, J. M. R. Parrondo, and C. Van den Broeck, Phys. Rev. Lett. **98**, 080602 (2007).

[6] E.A. Galburt, S.W. Grill1, A. Wiedmann, L. Lubkowska, J. Choy, E. Nogales, M. Kashlev, and C. Bustamante, Nature **446**, 820-823 (2007).

[7] J. M. R. Parrondo, R. Kawai, and C. Van den Broeck, Entropy production and the arrow of time, arXiv:0904.1573v1 [cond-mat.stat-mech] (2009).

[8] T. M. Cover and J. A. Thomas, *Elements of Information Theory*, (Wiley, Hoboken, New Jersey, 2nd ed., 2006).

[9] P. Martin, A.J. Hudspeth, F. Jülicher, Proc. Natl. Acad. Sci. USA **98**, 1438014385 (2001).

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**.

- *Aging in Fission Yeast* with I. Tolic (Dresden)
- *Self-compression by femtosecond pulse filamentation* with G. Steinmeyer (Berlin)
- *Nonlinear localized waves in nonlocal media* with W. Krolikowski (Canberra, Australia)
- *Analysis of turbulence in the atmospheric boundary layer* with J. Peinke (Oldenburg)
- *Negative interval correlations in neural firing and its effect on information transfer* with M. Chacron (Montreal, Canada)
- *Farfield characteristics of oval microlasers* with T. Harayama (Kyoto, Japan)
- *Farfield characteristics of microlasers of spiral shape* with F. Capasso (Cambridge, USA)
- *Propagation and filamentation of ultrashort laser pulses in air* with S. L. Chin (Quebec, Canada)
- *Strong field double ionization of atoms* with P. B. Corkum (Ottawa, Canada) and (Frankfurt/Main)
- *Spin dynamics of spin ladder systems* with C. Rueegg (London, Great Britain)
- *Spin dynamics of frustrated spin chains* with M. Enderle (Grenoble, France)
- *Analysis of exotic magnetic materials* with P. Schiffer (Penn State University, USA)
- *Analysis of turbulence in the atmospheric boundary layer* with J. Peinke (Oldenburg)
- *Control of neuronal firing by dynamic parallel fiber feedback* with J. E. Lewis (Ottawa, Canada)
- *Cell Division, cellular pattern formation and dynamics* with J. Howard, A. Hyman (Dresden)
- *Dynamic Organization of epithelia* with S. Eaton, C. Dahmann (Dresden)
- *Segmentation of vertebrates through oscillating and spatio-temporal gene expression patterns* with A. Oates (Dresden)
- *Study of cell movements and flows during the development of zebrafish* with C.-P. Heisenberg (Dresden)
- *Dynamics of the endosomal network in cells* with M. Zerial (Dresden)
- *Physics of active gels, the dynamics of the cytoskeleton and cell locomotion* with J.-F. Joanny, J. Prost (Paris, France)
- *Physics of mechanosensory hair cells* with P. Martin (Paris, France)

- *Physics of cell division with M. Bornens (Paris, France* with M. Bornens (Paris, France)
- *Cytoskeletal dynamics* with M. Dogterom (Amsterdam, Netherlands)
- *Physics of hearing and active wave phenomena in the cochlea* with T. Duke (Cambridge, Great Britain)
- *Role of morphogens in tissue patterning and growth* with M. Gonzalez-Gaitan (Genf, Switzerland)

3.3.5 Joint Workshop Program

Since 2008 mpi**pks** has been running a 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 splitted in even parts. To ensure a smooth operation and mpi**pks** quality standards from the beginning, we have provided substantial transfer of experience in logistical 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 call for proposals was very successful. We received a large number of workshop proposals of high quality. A referee board with international experts helps with the evaluation of the proposals. The first workshop *Extreme events: Theory, Observations, Modelling and Prediction* took place in November 2008 in Mallorca (see workshop report p. 169). Four more workshops are in preparation for the years 2009 and 2010.

3.3.6 Conferences, Workshops and Symposia

1. *Mobile Fermions and Bosons on Frustrated Lattices*
   Workshop: January 11 - 13, 2007 — 90 participants
   Scientific coordinators: P. Fulde, Z. Hiroi, P. Lemmens, R. Moessner

2. *Korrelationstage 2007*
   Workshop: February 26 - March 2, 2007 — 184 participants
   Scientific coordinators: R. Claessen, P. Fulde, M.-R. Valenti

3. *Nonlinear Physics in Periodic Structures and Metamaterials*
   Seminar and Workshop: March 19 - 30, 2007 — 83 participants
   Scientific coordinators: S. Flach, R. Hulet, Y. Kivshar

4. *Strong Correlations and Angle Resolved Photo Emission Spectroscopy*
   Seminar and Workshop: April 10 - May 11, 2007 — 101 participants
   Scientific coordinators: Ph. Aebi, D. Dessau, K. Matho, M. Potthoff

5. *Nanospintronic Design and Realization 2007*
   Workshop: May 21 - 25 , 2007 — 101 participants
   Scientific coordinators: S. Blügel, P. Bruno, D. Weiss

6. *From Complex Systems Theory to Clinical Neurology*
   Workshop: June 4 - 8 — 66 participants
   Scientific coordinators: H. A. Braun, E. Mosekilde, F. Moss

7. *Physical and Chemical Foundations of Bioinformatics Methods*
   Workshop: June 18 - 22 — 81 participants
   Scientific coordinators: M. Porto, H. E. Roman, M. Vendruscolo

8. *Physics of Fluctuations far from Equilibrium*
   Workshop: July 2 - 6, 2007 — 53 participants
   Scientific coordinators: P. Hänggi, F. Marchesoni, M. Rubi

9. *Fluctuation and Dissipation Phenomena in Driven Systems far from Equilibrium*
   Workshop: July 16 - 18 — 41 participants
   Scientific coordinators: M. Henkel, H. Hinrichsen, S. Lübeck, G. Schütz

10. *Attosecond Physics*
    Workshop: August 1 - 5, 2007 — 131 participants
    Scientific coordinators: P. Corkum, F. Krausz, J. M. Rost

11. *New Frontiers in Quantum Impurity Physics: From Nano-Structures to Molecular Devices*
    Seminar and Workshop: August 13 - 24, 2007 — 79 participants
    Scientific coordinators: R. Bulla, D. E. Logan, A. Schiller

12. *Minerva Summer School on Laser-Matter Interaction*
    Seminar: August 27 - September 8, 2007 — 31 participants
    Scientific coordinators: N. Moiseyev, J. M. Rost

13. *Local Correlation Methods: From Molecules to Crystals*
    Workshop: September 12 - 15, 2007 — 61 participants
    Scientific coordinators: U. Birkenheuer, B. Paulus, C. Pisani, M. Schütz

14. *Path Integrals - New Trends and Perspectives*
    Conference: September 23 - 28, 2007 — 120 participants
    Scientific coordinators: W. Janke, A. Pelster

15. *From Statistical Physics to Computer Science: Analysis of Biological and Medical Data*
    Seminar: October 1 - 20, 2007 — 34 participants
    Scientific coordinators: M. Biehl, B. Hammer, W. Kinzel

16. *Noise in Life 2007*
Workshop: November 07 - 09, 2007 52 participants
Scientific coordinators: Schimansky-Geier, J. Garcia-Ojalvo, B. Lindner

17. *Strongly Interacting Systems: Past, Present and Future. A Symposium in Remembrance of Richard A. Ferrell*
Symposium: November 16 - 17, 2007 41 participants
Scientific coordinators: P. Fulde, P. Hohenberg, R. Prange

18. *Atomic Physics 2007*
Workshop: November 26 - 30, 2007 92 participants
Scientific coordinators: P. Pillet, J.-M. Rost, M. Weidenmüller

19. *Pattern Formation: Self-Organization versus Self-Assembly?*
Workshop: December 10 - 12, 2007 47 participants
Scientific coordinators: U. Thiele, Ph. Moriaty, B. A. Grzybowski

20. *Epidemics in Evolving Networks*
Workshop: December 16 - 18, 2007 14 participants
Scientific coordinators: T. Gross, B. Blasius

21. *Interaction and Interference in Nanoscopic Transport*
Workshop: February 18 - 22, 2008 88 participants
Scientific coordinators: K. Ensslin, Y. Gefen, J. König

22. *Chaos and Collectivity in Many-Body Systems*
Workshop: March 05 - 08, 2008 46 participants
Scientific coordinators: M. Hussein

23. *Bio-inspired Complex Networks in Science and Technology: From Topology to Structure and Dynamics*
Seminar and Workshop: April 14 - May 09, 2008 88 participants
Scientific coordinators: S. Boccaletti, J. Kurths, T. Gross

24. *New Frontiers of Quantum Chaos in Mesoscopic Systems*
Seminar and Workshop: May 19 - 30, 2008 71 participants
Scientific coordinators: M. Hentschel, M. G. Raizen, J. Wiersig

25. *Unconventional Phases and Phase Transitions in Strongly Correlated Electron Systems*
Seminar and Workshop: June 02 - 27, 2008 142 participants
Scientific coordinators: A. Chubukov, M. Vojta, T. Vojta

26. *Quantum Phases and Excitations in Quantum Hall Systems*
Workshop: June 16 - 20, 2008 75 participants
Scientific coordinators: A. Mirlin, F. von Oppen

27. *Competing Orders, Pairing Fluctuations, and Spin Orbit Effects in Novel Unconventional Superconductors*
Seminar and Workshop: June 30 - July 11, 2008 92 participants
Scientific coordinators: J. F. Annett, I. Eremin, D. K. Morr

28. *Advanced Methods of Pharmacokinetic/Pharmacodynamic Systems Analysis Using ADAPT 5*
Workshop: July 15 - 16, 2008 23 participants
Scientific coordinators: D. Z. D Argenio, M. Weiss

29. *Optical Properties of Coupled Semiconductors and Metallic Nanoparticles*
Workshop: July 21 - 25 93 participants
Scientific coordinators: A. Eychmüller, A. O. Govorov, U. Woggon

30. *International Workshop on Time-Resolved X-Ray Dynamics*
Summer School in Time-Resolved X-Ray processes in Atoms, Molecules and Solids
Workshop and School: July 28 - August 08, 2008 73 participants
Scientific coordinators: I. S. Ko, J.-M. Rost, G. Schütz, W. Wurth

31. *Quantum Dynamical Concepts: From Path Integrals to Semiclassics*
Seminar and Workshop: August 11 - 23, 2008 77 participants
Scientific coordinators: F. Grossmann, L. S. Schulmann

32. *Dynamics of Intertial Particles: From Ocean and Atmosphere to Planets*
School and Workshop: September 01 - 26, 2008 75 participants
Scientific coordinators: E. Bodenschatz, U. Feudel, T. Tel

33. *Blebs and Cell Cortex Mechanics in Cell Movement*
Workshop: October 06 - 08, 2008 70 participants
Scientific coordinators: F. Jülicher, E. Paluch, E. Raz

34. *Correlated Electron Systems in High Magnetic Fields*
Workshop: October 13 - 17, 2008 75 participants
Scientific coordinators: V. Fleurov, V. Kagalovsky, B. Spivak, J. Wosnitza

35. *Computational Magnetism and Spintronics*
Workshop: November 03 - 07, 2008 86 participants
Scientific coordinators: P. Zahn, I. Mertig, O. Eriksson

36. *TCS-Program: Extreme Events: Theory, Observations, Modelling and Prediction*
Workshop: November 10 - 14, 2008 in Palma de Mallorca 66 participants
Scientific coordinators: H. Kantz, M. Matias

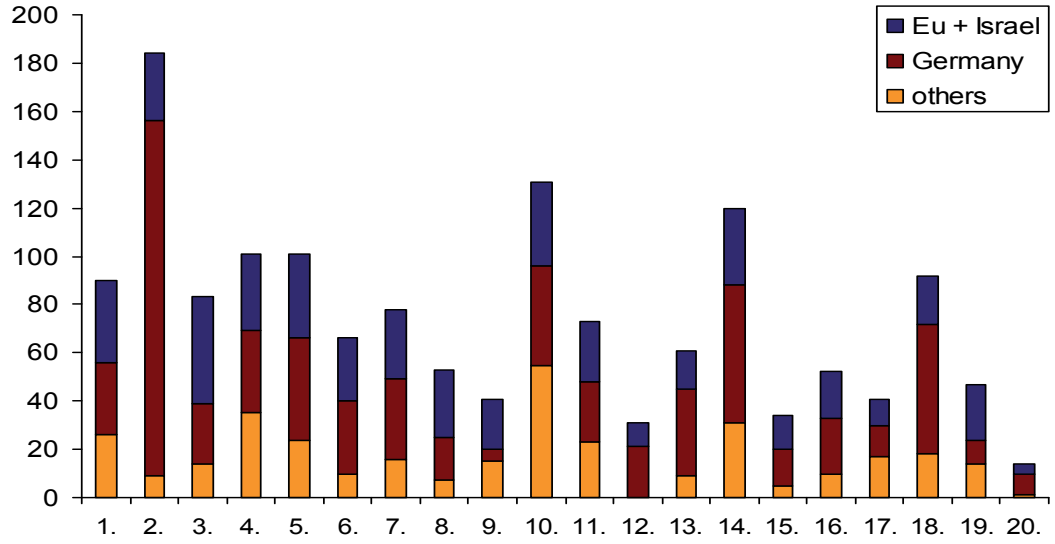
37. *Phasefield-Simulations: Materials Science meets Biology and Medicine*
Workshop: November 12 - 14, 2008 47 participants
Scientific coordinators: H. Emmerich, R. Spatschek, A. Hernandez-Machado

38. *Atomic Physics 2008*
Workshop: November 24 - 28, 2008 64 participants
Scientific coordinators: J.-M. Rost, W. Strunz

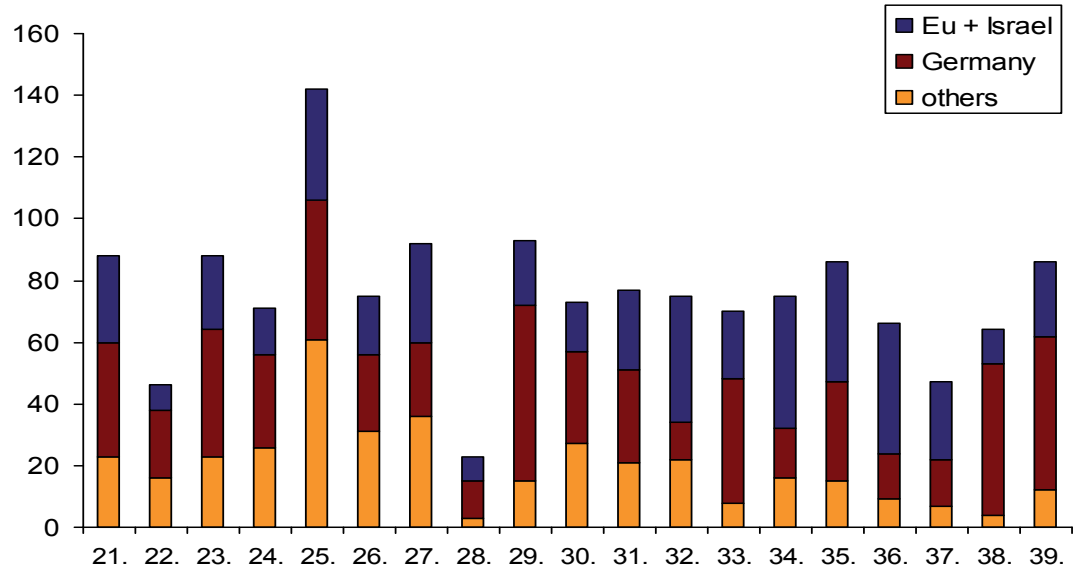
39. *Nonequilibrium Nanostructures*
Workshop: December 01 - 06, 2008 86 participants
Scientific coordinators: M. Helm, P. Lipavsky, K. Morawetz

3.3.7 Workshop Participation and Dissemination of Results

Statistics of Workshop participation



Number of Workshop/Seminar participants in the year 2007.



Number of Workshop/Seminar participants in the year 2008.

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:
  Nonlinear Physics in Periodic Structures and Metamaterials, March 2007
  Nonlinearities in periodic structures and metamaterials. Eds. C. Denz, S. Flach Y.S. Kivshar. Lecture Notes in Physics, Springer Verlag. (in preparation)
- Workshop:
  From Complex System Theory to Clinical Neurology, June 2007
  Complexity in Neurology and Psychiatry. Eds. H.A. Braun, E. Moskilde, F.E. Moss and S. Postnova In: Journal of Biological Physics 34 (2008) 249 - 457
- Workshop:
  Physical and Chemical Foundations of Bioinformatics Methods, June 2007
  Physical and Chemical Foundations of Bioinformatics Methods. Eds. M. Porto, H.E. Romand and M. Vendruscolo In: Gene Vol. 422, Issues 1-2, Pages 1-52 (1 October 2008)
- Workshop:
  Minerva Summer School on Laser-Matter Interaction, August 2007
  Gilary, I., Y. Sajeev, M.F. Ciappina, A. Croy, C.M. Goletz, S. Klaiman, M. Sindelka, M. Winter, W. Wustmann and N. Moiseyev: Supression of Photoionization by a static field. In: Physical Review Letters 101 (2008) 163002
- Workshop:
  Path Integrals - New Trends and Perspectives, September 2007
  Path integrals - new trends and perspectives. Proceedings of the 9th International Conference. Eds. W. Janke and A. Pelster. World Scientific, 2008
- Workshop:
  Bio-inspired Complex Networks in Science and Technology: From Topology to Structure and Dynamics, April 2008
  Adaptive Networks Eds. T. Gross and H. Sayama Springer Verl. 2009 (in preparation)
- Workshop:
  Phasefield-Simulations: Materials Science meets Biology and Medicine, November 2008
  Emmerich, H.: In: Philosophical Magazine (to appear spring 2009)

3.3.8 Workshop Reports

Mobile Fermions and Bosons on Frustrated Lattices

Workshop
Scientific coordinators: P. Fulde, Z. Hiroi, P. Lemmens, R. Moessner

The workshop was organized within the scientific program Highly Frustrated Magnetism (HFM) supported by the European Science Foundation (ESF) and the Max-Planck Institute for the Physics of Complex Systems (mpi**pks**) Dresden. The organizers were: P. Fulde (Dresden, Germany), Z. Hiroi (Tokyo, Japan), P. Lemmens (Braunschweig, Germany), and R. Moessner (Oxford, United Kingdom). The local organization of the workshop was performed by K. Lantsch from the mpi**pks** Dresden, Germany

The initial planning for the workshop and first announcement happened during the HFM steering committee and the first workshop held in La Londe les Maures in France, November 2005. The focus on a restricted set of topics allowed adding well-established experts in the field, both contacted directly by the organizers and from the numerous applications. A webpage for the workshop was set-up and updated until the workshop started: `http://www.mpipks-dresden.mpg.de/~itfrus07/` with a brief report at `http://www-public.tu-bs.de:8080/~plemmens/esf-hfm/hfm-workshop-2007.html`

The topic 'frustrated systems with itinerant aspects' was divided into several subtopics that where represented by key speakers in addition to posters. These were: cobaltates, triangular organics, itinerant pyrochlores, spinels, frustration and ordering, quantum criticality, bosons and supersolids, fundamental mechanisms, checkerboard physics. Material science, modeling as well as theoretical aspects were discussed.

The workshop had 96 participants (36 oral, 63 poster contributions and one concluding remark). The organizers tried to bring together a mix of young scientists on the level of PhD students, and postdocs together with senior researchers. The interdisciplinary approaches of the workshop lead to the additional advantage of a mutual exchange about all material related aspects.

All scientific activities as well as lunch and dinner were organized in the central building of the mpi**pks** in Dresden. This led to close contact and intensive discussions between the participants, and optimized the use of the time available.

Description of the scientific content

Materials physics topics:

The topic cobaltate was represented using the experimental techniques neutron scattering (Keimer, Lee), photo emission (Hasan), NMR (Alloul, Yoshimura), preparation and thermodynamic investigations (Yoshimura) and theory (Maekawa, Eremin, Mochizuki). The compound NaxCoO2 is one of the novel systems that motivated this workshop due to its exceptional ground state and transport properties. Especially noteworthy is the very large thermopower that reaches application relevant magnitudes. The observation of unconventional superconductivity is an additional highlight and motivation. Strong activities exist in Japan, where the system has been established. In France important spectroscopic investigations have been performed. In Germany activities started with

one of the organizers at the MPI-FKF in Stuttgart and recently spread out to the TU Braunschweig in the frame of a project supported by the German Science Foundation (DFG).

The case of triangular organics is similar with respect to the strong position of Japan and the prospects of the materials. In our workshop thermodynamic aspects and the phase diagram have been discussed by Lang and Kanoda. Theoretical modeling relevant for these materials is more widespread. All important aspects were discussed by Baskaran and McKenzie. In general the interest in organic materials with competing interactions is recently growing in Europe.

Pyrochlores and spinels are two classes or families of compounds characterized by well-known and long-investigated crystallographic structures. These families of compounds show an enormous variety of compositions and physical properties. The interplay of magnetism (or other long range ordered states) and competing interactions is more recently in the center of interest. Accordingly, the speakers touched different aspects ranging from unconventional ground states to more materials related or application based interest. The respective seminars touched electron-phonon coupling and superconductivity (Hiroi), multiferroicity (Loidl), metal-insulator transitions (Kremer, Takagi), Kondo-type physics (Nakatsuji) and different theoretical approaches (Valenti, Lacroix, Tsunetsugu) with an emphasis on unconventional transport properties. During the workshop it has been widely accepted that both the pyrochlores and the spinels will be of increasing importance in the field of frustrated magnetism.

Conceptual foundations:

Additional emphasis was placed on addressing, mainly from a theoretical vantage point, a range of fundamental issues raised in the context of itinerant frustration. These included questions as fundamental as the origin of magnetic behaviour, with a talk by Oshikawa demonstrating the presence of ferromagnetism by statistical transmutation, and one by Shastry on kinetic antiferromagnetism. A classification of topological insulators was discussed by Moore. Vojta's talk considered the possibility of dimensional reduction near a critical point in the framework of an RG treatment.

The nature of ordering in the presence of frustration was also extensively discussed. Emphasis was placed on the interplay of magnetic with 'ferroic' ordering behaviour by Ramirez, while Mila addressed field-driven crystallization phenomena manifesting themselves in magnetization plateaux.

A pair of talks (Becca, Poilblanc) was devoted to different aspects of dimer model physics. These models are used to describe the properties singlet-dominated magnetic phases. One aspect concerned the details of the ordering behaviour of the triangular dimer model, the phase diagram of which includes not only a topological liquid but also a complex plaquette RVB state. The other dealt with the problem of doping such models — a topic of great interest due to their provenance from high-temperature superconductivity. The related topic of physics on the checkerboard lattice — one of the most highly frustrated lattices in $d = 2$ — was given much emphasis, including talks on connections with the lore of high-energy physics (Fulde), as well as on its peculiarities of ordering (Penc) and Fermionic quantum-dynamics (Shtengel). This was backed up with a talk on numerical studies on 1-d ladder-type systems (Brenig).

Finally, the workshop reached out to closely related topics of interest to the Helium and cold atom communities. Saunders discussed the properties of Helium films adsorbed on different substrates. On the topic of supersolid phases and Bosons in magnetic fields, lattice models and their ordering properties were discussed by Troyer, Melko and Auerbach.

Impact of the event

As discussed in the preceding paragraphs, the combination of competing interactions with itinerant aspects is a very strong and rapidly developing field which links fundamental conceptual, modeling as well as materials related questions. Given the well-focused topic of the workshop, it was possible to accommodate almost all of the applications for participations (application to the workshop was open to everyone). This gave a large number of younger participants on the student and postdoc level the chance to interact with world-renowned experts in the field on the highest scientific level. The excellent local organization of the workshop by K. Lantsch and the team at the mpi**pks** helped to prepare a very productive environment. The importance of the meeting was also highlighted by the large number of steering committee members present, as well as by a strong participation from outside Europe, despite the short duration of the workshop.

Korrelationstage 2007

Workshop
Scientific coordinators: R. Claessen, P. Fulde, M.-R. Valenti

Main focus The Korrelationstage are a well-established medium-to-large conference with a tradition going back to the 1980s. This event is certainly the single most important general conference on correlated electron systems in the German speaking world. The main focus of the Korrelationstage is to review the recent developments of research on strongly correlated electron systems. Since this field of research is many-sided and highly complex (with interdisciplinary extensions into other fields such as biophysics or atomic physics), the Korrelationstage are intended to stimulate discussions between theorists and experimentalists, to interrelate the various research subjects, and to critically evaluate the merits of competing methodical approaches. The Korrelationstage bring mathematical physicists, phenomenologists, experts on various numerical approaches as well as experimentalists working on a broad range of highly correlated materials together, aiming at a close interaction and intense exchange between the different players.

Participants The Korrelationstage 2007 were attended by many prominent and important physicists from Germany, and more and more also from other European countries. A total of 184 physicists participated, with most of them providing an oral or poster presentation. A full list of all participants is available at www.mpipks-dresden.mpg.de/ korrel07/. With stronger international participation the conference language has now changed from German to English, in contrast to a long-standing tradition from previous Korrelationstage.

Participation of younger scientists The Korrelationstage have always provided a forum for young scientists at an early stage of their career (i.e., advanced PhD students and

young postdocs) to present and discuss their research results. They were presented in a variety of ways. Most of the "scientific newcomers" gave poster contributions, which raised a lot of attention and generated vivid discussions. Others were given the chance to present their work in oral talks, some of which constituted highlights of the Korrelationstage 2007, such as that by M. Zwierlein on "Ultracold atoms - dilute gases with strong interactions", to name one example.

Scientific program and results The full program of the Korrelationstage 2007 is also available at www.mpipks-dresden.mpg.de/ korrel07/. Among the many scientific results presented at the conference that should be highlighted, are, e.g., the beautiful correlation physics studied in ultracold quantum gases and its impact on electronic solid state problems, the increasing understanding of the role of multi-orbital degrees of freedom in transition metal compounds, the successful development of novel theoretical techniques, as well as new insights from various joint experimental-theoretical approaches to real correlated electron materials.

Panel discussion on "Strongly correlated systems: Problems, progress, and perspectives" Wednesday night was dedicated to an attempt to identify important topics of recent fundamental progress in, and relevant scientific perspectives for the field of correlation physics. This was done in form of a panel discussion under participation of the entire conference forum. Although of course such an endeavor cannot seriously be expected to lead to a consensual or even definite result, the extremely high interest in this session (practically all conference participants attended it) and the very lively public discussion proved the importance of such an attempt. Several scientific directions have been identified which may become important for the field in the future. Some of them have indeed developed very rapidly and already become central topics of the upcoming Korrelationstage 2009, such as, e.g., electronic correlation phenomena at the interface of artificial transition metal oxide heterostructures.

Conference site An important non-scientific cornerstone for the big success of the Korrelationstage 2007 was apart from the extremely helpful financial support the ideal infrastructure and the inspiring scientific atmosphere at the mpi**pks**. On behalf of all participants the coordinators of the Korrelationstage 2007 would like to express their great gratitude for providing such an ideal environment and also thank the very friendly and helpful staff for making the conference such a memorable experience.

Korrelationstage 2009 The Korrelationstage 2007 have generally been considered so successful that all participants agreed on the necessity of a follow-up conference. The next Korrelationstage are scheduled March 2009.

Nonlinear Physics in Periodic Structures and Metamaterials

Workshop and Seminar
Scientific coordinators: S. Flach, R. Hulet, Y. Kivshar

The purpose of the seminar and workshop was to combine experimental and theoretical expertise in the study of nonlinear effects in seemingly different types of periodic systems, to unite fundamental concepts and to develop novel theoretical and experimental approaches and techniques for analyzing nonlinear excitations, nonlinear wave

propagation and interaction in highly anisotropic and periodic structures. These structures are characterized by the simultaneous existence of continuous and discrete modes, and include photonic lattices and photonic crystals in optics, optically trapped Bose-Einstein condensates in atomic physics, and left-handed metamaterials in the physics of microwaves.

We brought together leading experts in these fields to advance the nonlinear physics of periodic systems and to facilitate key experimental observations. The seminar during the first week was aiming at an audience of young scientists. Lecture series by G. Assanto, J. Brand, V. Fleurov, I. Goldobin, W. Krolikowski, G. Tsironis, M. Wegener and the coordinators offered insights into the basic mathematical principles of localization, wave scattering, transport, quantization methods, as well as computational aspects. With that program accomplished, we moved into the second week of an intense workshop. The young participants were now well trained to follow and actively participate in the scientific debates of the second week.

During the workshop we had an intense discussion of the front research in the fields, including resonant wave scattering, gap solitons in optical lattices and Bose-Einstein condensates in optical lattices, and the different physics in micro-structured metamaterials. We received very positive feedback from the more than 70 participants, who enjoyed both the productive atmosphere of the meeting, and also the highly professional support provided by the mpi**pks**. In the framework of the workshop, we organized the mpi**pks** Colloquium on Anderson localization of optical waves in photonic lattices presented by Prof. M. Segev (Technion).

As an aftermath of that inspiring and productive meeting, we prepared a special volume of Lecture Notes in Physics (Springer) which is scheduled for publication in 2009. It contains contributions from major lecturers of the seminar week, and from a majority of invited speakers of the second workshop week.

Strong Correlations and Angle Resolved Photo Emission Spectroscopy

Workshop and Seminar
Scientific coordinators: Ph. Aebi, D. Dessau, K. Matho, M. Potthoff

Main focus of the conference: The overall objective of the CORPES workshops and seminars is to investigate the electronic structure of highly correlated materials by studying their low-energy (one-electron) excitations. Participants are situated at the crossing between many-body theory for correlated electrons and angle-resolved photoemission spectroscopy (ARPES).

A detailed modeling, realistic calculations, and the understanding of the effects of electronic correlations on photoemission spectra is particularly important when the standard quasi-particle picture no longer applies. The main focus is the complex electronic self-energy $\Sigma(k; E)$, but various intrinsic and extrinsic influences stand in the way of quantitatively extracting its momentum and energy dependence from the experimental data. These influences can obstruct the desired focus and also lead to erroneous interpretations. The program of CORPES07 was to concentrate decidedly on such refinements of the theory that either eliminate the perturbing influences or else

turn them into assets of additional information. Participants: A total of 101 participants was evenly divided between theory and experiment. Among these, 52 assisted only in the workshop, 45 in both workshop and seminar, 4 only in the seminar. The geographical distribution was as follows: Western Europe - 61, North America - 15, Asia - 11, Eastern Europe - 10, Central and South America - 3, Nigeria - 1. We strove to have a wide spectrum, reaching from the most established leaders in the field (among them: Franz Himpsel, winner of the 2007 Davisson-Germer Prize, James Allen, winner of the 2002 Isakson prize, Gabriel Kotliar and Dieter Vollhardt, winners of the 2006 Agilent Europhysics Prize) to scientific newcomers (defined as grad students and postdocs, 22 participants). All participants presented either a talk during the workshop or seminar, or gave a poster during the workshop (many did two of the above). Our policy was to not have any invited speakers for the workshop who had given a talk during the CORPES05 workshop. The majority of the talks is again available online: `http://www.mpipks-dresden.mpg.de/corpes07/`. Additional funding: In addition to the generous support from the mpi**pks**, we succeeded in raising extra support for the conference. We received over 12000 from various synchrotron facilities around the world, and travel support for 10 junior participants from IICAM (International Institute for Complex Adaptive Matter). Scientific results of the conference in the broader sense: Different material classes have been in the focus of the discussions: transition-metal oxides, heavy fermions, graphene, Luttinger liquids, nanostructures, etc. Substantial advances have been reported in the understanding of the spectrum of one-electron excitations, both for low-dimensional lattice models of correlated electrons and for realistic multi-orbital systems, also including phonon degrees of freedom, more complex electron spectroscopies, ab initio approaches to the electronic structure of correlated materials, final-state effects and effects of transition-matrix elements. High-temperature superconductors continue to attract the main attention, but also fertilize the interpretations in other systems. A major goal of the organizers, which we feel has been successfully promoted during CORPE07, is to encourage interactions between theory and experiment in a more sustained way and thus improve the understanding of ARPES data on correlated systems. Future of CORPES: During this workshop, new generations of synchrotron beamlines were presented, dedicated to ARPES with unprecedented resolutions. In view of the important investments in these facilities and the expected explosion of experimental data, it was generally agreed that a sustained and long term effort for improved understanding of ARPES is required. A great and clear enthusiasm for continuing this series of conferences in future years prevailed among the participants. Representatives of leading synchrotrons expressed their support and ordered venues for future workshops.

From Complex Systems Theory to Clinical Neurology

Workshop
Scientific coordinators: H. A. Braun, E. Mosekilde, F. Moss

Around 70 scientists from different disciplines came together for a four days highly interdisciplinary workshop at the mpi**pks** Dresden to discuss the issues of mathematical and biophysical modeling for a better progress in neuron clinical and pharmaceutical research. The workshop was organized in collaboration with the EU Network of

Excellence (BioSim) which is devoted to the implementation of computer simulations at a molecular, cellular and systemic level in the process of drug development, e.g. for a more rational planning of animal experiments and clinical trials on the basis of mathematical models.

The focus of this workshop was laid on neurological and psychiatric diseases, specifically Parkinson's disease, epilepsy, mental depression and schizophrenia, and also including associated disturbances in autonomous functions which are under neural control, e.g. disturbances of sleep wake cycles and stress axis (cortisol release). These diseases were discussed in context with mathematical and biophysical approaches which have been developed for a better understanding of brain dynamics and their modulation and disturbances. Specific attribution was paid to the origin and disturbances of brain rhythms and their synchronization as apparently most relevant parameters and indicators for a diversity of neurological and psychiatric disorders.

There were 43 oral presentations and more than 20 poster presentations. Oral and poster presentations were arranged according to different topics, partly with several subtopics.

The main topic and subtopics of the oral presentations were: 1) Brain Dynamics 1.1) Spatio-Temporal Patterns and Synchronization 1.2) Complexity and Cognition 1.3) Nonlinearities and Time-Delays 2) Rhythmogenesis and Synchronization 2.1) Neural System and EEG dynamics 2.2) Biophysical Approaches and Pathophysical Aspects 3) Comparison with Non-Neuronal Systems 3.1) Neuromodulation 3.2) Network Excitability and Sensitivity 3.3) Ions, Hormones, Genes and Glia 4) Neural Disorders 4.1) Epilepsy 4.2) Parkinson's Disease 4.3) Mental Disorders 5) System Dynamics 5.1) Autonomous Functions 5.2) Therapeutical Concepts Most of presentations were scheduled for 35 minutes

The posters were on display all over the meeting with poster presentations at three evenings. They were subdivided according to the following topics: a) Concepts of Biosimulation b) Experimental and Clinical Data Analysis c) Oscillations, Synchronization and Self-Organization d) Information Processing

Additionally, there was an 40 minutes introductory talk about Concepts of Biosimulation Their were two special mpipks lectures of 45 minutes in context with "Rhythmogenesis and Synchronization" about Biophysical and Physiological Concepts We also had a scientific "After dinner speech" about The History of Probability Moreover, there was the mpipks Public Evening Lecture (in German) about "Sonifikation - Dem Gehirn zuhören" which found excellent acceptance by a big number of external attendants.

For the realization of this extensive program, we have succeeded to bring together a group of highly reputated clinicians and experimental physiologists with outstanding experts from nonlinear systems theory. The concept of this workshop also has attracted many promising young scientists with high quality talks and poster presentations.

The clinicians and experimentalists on the one hand and the theoreticians on the other hand were almost equally distributed although such a separation cannot easily be made because many participants, due to their interdisciplinary work, can equally well be associated with one or other group.

The interdisciplinary background of most of the contributors essentially facilitated the

communication between the different groups. Most of the contributors carefully followed the organizers requests who have asked the experimentalists and clinicians to spend some more time than usual to explain the physiological systems which are under examination while the physicists and mathematicians were asked to more clearly explain their specific approaches and also to indicate the potential relevance for biological and clinical problem solving.

Moreover, despite of a full program, there was additional time also for informal meetings with further discussions of more specific questions. These possibilities were essentially used during extended poster sessions at three evenings as well as during an half day excursion with following conference dinner.

In the course of this workshop many new contacts have been and many new ideas came up which may lead to future interdisciplinary cooperation towards a better understanding of complex dynamics in physiological and pathophysiological mechanisms with applications of nonlinear system theory in physiological, clinical and pharmacological research.

Physical and Chemical Foundations of Bioinformatics Methods

Workshop
Scientific coordinators: M. Porto, H. E. Roman, M. Vendruscolo

Bioinformatics is a relatively recent discipline that has been emerging in response to the need to the need of organizing and analyzing the wealth of biological data generated by large scale programmes such as genome projects and structural genomics initiatives. Today, this discipline constitutes a very active area of research that provides efficient algorithms for a variety of applications, including sequence alignment, gene detection, and structure comparison. The idea of the workshop originated from the recognition that the physical and chemical foundations of the methodologies developed in Bioinformatics have not been, however, explored with the necessary depth. The goal of the meeting has been to bring together experts from Bioinformatics and Physics, since we believe that progress in understanding the structural properties of biological entities, including their physical and chemical interactions, can greatly help to improve existing bioinformatics methods, and ultimately suggesting new approaches.

The workshop provided an excellent opportunity to promote discussions among researchers from different scientific communities working within the following three main areas: (i) methodological developments in Bioinformatics, (ii) experimental and (iii) computational studies of the properties of biological macromolecules. Possible synergies between these experimental, theoretical, computational, and statistical analysis approaches are anticipated to take place on two main fronts. On the one hand, to improve our understanding of biological information storage and processing, and, on the other hand, to suggest new methods to extract this information from biological sequences. When achieved, such synergies will provide us with an integrated view of the subject. Our workshop has been fully successful in stimulating such an integration, by letting explore the connections between these different disciplines and providing a suitable framework for interaction.

The workshop has been organized in several sessions, 'Networks' (D. Segrè and M. Schroeder), 'Transcriptional Regulation' (M. Lässig S. Bornholdt, and E. Domany), 'Protein Structure and Function' (A. Ortíz, C. Orengo, and R. Russell), 'Protein Structure, Folding, and Complexes' (H. Fraser, L. Holm, M. Sternberg, and A. Horovitz), 'Bioinformatics' (P. Baldi, S. Teichmann, and J. Meiler), 'Protein Structure Space' (S.-H. Kim, D. Frishman, A. Lee, and S. Pietrokovski), 'DNA and RNA' (R. Bundschuh, L. Mirny, and C. Kiel), 'Genetics and Epigenetics' (C. Ouzounis and E. Kussel), and 'Systems Biology' (H. Westerhoff). 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.

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 special issues of the renowned journal 'Gene' edited by us.

The organizers wish to express their sincere gratitude to the mpi**pks** for hosting and financing this workshop and for the very generous support.

Physics Of Fluctuations Far From Equilibrium

Workshop
Scientific coordinators: P. Hänggi, F. Marchesoni, M. Rubi

This workshop took place on July 1st-6th, 2007 and was endorsed by IUPAP as a Satellite Meeting of the XXIII International IUPAP Conference on Statistical Physics (StatPhys23, Genova, Italy, July 9th-13th, 2007). The workshop program had its focus on the comprehensive collection of phenomena which originate from fluctuations occurring in nonlinear systems far from equilibrium. Special emphasis has been put on applications in physics, engineering sciences, chemical and biological physics. In addition, an attempt was made to feature also other fluctuation phenomena that appear to characterize the statistical physics of devices at the submicron scale. The notion of linear response, which, in turn, is related to the fluctuation properties of the observable of interest, can be extended to arbitrary systems that operate far from equilibrium; the corresponding fluctuation theorem relations provide most valuable information on the role of non-equilibrium fluctuations (for an overview see in P. Hänggi and H. Thomas, Stochastic Processes: Linear Response and Fluctuation Theorems, Phys. Rep. 88: 207319 (1982), Chapt. V).This notion of fluctuation theorems should not be confused with the recently proposed non-equilibrium work relations, also termed fluctuation theorems. This new branch of the fluctuation theory was formalized in the chaotic hypothesis by Gallavotti and Cohen; independently, Jarzynski derived an interesting equality, which is valid for both closed and open classical statistical systems, that relates - a priori surprisingly - the difference of two equilibrium free energies to the expectation of a particularly designed, stylized non-equilibrium work functional. Prof. Ch. Van den Broeck and Prof. L. Peliti delivered an overarching review of these recent developments "beyond the second law of thermodynamics". Prof. G. Gallavotti, this

year's recipient of the IUPAP Boltzmann medal, attended our meeting and reported on his interpretation of the notion of temperature in the context of the fluctuation theorems. Current research updates on this topic were presented, among others, by A. Imparato, J. M. Ortiz de Zarate, and B. Wynants. The implications and the role of fluctuations in the design and operation (with the characteristic manipulations occurring at differing time scales) of fabricated nanodevices was addressed by several speakers such as S. Savelev, A. Wixforth, P. Talkner, D. Reguera and M. Borromeo. A particular challenge presents the extension of the work/fluctuation theorems to open quantum systems: Here, in clear contrast to the classical situation, or also a closed, thermally isolated quantum case, a time-dependent non-equilibrium manipulation distinctly impacts the coupling strength to the heat bath (i.e. the "dissipation" strength) and thus the effective free energy and entropy. An entire morning session was devoted to this and related issues: The fundamental question as how to define work in a quantum context and the extension of work theorems to micro-canonical initial conditions was discussed by P. Hänggi, whereas new applications of great technological potential were proposed by A. Nitzan, J. Gong, S. Kohler, M. Rey-Mazon, and L. Arrachea. The multi-facetted role of non-equilibrium fluctuation in biological systems is attracting increasing interest. This topic occupied as well a whole session with illuminating contributions by M. Ehrenberg on fluctuations in gene expression, U. Gerland on conformational transitions in bio-molecular complexes, or also by D. Petrov with single molecule experiments in optical traps. Finally, widespread interest seems to persist on the issue of particle diffusion in low dimensional structures: Anomalous diffusion (I. Sokolov), diffusion enhancement (B. Lindner), absolute negative mobility (J. Luczka), Levy flights (E. Lutz), ratchet effects in higher dimensions (I. Zolotaryuk) and at the cross-over between classical and quantum regime (S. Flach) raised renewed attention in the audience. The colloquium was given by Professor L. Schimansky-Geier: He presented a most illuminating and exciting overview of the physics and applications of coupled noisy oscillators in physics and physical biology, topics that had been addressed earlier that same day by H. Park and N. Janson. As a final remark we stress the increasing interest of scientists from the Korean Advanced Institute of Science and Technology (KAIST), namely H. Park, E. K. Lee, and J. Lee, in the activities of the mpi**pks**. Closer contacts and joint initiatives between mpi**pks** and KAIST might develop in the next future.

Attosecond Physics

Workshop
Scientific coordinators: P. Corkum, F. Krausz, J.-M. Rost

The interaction between intense ultra-short laser pulses and matter constitutes a new field of research. It challenges the experiment and also theory, since a non-perturbative description with regard to high non-linear multi-photon processes is required. So far, the biggest breakthrough which has emerged from the experimental and theoretical attosecond research in this highly non-linear non-perturbative regime of laser-matter-interaction, was the creation and measurement of attosecond pulses. Having them at our disposal we are at the beginning of a new scientific era, the age of attosecond science. It will give researchers a completely new microscopic insight into electron processes,

taking place in atoms, molecules, biosystems, clusters, semiconductor nanostructures or plasmas. They can be observed in real-time and even controlled to an increasing extent on their natural (attosecond) time scale. The main purpose of this workshop was to discuss the current status of attosecond research and the obstacles for further development of attosecond measurements towards shorter time intervals and higher intensities, as well as methods to resolve them. A second important motivation was to understand and propose new applications of attosecond technique in biology, chemistry, physics and plasma physics. This happened during very intense 4 days in 40 talk and more than 60 posters. Naturally, such a new field attracts a lot of young people. 30 students and 59 postdocs participated in the conference, apart from 42 professors from all over the world, with 41 from Germany, 35 from Europe including Israel and 55 from the rest of the world. The workshop was also financially supported in form of the 391. WE-Heraeus-Seminar by the Else und Werner Heraeus foundation, Bad Honnef.

During the workshop, a steering committee was established for a new conference "Attosecond Science" with this Dresden meeting as the first conference of the new biannual series. The next one will take place in Manhattan, Kansas (USA) in 2009.

New Frontiers in Quantum Impurity Physics: from Nano-Structures to Molecular Devices

Workshop and Seminar
Scientific coordinators: R. Bulla, D. E. Logan, A. Schiller

From its historical origins in the unusual behaviour of magnetic impurities in metals, quantum impurity physics has served over the last forty years as an important arena for the development of new concepts and methods for treating correlated electron systems. The remarkable progress of recent years in the fabrication and design of nano-devices, has opened a new world of possibilities hitherto inaccessible in bulk systems. Following its first detection in semiconductor quantum dots, the Kondo effect has been observed by now in numerous nano-devices, each offering its own unique advantage. From the exquisite control of microscopic parameters in semiconductor quantum dots, to the accessibility of orbital degeneracy in carbon nanotube dots, and electronic coupling to vibrational modes in single-molecule transistors, these systems have stimulated a host of new and fundamental theoretical questions. These, in turn, have triggered significant progress in theoretical methods for handling quantum impurity and related models, both in and out of equilibrium. Recognizing the exciting experimental and theoretical developments in the field, the intent of the workshop/seminar was to bring together a wide range of workers in the field, with two central aims in mind.
1. To provide a comprehensive, up-to-date perspective of this rapidly developing field.
2. To promote communication and cooperation between researchers, most especially between theorists and experimentalists.
The main topics covered at the workshop/seminar included: • single-molecule transistors;
• dissipation, dephasing and non-equilibrium physics in the presence of strong electronic correlations; • orbital physics in quantum dots; • quantum criticality in confined nanostructures and its comparison to heavy fermions; • developments in theoretical approaches to quantum impurities and related systems.

The mpi**pks** proved to be an ideal venue for the meeting. Its location, facilities and support, as well as the superb organization and extracurricular activities, were uniformly commended by all participants. They in turn contributed immensely to the success of the workshop/seminar, which was certainly an international activity: researchers from 19 countries were present, with more than 70 participants in total. These numbers would have been larger yet were it not for inevitable space limitations – some 15 applications had to be rejected on these grounds. Highlight lectures included the QIPN2M07 Colloquium, given by D. Goldhaber-Gordon (Stanford) on observation of the two-channel Kondo effect in a semiconductor nanostructure; lectures given by D. Ralph (Cornell) and D. Natelson (Rice) about the fabrication and aspects of strong correlations in molecular devices; and a lecture given by N. Andrei (Rutgers) about new and exciting developments in the theory of quantum impurities out of equilibrium. Additional perspectives on a diverse array of subjects were given by a range of 'senior scientists', including T. Costi, K. Ensslin, M. Fabrizio, L. Glazman, A. Hewson, K. Ingersent, H. Johannesson, H. R. Krishnamurthy, H. Kroha, M. Lavagna, K. Le Hur, T. Pruschke, H. Schoeller, Q. Si, F. Steglich, M. Vojta, F. von Oppen, P. Wölfle, G. Zárand, and V. Zlatic.

One aim of the workshop/seminar was also to expose and encourage active, but younger or less established researchers, working in the field. They were well represented on the list of speakers by F. Anders, C. Bolech, L. Borda, L. De Leo, G. Finkelstein, J. Folk, J. Paaske, M. Pustilnik, and R. Zitko. Participants also had the opportunity to present their work in two poster sessions, one each during the workshop and seminar. With the same aim in mind, overview/tutorial lectures were also incorporated into the workshop programme, leading overall to an intellectually healthy balance between research talks, tutorials, and ample time for the individual discussions that are so central to science.

Reactions to the workshop/seminar were enthusiastic. In particular, participants felt it had succeeded in solidifying the community focused on quantum impurity physics, and hopes were frequently expressed for future programmes of similar nature and goals aimed at this community. The organizers would simply like to express their gratitude to the mpi**pks** for the hospitality and generous support that made the venture possible.

Local Correlation Methods: from Molecules to Crystals

Workshop
Scientific coordinators: U. Birkenheuer, B. Paulus, C. Pisani, M. Schütz

The aim of the workshop was to bring together physicists, chemists and mathematicians who work on the development of local correlation methods especially with the focus of large extended systems and crystals.
LCC2007 took place in Dresden from the September 12 to September 15, 2007. There were in total 61 participants, 9 from oversea, 16 from Europe and 36 from Germany. The program included 12 invited talks (40 min), 13 contributed talks (25 min, mostly by younger scientists), and 21 posters, which were discussed intensively in two poster sessions.
Rodney J. Bartlett (QTP, Florida) explained his approach of the linear scaled coupled cluster theory, Gustavo Scuseria (Rice University, Houston) bridged the gap between

Density Functional Theory and the Hartree-Fock approach with screened hybrid functionals for solid state calculations. Kazuo Kitaura presented for the first time his results with the fragmented MO-based correlation method for biomolecules. Martin Head-Gordon (UC Berkeley) discussed the problems and possible solutions of local correlation methods. Jeppe Olsen (Aarhus) reported about their attempts to develop a domain free local correlation method and on how to overcome the inherent numerical problems in solving the required equation systems. Hermann Stoll (Stuttgart) presented recent advances about combining Density Functional Theory and wavefunction based ab initio methods based on a split Coulomb operator ansatz. Lorenzo Maschio (Torino) and Denis Usvyat (Regensburg) presented recent progress in the development of the CRYSCOR program, which provides a correlation treatment of crystals and other periodic systems at the level of second order Møller Plesset perturbation theory. Extensions of the existing local correlations treatments for metals and for adsorption energies on surfaces were discussed. Half a day was reserved for the ab initio treatment of transition metal compounds. An evening lecture was presented by Peter Fulde who combined in his talk "The correlation hole of an electron" the viewpoint of a theoretical physicist with the one of a quantum chemists.
Lively discussions after the talks and the individual exchange between the participants of the workshops had an significant impact in the success of the workshop. It was shown, that more and more groups in theoretical physics and chemistry are interested in the local correlation methods (15 students, mostly from Germany, who wanted to learn about the newly developed methods). Successful work is underway in different groups, where most of them had at least one member of the group attending the workshop, to provide powerful state-of-the-art tools of a rigorous ab initio description of electron correlations in extended systems.

Path Integrals New Trends and Perspectives

Conference
Scientific coordinators: W. Janke, A. Pelster

The 9th International Conference on Path Integrals New Trends and Perspectives (PI07) was held at the Max Planck Institute for the Physics of Complex Systems (mpi**pks**) in Dresden during the period September 23-28, 2007. The general format and style of the conference followed the accepted and well-developed pattern of the series, focusing on the development, refinement, and important applications of the techniques of path integration. Since its founding in 1983, the series of international path-integral conferences has been coordinated by an International Advisory Committee (IAC) whose permanent members are Jozef T. Devreese (Belgium), Hermann Grabert (Germany), Martin C. Gutzwiller (USA), Akira Inomata (USA), John R. Klauder (USA), Virulh Sa-yakanit (Thailand), Lawrence S. Schulman (USA), Valerio Tognetti (Italy), Ulrich Weiß (Germany), and Vladimir S. Yarunin (Russia). The previous conferences in Albany, NY (1983), Bielefeld (1985), Bangkok (1989), Tutzing (1992), Dubna (1996), Florence (1998), Antwerp (2002), and Prague (2005) have emphasized the broad range of path-integral applications in many fields of physics and chemistry. Thus, the series has an interdisciplinary role, bringing together scientists whose interest in the path integral spans many fields, allowing them to exchange opinions, discuss problems, and

disseminate new ideas. In particular, the series aims at fostering the exchange of ideas and techniques among physicists applying many-body techniques in such diverse areas as nuclear and sub-nuclear physics, atomic and molecular physics, quantum chemistry, condensed matter physics, complex systems, quantum field theory, elementary particle physics, and astrophysics. Continuing this tradition, the 9th International Conference under the motto Path Integrals New Trends and Perspectives focused on recent developments and new directions of the path-integral approach in this transdisciplinary setting. This topical diversity is reflected by the delivered talks and the presented posters at the conference. Nearly all contributions are collected in a Proceedings book which is published in autumn 2008 by World Scientific, Singapore. At the beginning the volume covers in two parts more traditional fields such as general quantum physics and quantum field theory. Applications of generalized path integrals to quantum gravity, astrophysics, and cosmology are separately collected in the next part. This is followed by articles on statistical field theory and an overview of the many modern Monte Carlo techniques based on the path integral approach. The next two parts deal with topical subjects such as atomic and molecular Bose-Einstein condensation and many other modern developments in condensed matter physics where path integrals have turned out to be a useful tool. Next, the part on spin models surveys phenomena that can be modeled by discrete lattice formulations. Finally, the concluding part reports on many other challenging applications, ranging from the study of thermal fluctuations of polymers and membranes in the realm of biophysics to the treatment of stochastic processes such as option pricing and risk management in econophysics. 1 The mpi**pks** in Dresden provided a truly perfect and stimulating environment for such a meeting. A total of about 120 scientists from all over the world attended, representing more than 20 different countries. The conference program was organized into 30 invited plenary talks, 56 contributed talks in two parallel sessions, and 27 posters. The poster session was scheduled intentionally on the afternoon of the first conference day and preceded by a plenary session where all posters were briefly presented in a short 23 minutes talk. This was particularly fruitful for the younger participants at the PhD student level, who mainly presented posters, since this gave them the chance to really actively contribute to the conference. The posters remained on display until the last day of the conference such that very intense discussions were initiated by this schedule. It should be emphasized that the great success of this type of poster presentation depended also on the splendid infrastructure at the mpi**pks** whose architecture provides many convenient "interaction points". The special social event was an excursion on Wednesday afternoon with Martin Gutzwiller's "River Elbe boat talk" posing the provocative question Quo vadis, physica?. The day was concluded by the conference dinner at Fortress Königstein. On Thursday evening, a very active round-table discussion among the most senior researchers, very efficiently and skillfully chaired by C'ecille DeWitt-Morette, continued the theme by providing controversial answers to the question Quo vadis, path integrals?. This was preceded by historical reflections on both the personal and the scientific relationship between Einstein and Feynman in the evening talk of Tilman Sauer. These three special events are also documented in the prologue of the Proceedings. We gratefully acknowledge generous financial support for the conference from the mpi**pks**, the German Science Foundation (DFG), and the Wilhelm and Else Heraeus Foundation. Furthermore, we cordially thank Marita Schneider from the mpi**pks** for her efficient assistance with all organizational matters, in partic-

ular for maintaining the conference website where all abstracts of the talks and poster could be found. Furthermore, we thank Andreas Nußbaumer for his invaluable technical assistance in producing the abstract booklet for the conference. It contained the conference schedule, all abstracts, a list of participants and some practical information on the conference site, which all participants received together with their conference bag upon registration on Sunday evening. Finally, we also thank Andreas Nußbaumer along with Elmar Bitter, Aristeu Lima, and Moritz Schütte for their help during the conference.

From Statistical Physics to Computer Science: Analysis of Biological and Medical Data

Seminar
Scientific coordinators: M. Biehl, B. Hammer, W. Kinzel

This seminar brought together about 35active researchers from an important interdisciplinary field on the borderline of physics, computer science and computational biology. Its main aim was to provide a platform for extensive discussions, exchange of results, and active collaboration. Only two or three talks per day were scheduled, in order to provide an adequate starting point for discussions and research activities. Participant's benefited very much from the excellent infrastructure and working conditions. Spontaneous working groups were formed, new collaborations have been outlined and existing joint projects were put forward. Young researchers were ideally integrated into the overall group dynamics based on their presentations of new results form their PhD resp. pesto research. In the following we can highlight only a few of the topics addressed in the presentations: Data analysis is most effective when supported by insights from modeling the underlying physics or biology. Therefore, modeling has been one of the major themes of the seminar. For example, oscillations in gene expression can be modelled either by deterministic rules or by stochastic processes. In the first case it turned out that for some cases the interaction between genes can be represented by a deterministic system of on-off elements, which can be used to predict cycles of gene expression. In other cases, stochastic processes cannot be ignored that been shown that some simplifying model systems can be analyzed analytically, and the predictions led to the design of new experiments on genetic oscillators. Modelling also plays an important role in understanding properties of neural networks. In the seminar a model has been introduced which emphasizes several main mechanisms: balanced inhibitory and excitatory input, excitation by external signals, stable synfire chains. The statistical properties of spike correlations and intervals are in good agreement with corresponding measurements in animals. On a more abstract level, modelling helps to understand the properties of general algorithms to analyze data. For example, an effective algorithm to find group structures in sparse networks was introduced and analyzed. When it was applied to random networks with predefined communities, the theoretical analysis showed a sharp transition between zero success and good overlap between the predefined and reconstructed community. Many contributions addressed the application of adaptive information processing and machine learning in the analysis of biological and medical data. These fields currently witness an enormous increase in both, the complexity and the amount of data that is to be analyzed. Besides many applications

to real world data, the theoretical background of the methods has been discussed extensively during the seminar. Training methods have to be modified and optimized to facilitate the analysis of very large data sets. For example, it was shown how the ideas of kernel based methods, such as the support vector machine, can be implemented with high efficiency. The incorporation of prior knowledge in the analysis of biological data sets and the selection of relevant features has been addressed in several presentations. Related, important issues were the choice of discriminative similarity measures for clustering and classification and the discussion of how to represent data in order to facilitate high-throughput analysis. The latter included topology preserving networks as well as multi-dimensional scaling and related methods.

Noise in Life 2007: Stochastic Dynamics in the Neurosciences

Workshop
Scientific coordinators: L. Schimansky-Geier, J. Garcia-Ojalvo, B. Lindner

Noise in Life 2007 brought together statistical and nonlinear physicists with computational neuroscientists and neurophysiologists, and presented a wide overview of the influence of random fluctuations in the behavior of neuronal systems. We were happy to welcome a number of great and well-known speakers on this general problem — among them Wulfram Gerstner, Peter Jung, Alexander Neiman, Nestor Parga, Arkady Pikovsky, Luigi Ricciardi, Nigel Stocks, and Henry Tuckwell.

A number of talks were concerned with noise in single neurons and discussed in this context the following problems: the faithful modeling of the neuron's nonlinearity (W. Gerstner, M. Richardson); novel methods to calculate interval histograms for spiking cells (L. Ricciardi, T. Engel, A. Porporato) or the response to periodic stimulation (N. Brunel, P. Talkner); noise-induced effects in neural models (A. Torcini); detailed models of intrinsic channel noise (G. Schmid, M. Falcke), synaptic noise (P. Jung), and external conductance fluctuations (L. Wolff); effects of the spatial extension of the neuron (H. Tuckwell); the quantification, the theoretical calculation, and the biological function of interval correlations in neural spike trains (M. P. Nawrot, E. Müller, A. Neiman).

The questions of how precisely and how strongly correlated different neurons respond to a stimulus, and the details of this response on a fine temporal scale, were addressed in the talks by A. Pikovsky, G. Schneider, and J. Ritt. There were a number of excellent talks on noisy neural networks devoted to one or more of the following issues: the detection of synchronous spikes in a neural population and the question of what these synchronous spikes code for (J. Benda, G. Pipa); the spontaneous and evoked stochastic activity in biological neural networks (N.Parga, M. V. Sanchez-Vives); the function of spike-timing dependent plasticity in the developmental phase of a network (O. Chibirova); experimental evidence for traveling waves in various extended neural systems (E. Manjarrez); and task performance by means of populations of spiking neurons (M. Mattia, R. Moreno-Bote).

There was also a lively Poster session of the remaining participants of the workshop (mostly students and younger scientists), including short oral presentation of

the posters. The various topics of the posters were all related to stochastic neural dynamics and discussed specific models in detail.

In general there was a good connection of the various theoretical approaches (for instance, the spike train analysis and theorems on point processes, but also approximate solutions of the Fokker-Planck and Master equations as well as linear response theory) with exciting experimental findings (for instance, the emergence of oscillations in the spontaneous and evoked activity of single resonant cells and of networks on various time scales).

In summary, the workshop *Noise in Life 2007* provided a fruitful forum for the presentation and exchange of ideas in the interdisciplinary community studying noise and fluctuations in neural systems.

Strongly Interacting Systems: Past, Present and Future: A symposium in memory of Richard A. Ferrell

Symposium
Scientific coordinators: P. Fulde, P. Hohenberg, R. Prange

Professor Ferrell, during his lifetime, initiated and advanced a number of important subfields of condensed matter and statistical physics. Recent advances in two such subjects were particularly prominent at the meeting. In the first, dynamical scaling, several recent advances were reported. Ferrell introduced this subject in 1965 with colleagues, several of whom were able to attend the meeting.

One of the first proposals for unconventional superconductivity, which he and Fulde, (and independently, Larkin and Ovchinnikov) suggested even earlier, 1962, is a truly remarkable story. For about 35 years, the proposal for this 'FFLO' state, as it is known, lay dormant. In the last five or ten years, the field has sprung to life, with a number of quite different systems, from certain crystals, to 'cold atoms', to neutron stars, giving results suggesting something like an FFLO state. In very recent work presented by Scalapino, it appears possible that well known high-T_c d-wave superconductors may be likened to a simple mathematical transformation of the FFLO state.

In addition to Douglas Scalapino, there were a number of other distinguished colleagues who were able to participate. To keep the list short, we mention only Michael Fisher, Jan and Anneke Sengers, and of course, Ferrell's four most successful students, John Quinn, Peter Fulde, Alan Luther and Jayantha Bhattacharjee. There were several younger physicists who were called upon to give talks, which were well received.

The meeting overall was a considerable success. It brought together over 40 physicists with a common regard for Richard Ferrell, who reminisced about their friendship with Richard and told of his considerable impact on their lives and careers. In addition to the cross fertilization afforded by hearing about recent research on related topics, we hope that the meeting will be fruitful in the longer run as a source for historians of physics. Fortunately, Ferrell's wife Miriam, and son Robert, also a physicist, were able to attend.

Pattern Formation: Self-Organization versus Self-Assembly?

Workshop
Scientific coordinators: U. Thiele, Ph. Moriarty, B. A. Grzybowski

It has been suggested that the study of complex systems represents the ultimate interdisciplinary field. Essentially, complex systems are assemblies whose collective behaviour is not interpretable solely in terms of the behaviour of the individual components. This definition in turn gives rise to the concept of emergent complexity, where very many simple individual parts interact to produce complex spatiotemporal behaviour/structure in the overall system. Although countless examples of complex systems are encountered in scientific disciplines ranging from physics to sociology, a key goal of the study of complexity lies in uncovering and elucidating universal behaviour spanning such apparently unrelated fields. A fundamentally exciting and technologically relevant sub-field of complex systems science is the area of spontaneous (non-equilibrium) pattern formation. At present, several groups are working on the extension of the state-of-the-art in nonlinear dynamics to encompass a detailed understanding of pattern formation and critical phenomena in micro-and nano-technologically relevant systems. One result of their work is the insight that the seemingly sharp distinction of self-assembly and self-organization that is often taken for granted frequently becomes rather vague. Traditionally, self-assembly is assumed to mean organization of discrete components into equilibrium structures; in contrast self-organization evolves spatially continuous fields or many interacting objects into spatio-temporal out-of-equilibrium structures. The scope of the workshop was to discuss the growing number of systems under investigation in which this sharp distinction is blurred. For example, self-assembled nanoparticle arrays on a small scale can self-organize on a large scale into network-like or branched structures. This implies that a hierarchy of self-assembled and self-organized structures may exist with length scales given by the interaction length between the microscopic entities (nano-particles) and the mesoscopic transport coefficients and external gradients, respectively. In addition, subjecting self-assembling systems to sustained external gradients also leads to a variety of structures that can neither be called self-assembled nor self-organized, prompting the notion of dynamic or non-equilibrium self-assembly or self-assembled dissipative structures. In a third class, relaxational systems initially out-of-equilibrium evolve towards equilibrium. However, the pathway might proceed through a sequence of (very long) transients showing patterns with length scales given by mesoscopic parameters. The workshop was co-financed by the Marie-Curie Research Training Network PATTERNS (Unifying principles in non-equilibrium pattern formation, MRTN-CT-2004 005728) and the Max-Planck-Institut für Physik komplexer Systeme (mpi**pks**). It was organized through the workshop program of the mpi**pks**. A special aim was to bring together leading researchers working on quite different problems in the field of self-assembly and self-organization in order to share experimental and theoretical approaches and methods and to foster future collaborations throughout Europe and the world. Two of the organizers and about half of the participants had an affiliation with one of the institutions forming the nodes of the PATTERNS network. The other half came from the wider community from all over the world. In order to make the exchange as fruitful as possible, we invited exceptionally active scientists of the different subfields. Long talks were given by renowned senior scientists like, for example, D. Bonn,

X.-M. Lin, L.M. Pismen, E. Rabani, G. Reiter, H. H. Rotermund, T. P. Russell, and U. Steiner. Furthermore, a number of short talks and one poster session allowed most participants to present their results. The short talks were mostly given by postdoctoral scientists or advanced PhD students. Nearly one third of the time for each talk was reserved for discussion, an opportunity that was well used. In a vivid 45 min session the participants had the opportunity to present their posters to the general audience. During the workshop the recent developments in the individual sub-fields were presented, with a special emphasis on common properties and differences. Central themes included, for instance, the dynamics of electrostatically induced dewetting of ultrathin polymer films, instabilities and particle assembly in thin films of evaporating nanoparticle suspensions, the interplay of pattern formation and phase changes in thin films, the collective motion of self-propelled particles, block copolymer ordering in thin films, self-organization in granular materials, the interaction of buoyancy and diffusive instabilities in reaction-diffusion systems, and pattern formation in catalytic surface reactions and in corrosion. Beside investigations of the basic mechanisms underlying the specific pattern formation processes, applications were discussed, e.g., of structured polymeric films in photovoltaic devices and of regular dewetting structures in photonics. The interesting talks and the vivid poster session gave a strong evidence for the broad interest in this scientific area. The workshop united about fifty researchers from about 20 countries and more importantly it brought together mathematicians, experimental and theoretical physicists and material scientists to discuss problems of common interest. It is to expect that the workshop initiated future collaborations and was instrumental to identify future challenges for the investigation of self-assembly and self-organization in systems relevant for applications in modern technologies.

Epidemics in Evolving Networks

Workshop
Scientific coordinators: T. Gross, B. Blasius

Over the last decades we have witnessed the emergence of new diseases such as AIDS and SARS and the return of old ones such as Cholera, Tuberculosis and Influenza. Because of globalization, population growth and environmental change, infectious diseases present an ever growing threat to the human population. In order to combat this threat epidemiologist have recently started to make use of network theory. It has been shown that in models that the vaccination level required to prevent major epidemics can sometimes be reduced up to 90 percent if the structure of the underlying contact network is taken into account. Presently several large research projects try to capture the structure of the human contact network in order to gather data for the optimization of vaccination campaigns and contingency plans. What these studies overlook is that the contact network itself can change quite radically in response to the arrival of the epidemic. For example in response to SARS a large number of people changed their travel plans, stayed at home, or even fled the affected region. While the primary effect of these behavioral changes is to reduce the prevalence of the epidemic, several recent results show that they can also significantly reduce the efficiency of targeted vaccination. The workshop Epidemics in evolving networks 2007 gathered a small group of 20 leading international experts in Dresden. The participation was by invitation

only, and the participants were selected because of their recent ground-breaking contributions to the understanding of disease-topology feedback. In order to facilitate the generation of new insights the workshop followed a very rough schedule. It was characterized by lively discussions, broken only by short talks spontaneously contributed by the participants to elucidate important points. The discussion focused mostly on the identification of important open question and the planning of future projects by which these could be resolved. Examples of important topics included for instance the effect of disease-related information spreading in the population, the choice of the right timescale on which changes in the contact network should be described, and strategies for data acquisition. The last of these questions was also the topic of a colloquium talk by Dirk Brockmann. We feel that in the workshop many insights have been gained by all participants; new ideas appeared and new promising approaches were formulated. During and after the workshop many of the participants praised the open and productive atmosphere and the high standard of facilities and service provided by mpi**pks**. Also several joint projects were initiated as a result of the work-shop. I would like to thank the institute for providing this unique opportunity.

Interaction and Interference in Nanoscopic Transport

Workshop
Scientific coordinators: K. Ensslin, Y. Gefen, J. König

Following its emergence in the early 1980's, the field of mesoscopic physics has reached a level of maturity in the late 1990's. The new phase of this field saw (1) its merger with topics taken from the discipline of strongly correlated electrons and (2) the emergence of new exciting research topics, including spintronics, noise and fluctuations, quantum statistics, quantum computation, and systems with exotic spectra such as Luttinger liquids and graphene. The new discipline is often related to as nanoelectronics. The idea of the workshop held at the mpi**pks** from February 18 – 23, 2008 was to bring together experts in the field of nanoelectronics, covering a broad range of topics. The key words "interaction" and "interference" represent the input brought from the more traditional fields of strongly correlated electrons and mesoscopics, respectively. The program consisted of 35 invited talks and about 50 poster contributions, presented by participants from 18 different countries. Originally, this workshop was strongly oversubscribed, attesting to the wide interest in the chosen topic. Junior scientists had to be selected according to their achievement so far and recommendations. Almost all of them used their opportunity to present their work in one of the two poster sessions. The latter were of very high quality and stimulated long and lively discussions until late in the evening. The young participants were also actively participating in the extensive discussion sessions that followed each talk. The message of the workshop was clear—the merger of the two disciplines alluded to above, and the range of exciting challenges, define a fast moving and lively field. Many talks underlined the close contact between theory and experiment. It is clear that regular meetings in this field are the call of the day.

Chaos and Collectivity in Many-Body Systems

Workshop
Scientific coordinator: M. S. Hussein

The workshop CCM08 was conceived as a multidisciplinary gathering of scientists at the Max-Planck-Institute for the Physics of Complex System to discuss topics of chaoticity and collectivity in the response of many-body systems of different sizes, such as the atomic nuclei, Bose-Einstein Condensates and mesoscopic devices such as quantum dots. The workshop was subdivided into blocks of 4 mornings and 4 afternoons over the period of four and a half days (one afternoon was put a side for an excursion). The number of registered participants was 47, with a larger number of attendees in the different session.

In the first morning on March 5, giant resonances in nuclei were discussed by leading nuclear physicists such as Thomas Aumann (GSI) and David Brink (Oxford). Eckart Grosse (FZD) gave a review on the decay of these collective nuclear states. The concept of "doorway states", of much use in nuclear physics, was then discussed in talks by Thomas Guhr (Duisburg-Essen) and Naftali Auerbach (Tel Aviv) among others. Whereas Auerbach emphasized the superradiance characteristics of these states, Guhr made the point of looking at these states as superscars in billiards using microwave oven analog computers. Eckart Grosse (FZD) gave a review on the decay of giant resonances.

The morning of the second day of the workshop was dedicated to condensed gases and ions. Ulf Saalmann (mpi**pks**) talked about ultrafast collectivity in finite systems, while Eddy Timmermans (LANL) talked about fermionic BEC mixtures. V. S. Bagnato (S ao Carlos) talked about the experimental effort of his cold atom group and about Quantum Turbulence. Masud Haque (mpi**pks**) spoke about vortices in BEC while A. F. R. de Toledo Piza (S ao Paulo) discussed cold bosons in cranked lattices and T. Kottos talked about quantum dissipation, irreversibility and pumping in Bose systems. The following morning was dedicated to quantum chaos, with Achim Richter (Darmstadt) speaking about Chaotic scattering study using microwaves, and Mauricio Pato (S ao Paulo) and Oriol Bohigas (Orsay) describing recent advances in Random Matrix Theory (RMT). Finally, Gary Mitchell (NCSU) described the study of nuclear spectroscopy using RMT. In the afternoon of the same third day of the workshop several talks were delivered concerning chaos in mesoscopic systems. Lev Kaplan (Luiziana) discussed chaos in quantum dots, Armando Perez decoherence in spin systems, N. Papanicolaou spoke about vortices in magnetic grains and S. Schmidt discussed the coexistence of superconductivity and ferromagnetism in chaotic metallic grains.

The last morning session held on Saturday, March 8, was dedicated to four talks on vortices in magnetic grains by Stavros Komineas (mpi**pks**), networks of topological defects, by D. Bazeia (Paraiba), chaos in open systems, by Martina Hentschel (mpi**pks**) and tunneling of composite systems by C. A. Bertulani (Texas A&M-Commerce). The poster session was had in the evening of Friday, March 7. There were about 20 posters. The attendance of the session was quite good, as more than 50 people were present.

The workshop was a success as it brought together people in seemingly different areas of physics under the same roof with ample opportunity to discuss the similarities and

differences in the systems being studied. The discussions which followed the talks were lively and very informative. Most of the sessions were very well attended, especially by young mpipks visiting scientists. A simple measure of the interest of the community in the Workshop can be attested by the number of attendees in the last, Saturday morning, session; there were more than 40 people present.

The success of the workshop owes a lot to the keen dedication of the secretary, Ms. Marita Schneider, whom I thank very much.

Bio-inspired Complex Networks in Science and Technology: From Topology to Structure and Dynamics

Workshop and Seminar
Scientific coordinators: S. Boccaletti, J. Kurths, T. Gross

The workshop on *Bio-inspired Complex Networks in Science and Technology 2008* (BioNet08) set out to achieve an ambitious goal: On the one hand we wanted to bring scientists from a diverse range of backgrounds together to encourage the transfer of insights between disciplines – from physics to medicine; from biology to engineering. On the other hand we wanted to focus specifically on certain topics in which significant progress has recently been made, in particular, the investigation of dynamics on weighted networks and the interplay between topology and local dynamics in adaptive networks.

The combination of a broad range of approaches and applications with a pronounced focus on certain phenomena proved to be very conductive for the success of the workshop. Right from the beginning the workshop attracted a large number of applications, in particular from international PhD students. In total 88 researchers from 18 countries participated in BioNet08. Of these 28 participants stayed for the entire duration of the workshop (04/14/08 – 05/09/08).

The workshop started with a summer school week, which aimed to provide students with a sound working knowledge of network theory. A total of twelve 90-minute lectures given by international experts covered a large range of basic topics, ranging from spectral-graph theory to non-linear dynamics in heterogeneous causal networks. The talks were supplemented by ten 2-hour tutorial sessions to provide practical in-depth work experience in modern techniques.

The second and third week of the workshop were devoted to a seminar phase. During this time the emphasis was on actual collaborative research work with typically one or two longer talks per day as well as several get-together events. Work focused for instance on the analysis of data from real world networks and embedding techniques and moment closure approximations for adaptive networks. We experienced a great enthusiasm in particular from the younger participants, who immediately began to apply techniques from the school and seminar to problems from their own work. From this time of intense interaction many interesting ideas and promising collaborations have emerged.

The majority of senior participants joined the workshop in the final conference week. Prominent international experts from different fields of science presented state-of-the-art advances in the investigation of complex networks. In total eighteen 20-minute

talks and twenty-three 40-minute talks were given as well as one 1-hour colloquium talk. In the talks many interesting connections between applications from different fields became apparent. For instance talks on synchronization phenomena connected nicely to a lecture on experimentally observed oscillations in growing fungal networks. With great pleasure we also noted that the younger participants took part very actively by asking many questions and discussing with the speakers over lunch and breakfast and during the coffee breaks.

In response to the conference we have received much positive feedback from the participants. In particular many participants mentioned the high quality of the talks and the friendly, open atmosphere at the institute. We feel that the conference has met our twin goals to facilitate the transfer of knowledge between different disciplines and to provide in-depth insights into selected topics of active research. Several of the young participants remarked that the workshop has greatly advanced there working knowledge of networks and has provided a good orientation for their future career. Finally let us mention that at least three of the young international participants will be coming to Germany to join the groups of researchers they met during the conference.

We would like to express our thanks to the mpi**pks** for hosting the workshop. In particular we are greatly indebted to the visitors program, whose great care and efficiency made BioNet08 such a pleasurable experience for all involved.

New Frontiers of Quantum Chaos in Mesoscopic Systems

Workshop and Seminar
Scientific coordinators: M. Hentschel, M. G. Raizen, J. Wiersig

The focus of the workshop and seminar was on subjects related to quantum chaos in mesoscopic systems. The workshop and seminar brought together theoreticians and experimentalists from all over the world in particular from the fields of electronic, photonic, and atomic systems and highlighted the latest theoretical insights. The aims were: (i) to share knowledge and foster further research collaboration on topical problems in mesoscopic systems, (ii) to review the most recent theoretical and experimental advances, (iii) to give an introduction to various aspects of the field to young scientists. The main scientific results of the workshop and seminar were on the areas of (a few key speakers are given) Atomic mesoscopic systems: potential of atom optics billiards and cold atoms cold atoms as designer lab for condensed matter physics and quantum chaos (Poul Jessen) Electronic mesoscopic systems: electronic transport through quantum dots and its experimental detection (Klaus Ensslin) fidelity and Loschmidt echo many-body effects from a quantum chaos perspective (Harold Baranger) Optical mesoscopic systems: directed emission from chaotic microcavities (Hui Cao) nonlinear interactions in random/microcavity lasers deviations from geometric optics and wave-ray correspondence Theory: periodic orbit theory for transport and decay in open systems survival of mesoscopic interference effects in the classical limit (Piet Brouwer) Discussion among the different communities as well as younger and more senior scientists were facilitated through long coffee breaks (that were very well received), two poster sessions in the first and one the second week, and a special evening session on "Facets of quantum chaos" on the first evening. The poster sessions as well as the second (school) week were actively used by the newcomers to the field for intensive

and long discussions among peers as well as with senior scientists. The feedback we obtained from these younger participants (mostly PhD students) was enthusiastic, especially also on the lectures in the second week. Their presentations (posters and talks) were all of high quality. We are confident that this will set a standard for their future work concerning both high quality of their research as well as a respectful cooperation. The conference, school and seminars were characterized by a very open and cooperative atmosphere and intensive scientific exchange that carried over even to a self-organized hike through Saxon Switzer- land of about 20 participants on Sunday. 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 mpi**pks** for the hospitality and Renate Seidel for the absolutely smooth local organization.

Unconventional Phases and Phase Transitions in Strongly Correlated Electron Systems

Workshop and Seminar
Scientific coordinators: A. Chubukov, M. Vojta, T. Vojta

The workshop and seminar are in the area of strongly correlated electron systems. At low temperatures, correlated electron systems display complex phase diagrams with unconventional ground state phases. In these phases and at the transitions that separate them, thermodynamic, transport and other properties deviate fundamentally from the properties of normal materials. Over the last years, it has become clear that understanding such unconventional behavior requires approaches beyond the established concepts of condensed matter theory. The purpose of the Seminar and Workshop was to bring together the leading experts in this field to discuss their latest work in an informal format, thereby fostering new and continued collaborations. A second important goal is to involve young scientists at the postdoctoral level in forefront research. To this end, we arranged 24 theory talks by leading theorists and 15 talks by leading experimentalists during the Workshop, and additional 15 talks by theorists during the seminar. We also arranged an informal but intensive and occasionally heated discussions on the interplay between metallic behavior and Mott physics, on the origin of the pseudogap in the cuprates (with short presentations from both experimentalists and theorists) , and on recently discovered superconductivity in Fe-pnictides, with talks from researchers from mpi**pks** and experimentalists from IFW.

The areas covered by the Seminar and the Workshop include high-temperature superconductivity in the cuprates, heavy-fermion and organic materials, grapheme, frustrated magnets, disorder and non-Fermi liquid physics. We succeeded in attracting the leading experts in these fields to our Workshop and Seminar.

We also had two lively poster sessions with the talks mainly by junior scientists. These sessions went very well, and both times the area around the posters on the second floor remained crowded long after the posted time for the discussions.

The two main results of the Seminar and the Workshop are (i) a focused exchange of ideas on the origin of non-Fermi liquid physics in correlated electron systems and the classification of theories for the pseudogap, and (ii) the involvement of young scientists

in the discussions. We deliberately gave a podium to young scientists during our discussion sessions.

We benefited a lot from having another workshop on strongly correlated electrons immediately after our workshop. A number of people came for both events, and, as a result, we had a larger than usual number of scientists present during the last week of our seminar.

The third week of our seminar was also the week of the International workshop on "Quantum Phases and Excitations in Quantum Hall Systems". That was a bit unfortunate as it turned out that there was only a small overlap between our seminar and that workshop. As a result, we could only arrange two talks during that week: on Wednesday, during the excursion/dinner for Quantum Hall workshop participants. We believe that it will be better in the future not to schedule a big workshop during an ongoing seminar activities on a similar subject.

We used the third week for discussion and collaborative works. Overall, we believe that the Seminar was a success, and participants got the feeling that the field is moving, and there is a real progress. The local organization was excellent, and we use this opportunity to thank the staff at mpi**pks** for their wonderful work.

Competing Orders, Pairing Fluctuations, and Spin Orbit Effects in Novel Unconventional Superconductors

Workshop and Seminar
Scientific coordinators: J.F. Annett, I. Eremin, and D.K. Morr

The seminar and workshop took place at the mpi**pks** in Dresden between June 30 - July 11, 2008 and were focused on a number of important open problems in the field of unconventional superconductivity. It brought together the leading experimental and theoretical experts to directly address some of the most pressing controversies in this field of research. The scope of the workshop spanned a large number of very different families of materials, and included: superconductivity in heavy-fermion compounds, the cobaltates, and the high-temperature superconductors, as well as non-centrosymmetric superconductors and the coexistence of superconductivity and magnetism. In particular the great excitement caused by the discovery in early 2008 of a new class of novel superconductors, the 'iron pnictides', led to a great deal of discussion about the relationship between these new materials and the other materials discussed at the workshop. This workshop was also of great relevance for other "hot" areas of contemporary condensed matter research, such as nanoscience, advanced spectroscopies, metal-insulator transition, and magnetism. Over 80 participants from Europe, USA, Canada, South America, Japan, and Australia took part in the meeting. The program included 55 oral presentations, both invited and contributed, as well as two poster sessions. Invited talks were presented by a number of leading experts in the field who covered major recent achievement in both theory and experiment. In addition, younger participants presented their results in the form of contributed talks and posters. The interchange of points of view between participants with distinct scientific interests gave rise to a highly stimulating atmosphere. During the workshop and seminar, a number of new and exciting results were presented by the following speakers: A. Huxley

on "Superconducting ferromagnets", A.V. Chubukov on "Pseudogaps near Quantum Critical Points", P. Coleman on "Qu-transitions. Phase transitions in the quantum era", C. Broholm on "Spin resonance in the d-wave superconductor CeCoIn5", G. Volovik on "Topology in momentum space, fermionic spectrum and quantum phase transitions", K. Ishida on "NMR in Fe-based superconductors", M. Sigrist on "How to form Cooper pairs without inversion symmetry?", B. Keimer on "Spectral anomalies in conventional and unconventional superconductors", C. Pepin on "Quantum criticality in 3He bi-layers", and A. Mackenzie on "Obtaining the experimental information on spin-orbit coupling in layered oxide metals", to name a few: Many other participants also made the important contributions and presented new and interesting results. It is also noteworthy that many young scientists presented talks of high quality and great interest. The talks, discussions, and posters at COFUS 2008 demonstrated that the field is developing rapidly and has great prospects. One of the highlight of our meeting was the session devoted to the recently discovered iron-based superconductors. Due to the enormous interest of the community in this new discovery we have had an extra informal round table discussion at one of the seminar days. Based on the feedback we received from the participants, this meeting was very well received and quite a success since it achieved the important goals we had set: (i) to bring together leading scientists working in the different subfields of low temperature physics and superconductivity in order to discuss the recent advances in the field, to visualize further research prospects and to promote new research collaborations and (ii) to bring together top level scientists and young researchers, to stimulate lively interaction and exchange of ideas between them. We would like to thank the mpi**pks** for its hospitality and excellent infrastructure provided to us and the participants of our workshop. We would also like to thank the team of secretaries and, in particular, Renate Seidel, for their kind assistance and always friendly support in organizing the meeting.

Advanced Methods of Pharmacokinetic/Pharmacodynamic Systems

Workshop
Scientific coordinators: D. Z. D. Argenio, M. Weiss

This hands-on software short course was designed to introduce the modeling platform ADAPT 5 to basic and clinical research scientists who are actively involved in the application of modeling, computational and data analysis methods to problems involving drug kinetics and drug response. The two-day short course attracted 22 participants from 11 countries, with participation limited to facility the instructional elements of the course. Background lectures were delivered by D.Z. D'Argenio (University of Southern California, Los Angeles) and M Weiss (Martin Luther University Halle-Wittenberg Halle(Saale)) and covered the following topics: estimation principles in pharmacokinetics/pharmacodynamics (PK/PD) including least squares, maximum likelihood and Bayesian methods; recirculatory models of drug disposition; absorption modeling via the inverse Gaussian function; modeling using inverse Laplace transformation; drug-receptor interactions; indirect and target mediated response models; principles of population PK/PD modeling; modeling covariates in population PK/PD; modeling principles with ADAPT 5. The participants then tested their understand-

ing of these concepts by implementing a series of 12 case studies using the ADAPT 5 software that included the following topics: doses and covariates; WLS/ML estimation; multiresponse estimation; recirculatory modeling; drug-receptor interaction models; direct response PK/PD models; absorption/disposition modeling; indirect response PK/PD models; modeling building with covariates. Participants also shared the modeling problems from their own research, which provided expanded opportunity to discuss how ADAPT could be applied to solve these problems. The short course was presented as part of the service function of the Biomedical Simulations Resource at the University of Southern California, which is supported by the National Institutes of Health under grant P41-EB001978 to develop and disseminate modeling and computational methods to advance biomedical research. We wish to thank the mpi**pks** and the visitors program staff for providing the opportunity to present the short course, and especially Ms. Claudia Pönisch for her expert organization of all aspects of the course.

Optical Properties of Coupled Semiconductor and Metallic Nanoparticles

Workshop
Scientific coordinators: A. Eychmüller, A. O. Govorov, U. Woggon

The OPCSMN08 workshop brought together about 100 researchers from Europe, US, Canada and India working in the field of optical properties of self-assembled quantum dots, colloidal nanoparticles and metallic nanostructures. In a very productive scientific environment provided by the mpi**pks** an interested mixture of young upcoming and established senior scientists enjoyed exciting discussions and exchange of ideas. During the five days of the workshop the participants could listen lectures given by highly recognized speakers from the field of theoretical physics, solid state physics, physical chemistry, ultrafast spectroscopy, and photonic engineering.

The central theme of the Workshop was many-body interactions in nanostructures. Now it is an extremely "hot" field of research, due to both new fundamental physics and applications. The concrete topics touched by the workshop were, e.g., different coupling and interaction phenomena in the area of quantum dot-quantum dot coupling and nanocrystal molecules, quantum dot-photon coupling, coupling of nanoparticles in assemblies (semiconductor/ metal/ molecule/ nanotubes/ supercrystals), quantum dot/exciton - plasmon coupling, and Coulomb interactions of charged carriers, excitons and multiexcitons.

Young scientists presented their results in short invited talks, posters or acted as session chairs during the lively scientific discussion. For some of the young participants, this was their first invited talk or session-chair role. In this way, the Workshop promoted young active scientists.

The participants used also a chance to contact and visit the researchers of the mpi**pks**, the Chemistry Department of the TU Dresden and of the Institute for Solid State and Materials Research. On the other hand, since the Workshop was open to public, non-registered visitors from several German institutions (local and other cities) used

the opportunity to attend the lectures and to get involved in the scientific atmosphere during the workshop.

Going back to their home institutions, all of us brought home new ideas, knowledge and information about cutting edge – developments in the field of optics of coupled and interacting semiconductor and metal nanostructures. The Workshop has received many good responses from the participants.

We thank the local organizers, Katrin Lantsch and Dr. Sergei Flach, for their excellent organization and support which was essential for the success of the workshop.

Summer School on Time-Resolved X-Ray Processes in Atoms, Molecules and Solids and International Workshop on Time-Resolved X-Ray Dynamics

Workshop and School
Scientific coordinators: I.S. Ko, J.-M. Rost, G. Schütz, W. Wurth

This two week event started with a summer school followed by an international workshop, both acknowledging the fast development of new light sources. Light pulses of soft X-ray frequency and attosecond pulse length open the way to "attosecond science". Light pulses of slightly longer duration but frequency reaching into the 10 keV range are being realized at the new X-ray free electron lasers. Finally, the next generation light sources evolve synchrotron radiation into a tool to resolve microscopic dynamics in the angstrom - sub-picosecond domain in space and time. Technologically, these light sources have a different background, but the physical processes one can initiate and monitor with them are growing together.

The workshop in connection with the summer school was intended to bring together scientists extending our knowledge about processes in nature with these new light sources in very different areas from biology to material science with an emphasis on the basic physical processes. At the same time young scientists who want to become involved in this research were encouraged to participate, in particular in the summer school.

The summer school had an intense format of two to three two-hour lectures a day, followed by exercises in two groups and concluded daily by a plenum, where all 30 students of the two groups summarized for each other the results. Lectures were given by Christoph Bostedt, Berlin on "experiments at FLASH", Alexander Fählisch, DESY on "ultrafast dynamics excited and probed on the atomic scale", Christian Schroer, Dresden on x-ray imaging techniques" and Robin Santra who gave an introduction to x-ray physics from a theorist's perspective. The latter was also published as a tutorial in Journal of Physics B.

The following workshop with about 75 participants presented through its 33 talks a wide range of topics, relevant for time-resolved X-ray processes, from the properties of the light sources over the dynamical features of matter under short pulses to questions of imaging such processes. One focus was the work of the Advanced Study Group at the Center of free electron laser studies in Hamburg, performed at FLASH, the free electron laser at DESY.

Special to this two-week event was its co-organization including financial support by a Korean partner, the Asian-Pacific Center for Theoretical Physics. This special format

allowed for a good overview of the status of Korean interest and status in this field through 5 invited talks, presented by Korean scientists. All in all 30 participants were from Germany, 16 from Europe and Israel and 27 from the rest of the world.

Quantum dynamical concepts: From path integrals to semiclassics

Seminar and Workshop
Scientific coordinators: F. Grossmann, L. S. Schulman

From the 11th of August until the 22nd of August 2008 an introductory seminar followed by an interdisciplinary workshop took place at the Max-Planck-Institut für Physik Komplexer Systeme in Dresden. The seminar week was attended by approximately 30 and the workshop by around 70 scientists from all over the world. Theoretical approaches to solve the time-dependent Schrödinger equation by using Feynman path integral techniques and semiclassical approximations were in the topical focus of the whole event. Applications ranged from quantum chaology to chemical dynamics in condensed phases. A total of 41 theoretical talks, 6 of which were contributed talks by younger scientists, were held during the central workshop. The interdisciplinary nature of the event manifested itself in the presence of physicists, chemists and mathematicians. Lively discussions after the talks and cross references between different talks made the event a very fruitful one. The mpipks colloquium by Ulrich Weiss from the University of Stuttgart demonstrated the feasibility of path integral calculations for qubits in a dissipative environment and the final workshop talk by William H. Miller from UC Berkeley was an impressive proof of what so-called semiclassical initial value methods can do in order to improve the quality of molecular dynamics simulations. Younger participants have used the two poster sessions and especially the preceding seminar week (which was held on a tutorial level) for intense discussions and contacts to the senior participants. Foundations of the theory underlying most of the workshop talks were laid out in great detail e. g. in the presentation by Uzy Smilansky from the Weizmann Institute of Science, who gave four 90 minute lectures on semiclassical theory.

Dynamics of Inertial Particles: From Ocean and Atmosphere to Planets

Workshop and School
Scientific coordinators: E. Bodenschatz, U. Feudel, T. Tel

This workshop very successfully fulfilled its goal, namely, bringing together scientists from various disciplines who investigate the advection of active and passive finite size particles in fluid flows. Scientists from physics, meteorology and oceanography were united at the school and the conference. Theorists as well as experimentalists contributed didactic lectures and scientific talks. One overwriting success, was that it mixed scientific communities - many scientists met for the first time and this lead to extremely stimulating discussions across the several disciplines. All participants learned a lot from each other by following talks from other areas of research. Many participants told us that they very much appreciated the very high level of the talks during the conference including the contributed talks given by young researchers. The discussions

after the talks, in the breaks and especially during the school led to new ideas how, e.g., to use methods developed for the description in raindrop formation to model the aggregation of marine aggregates. Particularly these analogies in modeling approaches resulted in a cross-fertilization of the different fields of research. The success of this event in initiating interdisciplinary research can be measured in the future by papers whose authors started a collaboration during this one month program. The students staying over the entire period on this International School and Workshop (about 20 in number) presented their work several times. In the beginning and at the end of the workshop they had to give short talks about their work and most of the students also presented a talk or a poster at the conference in the third week of the event. Comparing the short presentations of the students at the beginning and at the end revealed that some of them achieved very good new results based on the extensive discussions with the lecturers, organizers and invited speakers at the conference. Only during the short time of this school considerable progress has been made by Anton Daitche (Münster, Germany). The organizers gave an award to Jöran März (Oldenburg, Germany) as the most active student during the lectures of the school. Particulary, students at the beginning of their PhD work benefitted most from the comprehensive overviews given by the lecturers.

Blebs and Cell Cortex Mechanics in Cell Movement

Workshop
Scientific coordinators: F. Jülicher, E. Pauluch, E. Raz

The international workshop took place from the 5th of October until the 8th of October 2008 at the Max Planck Institute for Physics of Complex Systems in Dresden. The workshop included about 70 participants out of whom 25 delivered oral presentations and a bit over 30 participants presented their work in form of a poster.

The workshop focused on the mechanisms of bleb formation and cortex mechanics in the context of cell motility, apoptosis and cell division. The 15 invited speakers provided the scientific core of the meeting, which included the main figures in the field. The participation of leading researchers such as Michael Sheetz (Columbia University, New York), Eric Sahai (Cancer Research UK, London), L. Mahadevan (Harvard, Cambridge), Fred MacKintosh (Vrije Univ, Amsterdam) and Guillaume Charras (UCL, London), among others is an evidence for the significance and the interest in this emerging topic.

A unique feature of this workshop was the representation for a wide range of approaches, methodologies and model systems for studying blebs and cortex mechanics. Presentations of analysis of mathematical and physical properties of blebs, membrane and cortex combined with description of results from the developmental and cell biology fields encouraged interesting discussions.

A proportionally large number of young participants presented their results in talks. The poster session provided yet another opportunity for the others to discuss their findings and receive advice from more senior researchers.

This international meeting allowed the bleb community to meet for the first time, exchange ideas and establish interdisciplinary interactions and collaborations. It is

expected that this successful workshop will be followed by similar events where the issue of blebs and cortex mechanics are discussed.

Correlated Electron Systems in High Magnetic Fields

Workshop
Scientific coordinators: V. Fleurov, V. Kagalovskii, B. Spivak, and J. Wosnitza

The main focus of the workshop was to foster exchange of ideas between theoreticians and experimentalists using high magnetic fields as a tool for the investigation of electronic and magnetic properties of strongly correlated electron systems (SCES) both in three-dimensional and low-dimensional systems. For this sake, the leading experts from the high-magnetic field centers of the EuroMagNET consortium and other key experimental labs were invited as well as theoreticians active in the studies of SCES under extreme conditions. We may indicate the following names of participants: C. Berthier, T. Giamarchi, N. Hussey, M. Jaime, J. Mydosh, M. Potemski, C. Proust, U. Zeitler, S. Zvyagin as well as many others.

Among the young scientists the most impressive presentations were given by I. Burmistrov, A. Coldea, D. Kovrizhin, A. Laeuchli, N. Laflorencie. There were a large number of young researchers, such as PhD students from mpi**pks**, MPI-CPfS, FZD Rossendorf, and the Dresden University of Technology who were attracted by the talks and were active participants of the workshop.

The conference was devoted to experimental and theoretical studies of various systems carried out in high magnetic fields. The first talk by J. Mydosh served as perfect introduction to the importance of research in the highest experimentally accessible magnetic field with a special reference to heavy-fermion systems. This day was completed by the mpi**pks** colloquium given by N. Hussey.

There were several sessions on frustrated antiferromagnetic systems which exhibit various phase transitions analogous to Bose-Einstein condensation and other nontrivial phenomena. Exchange interaction is the most relevant parameter in these systems, which requires very high magnetic fields (above 40 T) in order to drive the system into new phases. Two sessions were devoted to the hot topic of graphene systems, which are characterized by an unusual type of Landau quantization and correspondingly quantum Hall effect in high magnetic fields. According to the talks given by E. Shimshoni (theory) and by U. Zeitler (experiment) the most interesting phenomena may be achieved in extremely high magnetic field. The workshop was complemented by a visit to the high magnetic field facilities at the FZD in Dresden-Rossendorf.

Computational Magnetism and Spintronics

Workshop
Scientific coordinators: P. Zahn, I. Mertig, O. Eriksson

The workshop was attended by about 90 scientist from 22 countries from Europe and overseas. They presented new theoretical developments and methods, and actual experimental results in 30 talks. Nearly all participants took the chance to present their

own results on 52 posters. Younger scientist were invited to present their findings on an international podium (C. Heiliger, Cs. Jozsa, C. Ederer, V. Garcia, N. Stern). This, in addition to talks of internationally highly-ranked specialists provided an aspiring atmosphere for discussions and lively exchange of ideas, which were centered at computer simulations of known, as well as brand new spintronics phenomena. This includes the understanding of the magnetic order and dynamics of nanostructures, spin dynamics under the influence of magnetic and electrical fields, the currently discovered Spin Hall effect, and the behavior of electrons in Graphene.

The addressed topics of the invited talks were:

- Spin Hall Effect (Stern, Buhmann, Jin, Bruno)
- Graphene (Katsnelson, Józsa, Louie, Nieminen, Kelly)
- Multiferroics (Picozzi, Alexe, Ederer, Garcia, Ravindran, Dörr)
- Electronic correlation effects (Schulthess, Temmermann, Lichtenstein)
- Magnetic structures and spin dynamics (Blügel, Wulfhekel, Nordström)
- Diluted magnetic semiconductor (Sanyal, Sato)
- Spin dependent transport (Turek, Ebert, Györffy, Heiliger, Resta, Tosatti)

The intense interaction of experiment and theory will boost the field for the future. Financial support of the Max-Planck-Institute, the psi-k.org network and the ESF Activity 'Towards Atomistic Materials Design' is kindly acknowledged.

The workshop is the second in the series CompMag, which started 2006 in Jülich. It provides a European forum for the development of computational solid state physics with special emphasis on magnetism. The next meeting of the series will be organized by Stefan Blügel in Jülich in spring 2010.

TCS-Program: Extreme Events: Theory, Observations, Modelling and Prediction

Workshop
Scientific coordinators: H. Kantz, M. Matias

Main focus: The workshop focused on the emerging field of very large self-generated short-time fluctuations in complex systems, so called extreme events. This involves theoretical physics and mathematics as far as theory and simple models are concerned, as well as many other disciplines where the real-world phenomena are observed and analyzed quantitatively. Altogether 17 invited speakers, 46 participants and the two coordinators participated in the conference.
Senior participants: The participants included leading experts working in these fields, such as M. Ghil, N. Johnson, J. Kurths, B. Malamud, E. Ott, J. Peinke, S. Redner, L. Smith, S. Solomon, D. Sornette R. Toral
Young scientists: 9 out of the 35 talks given in the Workshop were presented by

young scientists without tenure, typically at the postdoctoral level, and even a few of the talks were given by senior PhD students. A "best contribution award" (consisting in a book present sponsored by the European Physical Journal B) was awarded to Anja Garber, a PhD student, for her talk on finite size effects on extreme events, while the talk presented by Angeles Serrano (postdoc at IFISC) showing the occurrence of extreme events in texts was ranked second. The majority of the posters was presented by young people at the PhD or postdoc level. A three-minute presentation of each poster was arranged, so that the poster presenters could reach a wider audience.

Scientific results: Extreme events, for which the usual statistical prediction techniques fail, have tantamount importance in a number of fields, both related to Earth Sciences and also to Social Sciences. A dramatic example, addressed in Prof. Sornette's talk, is the economic crisis we are living nowadays originated in subprime mortgages. The talks presented in the workshop covered a wide range of topics from listing systems and model classes where evidence for extreme events exists (for example, Prof. Ghil's opening talk, who offered a review of the field), presenting current statistical tools for the characterization of extreme events including temporal and spatial correlations, and highlighting examples where a detailed understanding of underlying mechanisms has been achieved. This was completed by the issue of prediction and predictability, of scoring and evaluating predictions, and control of extreme events, as well as considerations about the discrepancy between physical impact of some event and societal impact. The combination of contributions from experts primarily working in different areas, like Statistical Physics, Meteorology, Statistics, Nonlinear Dynamics, Sociophysics, etc. is a very unique and outstanding aspect of this meeting, which helped to create an stimulating atmosphere of discussions that can result in potentially important collaborations across disciplines. Our overall evaluation of the meeting is very positive. The meeting generated stimulating discussions, the average attendance in the activities was high, and the level of most contributions was excellent.

Acknowledgments: We would like to thank IFISC and Govern Balear (Conselleria d'Hisenda) for generous support and the ideal environment to carry out the Conference. Also the mpipks Visitor's Program for their help with the organization, specially Claudia Pönisch, Workshop Secretary, for efficiently and competently handling all kind of organizational issues. We also thank Rosa Rodríguez and Marta Ozonas for their help with all local aspects of organization.

Phase-Simulations: Materials Science meets Biology and Medicine

Workshop
Scientific coordinators: H. Emmerich, R. Spatschek, A. Hernandez-Machado

The workshop "Phase Field Simulations: Materials Science meets Biology and Medicine" which was held at the Max-Planck Institute for the Physics of Complex Systems during Nov 12-14 2008 brought together scientists from different fields who work on various aspects of nonlinear and no equilibrium pattern formation processes. The common link between the participants from physics, materials science, biological physics and medicine, was the phase field method, which is nowadays probably the most prominent

and flexible numerical technique to solve problems with moving boundaries. This motivation of the workshop, to exchange ideas from very different scientific fields was very fruitful, since the common background on a mainly computational method bridged the gap between the participants and allowed to get new insights into very different questions at the frontier of current research. Both the oral and poster presentations covered a wide range of applications of phase field methods. A strong focus was on the classical aspect of solidification processes, which was originally the foundation of the phase field method. Here, also the influence of fluid flow on dendritic growth, elastic effects on solid-solid transformations as well as complex polycrystalline solidification processes, which are highly important for many technological applications, were discussed. Other presentations were dedicated to crack front instabilities under combined tensile and shear loading and heterogeneous nucleation processes. An emphasis was on a more recent development, the phase field crystal method, which incorporates also atomistic effects, and which is related to the classical density functional theory of freezing. A strong accent during the workshop was on soft matter physics, ranging from phase field descriptions of liquid crystals to viscous fingering and pinch-off singularities during Hele-Shaw flow. New insights on the dynamics of vesicles under shear flow shed light on the dynamics of e.g. red blood cells. Concerning applications of the phase field method in medicine and biology, new ideas towards and understanding and modelling of the growth and angiogenesis of tumors were presented. The development of suitable approaches from fundamental processes like the spreading of blood vessels was carefully elucidated. The strength of the meeting was to bring together scientists from very different fields, and to stimulate valuable discussions between them. Intense discussions suggest the formation of European networks to further link the activities of the groups, and steps towards such an integration were undertaken during the meeting. The success of this workshop reflects the importance of the prospering phase field method and its fast evolution, and a perpetual repetition of such meetings is a strong desire for the future.

Atomic Physics

Workshop
Scientific coordinators: J.-M. Rost, W. Strunz

A wide variety of topics were covered at the "Atomic Physics" International Workshop 2008 (November 24 - 28), ranging from atomic and molecular dynamics to more fundamental and conceptual issues. There were 64 participants from many European and some non-European countries of which a balanced mixture of well established and promising young scientists gave about 40 invited talks. Other participants presented their research during two poster sessions on Tuesday and Thursday evening.

The first two days were devoted to the "focus topic" on dissipative quantum dynamics in atomic and molecular systems. Invited speakers both from Theoretical Physics and Theoretical Chemistry reported on current developments in the description of complex quantum dynamics. On Monday many speakers gave an account of their research on quantum transport phenomena in biologically or chemically relevant complex molecules and we had the pleasure to witness the full catalogue of possible approaches to these highly complex systems (fully quantum approaches, master equations, path integrals,

stochastic Schrödinger equations, quantum-classical hybrid approaches, MD simulations, etc.). Focus was directed at questions on the relevance of coherent phenomena in such systems, the role of structured reservoir spectral densities, and non-perturbative results. A subject that could be felt permeating through many talks was concerned with the question whether – for some applications – dynamics may well be described classically, while all the quantum features are merely reflected in the initial phase space distribution. On Tuesday we heard talks on a variety of topics ranging from (quantum) control and quantum error correction under the influence of noise, the quantum strong damping limit, test of Bell inequalities featuring massive particles, and once again talks that highlighted the intricate difficulties when faced with an efficient description of complex quantum dynamics. Wednesday started with experimental accounts of quantum dynamics in or on Helium nanodroplets, a field of fascinating possibilities as these droplets are not only interesting many-body quantum systems themselves but they provide ideal refrigerators for molecular spectroscopy. These talks were followed by two sessions on the topical issue of (ultracold) Rydberg physics. Thursday was dedicated to the whole spectrum of topical research in atomic and molecular physics, ranging from Bose-Einstein condensates over femtochemistry and attosecond pulses to quantum chaos. The international workshop came to a close on Friday with the presentation of experimental results in laser-atom and laser-molecule interaction; again we heard some speakers touching more conceptual issues concerning coherence and entanglement in atomic and molecular processes.

The workshop was attended by researchers from divers backgrounds such as theoretical and experimental atomic, molecular and solid state physics, quantum optics, theoretical chemistry and theoretical biophysics, statistical physics and quantum information. As on so many occasions before, supported by the excellent local organization, the mpi**pks** provided an ideal environment for stimulating scientific discussions and an exchange of ideas between these various fields. It became very clear that a successful framework for the description of complex quantum dynamics will have to merge concepts from all these research areas.

Non-equilibrium Nanostructures

Workshop
Scientific coordinators: M. Helm, P. Lipavsky, K. Morawetz

As a result of the cooperative effort of the Forschungszentrum Dresden-Rossendorf, the International Center for Condensed Matter Physics in Brasilia (ICCMP), and the Max-Planck-Institut für Physik komplexer Systeme in Dresden (mpi**pks**), the international workshop Non-equilibrium Nanostructures (NONNA 08) took place at the mpi**pks** from 01.12.08 to 06.12.08. The workshop was supported by the Deutsche Forschungsgemeinschaft and the Government of Saxony. It was attended by 92 scientists from 24 countries and 5 continents. This high level of international interest in the subject pleasantly exceeded the expectations of the organizers. The highly ranked participating scientists assembled for the 6 days of the workshop and exchanged exciting new experimental and theoretical results. The extraordinary density of the program, featuring 58 talks in 6 days, was a stimulating experience. Every session of 3 talks was followed by a

lively discussion break. All talks were characterized by an extremely high quality of presentation, and often unpublished results were communicated. In this respect it was of great advantage to allow 30 minutes to every speaker. Leading scientists were able to provide an excellent compact overview of their current work, while younger scientists had the opportunity to present their results to an international audience with enough detail. The daily poster sessions, the friendly atmosphere and the coffee and lunch breaks all stimulated discussions which brought the participants in contact with topics and subjects of research outside their own. An immediate result of the workshop is the agreement to apply for a European network in 2009. Also, an international working group is currently being established with the same name at the ICCMP in Brasilia (www.iccmp.br/ne) to take up the momentum of the workshop and develop new collaborations among the participants. Major experimental results and developments were presented in the field of nanostructures as well as in the field of short time scale dynamics. This demonstrates the broad variety of main stream experimental research areas discussed at the workshop. On the theoretical side, the current status of many-body quantum theory of finite systems in non-equilibrium was discussed. Different approaches were presented to include transient effects on short time scales as well as correlations in the description. It became clear that our theoretical understanding is currently behind the experimental knowledge of such systems. This motivates renewed efforts to attack the open questions of quantum transport in finite systems. During the next years, groundbreaking developments in the quantum kinetic theory of finite systems are expected. In conclusion, the workshop successfully unified the pictures of quantum theory with theories of systems out of equilibrium. By a remarkable mixture of talks from international outstanding experimentalists and theorists as well as young postdocs, it was possible to achieve a compact overview of the current status of research. According to a common reaction of all participants, the NONNA 08 workshop was extraordinarily fruitful and stimulating for the activities of the different groups. It is a pleasure to thank the Deutsche Forschungsgemeinschaft and the Government of Saxony for their generous support. With no impact on the scientific quality of the workshop it was possible to use only 80 of the available funds. We also owe a debt of gratitude to Claudia Pönisch for the extremely professional and effective organization of the workshop.

3.4 Externally Funded Research and Relations to Industry

3.4.1 DFG Projects

Individual Projects

- *Experimentelle und theoretische Untersuchung von räumlich lokalisierten Anregungen in nichtlinearen Gittern*, Dr. S. Flach
- *Probabilistische Verfahren zur Vorhersage raumzeitlicher Strukturen des Autobahnverkehres*, Prof. H. Kantz

- *Modellierung schneller chaotischer Freiheitsgrade durch stochastische Prozesse*, *Prof. H. Kantz*
- *Directed Transport within Hamiltonian Dynamics: From Theory to Cold Atoms Experiments*, *Dr. S. Flach*
- *Scattering systems with complex dynamics*, Prof. A. Buchleitner
- *Scattering systems with complex dynamics: Quantum Chaos in Optical Microcavities*, *Dr. M. Hentschel*

Schwerpunktprogramme

- *Elektronenstruktur und Magnetismus (SPP 1153)*, Dr. U. Saalmann
- *Development of a wavefunction-based ab-initio-method of group II metals applying (SPP 1145)*, Prof. B. Paulus
- *Deviations from ideal structures in metallic elements and simple intermetallics: Combined experimental and theoretical studies of electron distributions (SPP 1178)*, Prof. B. Paulus
- *Spectral proberties of interacting cold atoms in optical lattices (SPP 1116)*, Prof. A. Buchleitner

Sonderforschungsbereiche und Nachwuchsgruppen

- *Emmy-Noether-Gruppe: Vielteilcheneffekte in mesoskopischen Systemen*, *Dr. M. Hentschel*
- *SFB 463 Seltenerd-Übergangsmetallverbindungen: Struktur, Magnetismus und Transport*, Prof. P. Fulde

3.4.2 BMBF Funding

- *Verbundprojekt Windturbulenzen und deren Bedeutung für die Nutzung von Windenergie: Statistische Analyse und stochastische Modellierung von Windböen*, Prof. H. Kantz

3.4.3 EU Funding

- Marie Curie RTN *Unifying Principles in Non-Equilibrium Pattern Formation*, *Dr. U. Thiele*
- ESF-Research Networking Programme *Arrays of quantum dots and Josephson junctions*, *Dr. S. Flach*
- ESF-Research Networking Programme *Highly Frustrated Magnetism*, *Prof. R. Moessner*

3.4.4 Additional External Funding

- HFSP Research Grant *The driving microtubule forces for cytokinesis checkpoint and early G1 cell spreading*, Prof. Dr. F. Jülicher
- Robert Bosch Stiftung, *Netzwerk Lehrerweiterbildung in Sachsen*, Prof. H. Kantz, U. Gneisse
- Japan Society for the Promotion of Science, *Ultrafast Intense Laser Science*, Dr. A. Becker
- NSERC Canada, *Controlled electron rescattering: sub-A, sub-fs imaging of single molecules*, Dr. A. Becker
- VW-Stiftung, *New algorithms in charged soft and biological matter*, Dr. R. Everaers
- VW-Stiftung, *Neuronal Control of Flight in Drosophila*, Dr. M. Zapotocky
- VW-Stiftung, *Electron spin resonance of Kondo ions in heavy fermion compounds: experiment and theory*, Prof. I. Eremin
- DAAD, *Entanglement and decoherence in open quantum systems* , Prof. J.-M. Rost
- DAAD, *Dynamics of Molecules and Clusters* , Prof. J.-M. Rost
- DAAD, *Dynamik von Mehr- Elektronen-Atomen und Molekülen in intensiven Laserfeldern* , Dr. A. Becker, together with Dr. L. Plaja, Universidad Salamanca
- DAAD, *Spin excitations in the strongly correlated systems with competing orders*, Prof. I. Eremin
- 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
- ANU STAC grant, *Nonlocal Solitons*, Dr. W. Krolikowski

3.4.5 Scholarships

- *Anatole Kenfack*, Reimar-Lüst stipend
- *Grezogorz Urbanik*, Klaus-Tschira-Stiftung
- *Marek Pasciak*, Klaus-Tschira-Stiftung
- *Pawel Wielgus*, Klaus-Tschira-Stiftung
- *Wojciech Miller*, Klaus-Tschira-Stiftung
- *Vardan Apinyan*, Klaus-Tschira-Stiftung
- *Sang Wook Kim*, Emmy Noether Group
- *Jeong-Bo Shim*, Emmy Noether Group
- *Eduardo Mucciolo*, Emmy Noether Group

- *Justin Bois*, HFSP
- *Luis Guillermo Morelli*, HFSP
- *Andrea Cecilia Jimenez Dalmaroni*, HFSP
- *Justin Bois*, Innovation Fonds
- *Nicholas Licata*, Innovation Fonds
- *Ernesto Nicola*, VW Stiftung
- *Nenad Pavin*, VW Stiftung
- *Debasish Chaudhuri*, VW Stiftung
- *Paula Riviere*, Spanish Government

3.4.6 External Cofunding of Workshops and Seminars

2007

- Workshop (50% of budget)
  Mobile Fermions and Bosons on Frustrated Lattices
- Seminar and Workshop (24% of budget)
  Strong Correlations and Angle Resolved Photo Emission Spectroscopy
- Workshop (30% of budget)
  From Complex Systems theory to Clinical Neurology
- Workshop (18% of budget)
  Attosecond Physics
- Summer School (15% of budget)
  Laser-Matter Interaction
- Conference (18% of budget)
  Path Integrals
- Workshop (45% of budget)
  Noise in Life 2007

2008

- Workshop (25% of budget)
  Optical Properties of Coupled Semiconductors and Metallic Nanoparticles
- Workshop and Summer School (16% of budget)
  Time-Resolved X-Ray Dynamics
- Workshop (53% of budget)
  Correlated Electron Systems in High Magnetic Fields
- Workshop (26% of budget)
  Computational Magnetism and Spintronics
- Workshop (84% of budget)
  Nonequilibrium Nanostructures

3.4.7 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 06/07

Stochastic Processes - Dr. B. Lindner, TU Dresden

Quanten-Elektrodynamik - Prof. I. Eremin, TU Braunschweig

Gruppen-Theorie - Prof. I. Eremin, TU Braunschweig

Modern Topics in Quantum Physics - Dr. M. Hentschel, TU Dresden

Sommersemester 07

Biophysik III: Theoretische Biophysik - Prof. F. Jülicher,Dr. S. Grill, TU Dresden

Physik komplexer Netzwerke - Dr. T. Gross, TU Dresden

Computational Physics II - Prof. I. Eremin, TU Braunschweig

Wintersemester 07/08

Nonlinear Dynamics - Prof. H. Kantz, TU Dresden

Theory of Phase Transitions - Prof. I. Eremin, TU Braunschweig

Mathematik - Prof. I. Eremin, TU Braunschweig

Condensed Matter Physics in Nanostructures - Dr. M. Hentschel, TU Dresden

Mathematical Methods - Prof. R. Moessner, Universität Oxford

Sommersemester 08

Biophysik III: Theoretische Biophysik - Prof. F. Jülicher,Dr. S. Grill, TU Dresden

Wintersemester 08/09

Stochastic processes - Prof. H. Kantz, TU Dresden

Laser-matter interaction - Dr. T. Pohl, TU Dresden

3.5.2 Degrees

Habilitations

- *Saalmann, U.: Dynamics of atomic clusters.* Dresden 2007
- *Kenfack, A.: Coherent and incoherent control quantum systems - Quantum mechanics in phase space.* Tours 2008

Dissertations

- *Altmann, E.G.: Intermittent chaos in Hamiltonian dynamical systems.* Wuppertal 2007
- *Becker, N.: Sequence dependent elasticity of DNA.* Dresden 2007
- *Islam, R.: Noble-gas atomic clusters illuminated by intense femtosecond.* Dresden 2007
- *Holstein, D.: Generalized Markov approximations from information theory and consequences for prediction.* Wuppertal 2007
- *Requate, A.: S-matrix analysis of vibrational and alignment effects in intense-field multiphoton ionization of molecules.* Bielefeld 2007
- *Schötz, E.: Dynamics and mechanics of zebrafish embryonic tissues.* Dresden 2007
- *Baier, S.: Numerische Simulationen zur Einfach- und Doppelionisation von H2 in kurzen intensiven Laserpulsen.* Bielefeld 2008
- *Bittig, T.: Morphogenetic signaling in growing tissues.* Dresden 2008
- *Georgescu, I.: Rare gas clusters in intense VUV laser fields.* Dresden 2008
- *Hallerberg, S.: Predictability of extreme events in time series.* Wuppertal 2008
- *Liu, Ivan: Ultracold Rydberg Atoms in Structured and Disordered Environments.* Dresden 2008
- *Peruani, F.: From individual to collective motion of self-propelled particles: the role of particle shape, orientational ordering and clustering.* Berlin 2008
- *Pinto Rengivo, R. A.: Quantum breathers in small networks: Dynamics, tunneling, correlations and application to Josephson cells.* Dresden 2008
- *Rudolf, L.: Population dynamics in theory and experiment: An investigation of species interactions on different scales of complexity.* Potsdam 2008

Diploma

- *Clausznitzer, D.: An analytical two-state model for stochastic hair bundle dynamics.* Dresden, 2007
- *Lenz, F.: Data based modelling of motorway traffic with time-dependent Fokker-Planck equations and their validation.* Osnabrück 2007

- *Wolff, L.: Sub-threshold fluctuations of a conductance-based point neuron under the influence of synaptic shot noise.* Dresden, 2007
- *Garber, A.K.: Finite-size effects on extreme events in models exhibiting self-organized criticality.* Dresden, 2008
- *Ranft, J.: Interfaces in Growing Tissues.* Dresden, 2008
- *Uhden, O.: Interferenz von Wellenpaketen in periodischen Strukturen.* Dresden, 2008

3.5.3 Appointments and Awards

Appointments

- *Prof. A. Buchleitner* accepted the offer for a Professorship at the University of Freiburg
- *Prof. A. Becker* accepted the offer for a JILA fellow jointly with a faculty position at the University of Colorado
- *Dr. M. Zapotocky* accepted the offer for a lecturer at the Adademy of Sciences of the Czech Republic
- *Prof. P. Fulde* accepted the offer for a Distinguished Professorship at the POSTECH (Pohang University of Science and Technology)

Awards

- *Jülicher, F.:* The Raymond and Beverly Sackler International Prize in Biophysics administered by the University of Tel Aviv 2007
- *Fulde, P.:* Verdienstorden des Freistaates Sachsen 2007

3.6 Public Relations

3.6.1 Long Night of Sciences

On June 29, 2007 and July 4, 2008 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, video shows, a physics show, a physics quiz, a science cinema and poster presentations. The resonance was very good with about 3000 visitors counted at each event.

3.6.2 Science in the City Hall

April 23, 2008 - 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 (about 3 per year) called *Wissenschaft im Rathaus*. The following lectures were delivered during the period 2007-2008:

- 8. März 2007, Prof. Dr. Schellnhuber, *Der Klimawandel - Das Problem und seine Lösung*, about 500 participants
- 11. September 2007, Prof. Dr. Feuerbacher, *Landung auf einem Kometen: Die Rosetta-Mission*, about 350 participants
- 23. Oktober 2007, Prof. Dr. Kempermann, *Neue Nervenzellen für erwachsene Gehirne*, about 300 participants

- 23. April 2008, Prof. Dr. Wehner, *Minihirn mit Megaleistung: Der Navigator im Cockpit der Wüstenameisen*, about 350 participants
- 1. Oktober 2008, Prof. Dr. Baumeister, *Schluss mit Altern? Forschung über Anti-Aging, Alzheimer und Co.*, about 300 participants

3.6.3 mpipks School Contact Program

Public lecture with Prof. Beate Paulus (FU Berlin) for Junior Doctors in March 2008

mpipks offers lecturing at high schools on a permanent basis. High school teachers receive updated lists of available lecture topics offered. About twenty lectures are given annually. Together with the Technical University in Chemnitz, we have applied for and obtained funding from the Robert-Bosch foundation within the program *NatWorking*. This program aims at establishing links between academia and high schools. Our joint project consists of a series of three workshops for about 40-60 teachers. We arranged an entertaining and educating mixture of scientific talks. Our schools were extremely well received by the participating teachers.

3.6.4 Dresden-Journalist in Residence Program

The mpipks 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,

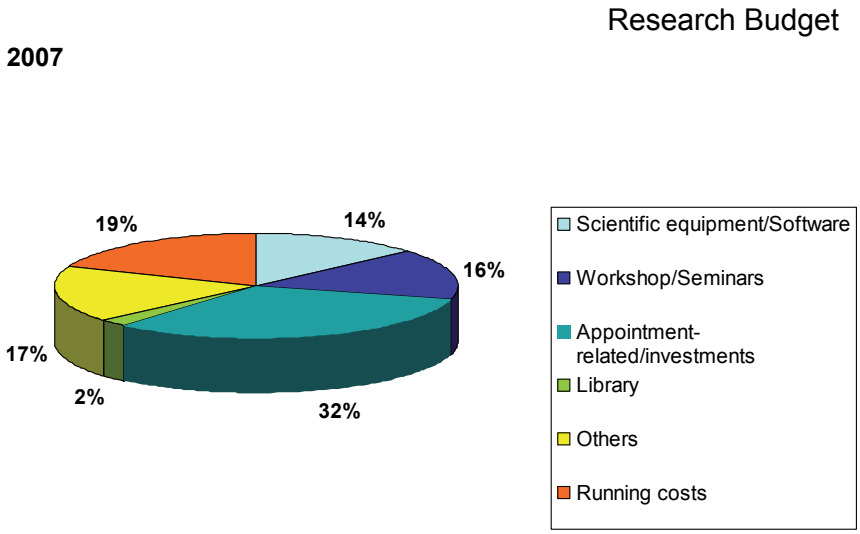
and conduct independent investigations which help to achieve the long-term goals of the fellow.

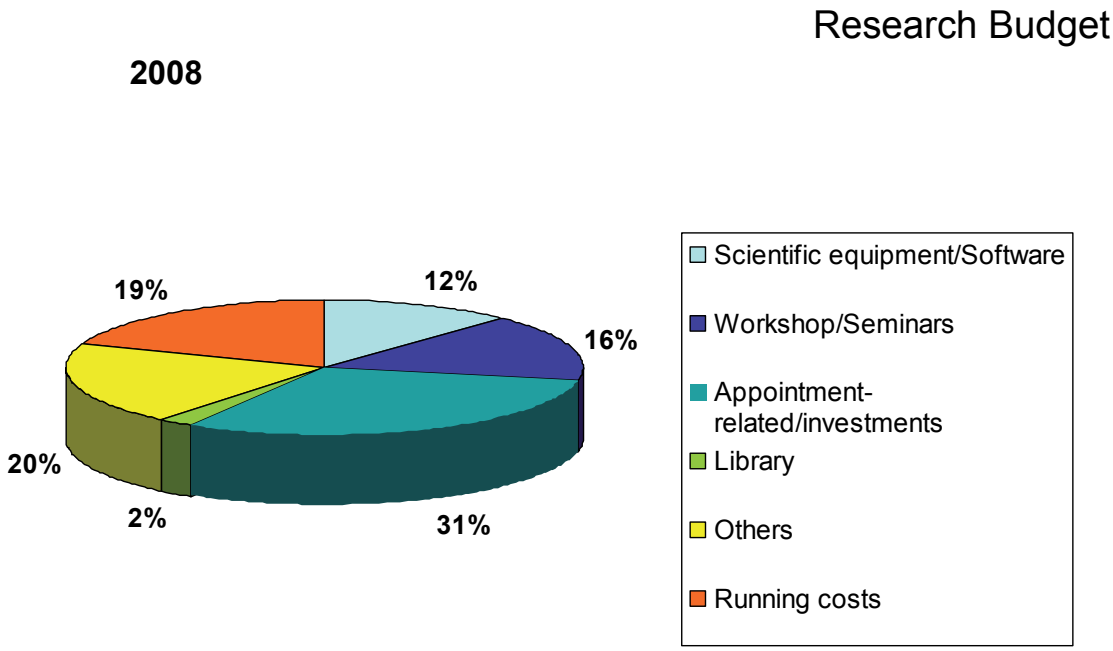
In return scientists at the institutes have a chance to interact closely and over an extended period with a journalist. They learn how their work can be communicated to the public and how to interact with journalists in the first place.

Mrs. *P. Dahl*, a free-lance TV-journalist, was the *Dresden-Journalist in Residence* fellow 2008. We discussed, whether it is possible to communicate the fascination of research and the atmosphere at a research institute to the general public. Among other results she produced an excitingly non-standard 10 minute episode movie about work and scientists at mpi**pks**. The *Dresden-Journalist in Residence* fellow 2009 is Mr. *M. Anhäuser*. He is a print journalist with ambitions towards new forms of publication, e.g., in the internet. His projects planned include a Lab-Diary (MPI-CBG) and a report about Path of a Substance (at MPI-CPFS).

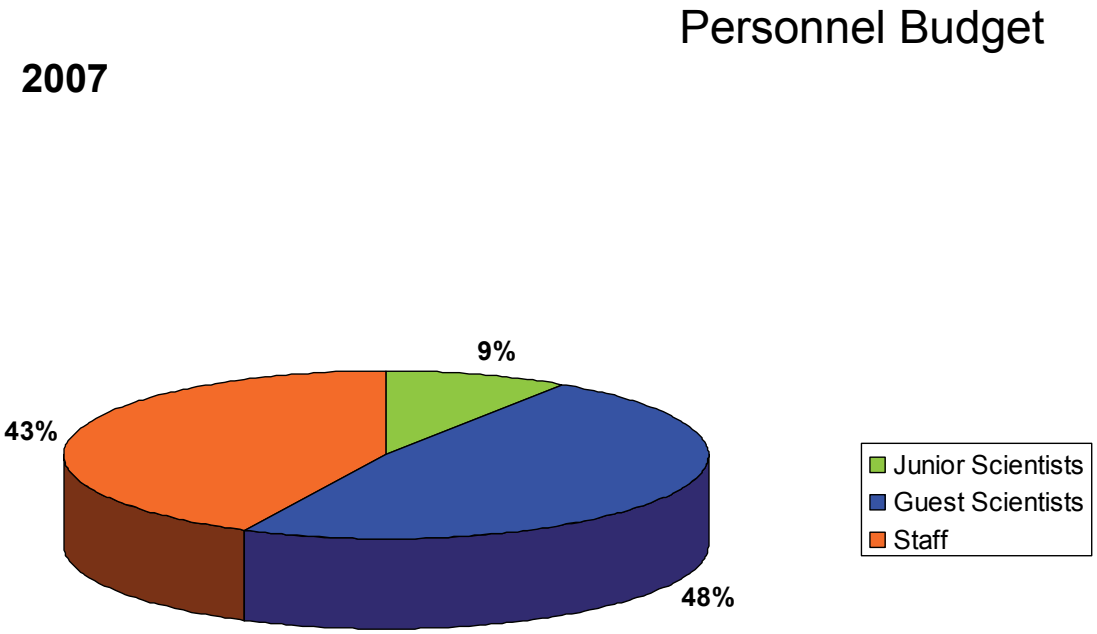
3.7 Budget of the Institute

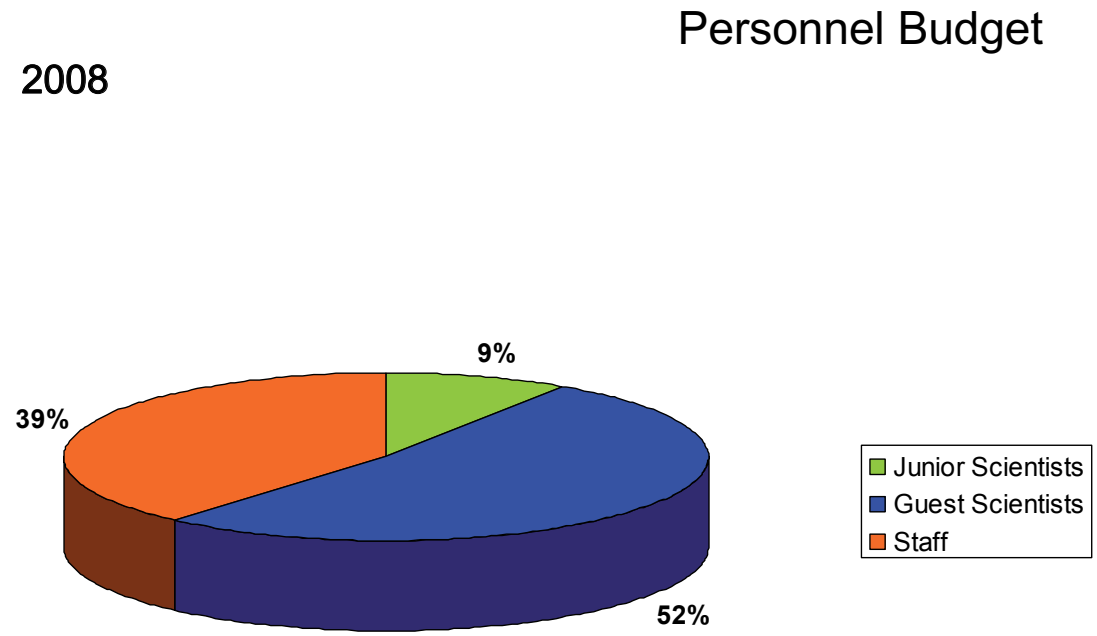
The following figures break the budget down according to costs for research and personnel, respectively for the two years 2007 and 2008.





Research budgets during the past two years





Budgets for personnel

3.8 Equipment and Premises

3.8.1 Computer Facilities

Computing facilities

Since many of our scientists are doing extensive numerical calculations, the main focus of our computer requirements in our institute is on the computational throughput, whereas the request for graphics is still rather moderate on average. This implies that most offices are equipped with X-Terminals (Thin Clients) while nearly all the compute servers are located in server rooms. At present the institute has approximately 360 computers with a total of 2400 CPU cores.

Our computers offer from one to 128 CPU cores and a maximum of 1 Terabyte of main memory and fifty Terabytes of local disk space. We use both Gigabit and Fast Ethernet as a local area network interconnect. By the end of 2008 about 92 % of the computing power available was based on Linux systems and 8 % 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 40 laptops for our scientists in order to give 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 that 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 which we share with our neighboring institute.

The computer department is run by four employees with their respective main tasks being Unix and networks, web and windows, hardware and general user support. In addition to those four people we employ two trainees and two students of the Berufsakademie Dresden. Smaller to medium programming tasks are done by our staff and six students who are working part-time in the computer department. Larger 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, running mainly on AMD Opteron based hardware. The now more or less

outdated operating system Tru64 Unix which has been the platform for running our most important services is being replaced by Linux.

History

In 1996 the institute occupied three buildings in Dresden and an outpost in Stuttgart. Before we moved to our new building, additional office in Dresden was needed. This implied that the interconnection of the offices and running the distributed infrastructure made up the biggest part of the work of the two employees in the computer department at that time. Moving to the new building in 1997 implied a boost in local network bandwidth from shared ethernet to ATM and an increased bandwidth of our internet connection from 128 kBit/s to 2 MBit/s. While during the first years nearly all the computing power was covered by workstations, starting from 2000 we switched to small and medium sized servers. 2002 was the first year to see an inhomogeneous Unix cluster in our institute when we introduced Linux on standard PC systems. By the end of 2002 we even decided to give away our 16 processor server in favor of a Linux based PC cluster that delivers several times the CPU performance of that server. 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. The following table shows the development of the computer resources at our institute over time.

year	computers	GFlops	main memory (GB)	disk space (TB)
1996	33	15	13	0.5
1998	66	60	60	2.0
2000	95	140	310	8
2002	162	400	590	22
2004	327	2100	2600	90
2006	345	5400	5500	190
2008	360	11600	15000	510

3.8.2 Library

The library is a special library offering services firstly to scientists working at the institute. Scientists from outside the institute are also welcome and may use the library. The library is permanently accessible for members of the institute including guests and provides the scientists with media and scientific information in many forms.

The annual growth rate in 2007/2008 of the library holdings increased in line with the budget and our holdings list consists of 4300 monographs, 15.000 bound journal volumes and 60 scientific journals subscriptions, which you can find in the online catalogue. Our users have access to more than 30.000 online journals, as well as numerous literature and

factual databases, online encyclopedias, dictionaries, the Virtual Max Planck Library, international catalogues etc.

Books or references, which are not available in the library can be ordered through document delivery (2007/2008 - 877 documents). The scientists receive articles within 24 hours as email files (this service is at the moment strongly affected by the new German law on intellectual property and copyright, Urheberrecht).

With an automatic lending system all users can borrow literature themselves 24 hours a day. In February 2007 we switched to a new library catalog and booking system - ALEPH from Ex Libris. For copying printed material there is a new scanner available especially for books and journals.

The reading room in the new D-wing of the institute. Copies of the most important books and journals for each research group are available there for easy access.

In the library steering committee scientists representing the departments and research groups of the mpi**pks** discuss new developments in quarterly meetings.

Since 2006 there is a reading room in the new D-wing of the institute. Copies of the most important books and journals for each research group are available there for easy access. The room invites to discussions and is very well accepted.

The library supports the electronic document server (eDoc) of the Max Planck Society. Via eDoc scientists can make their work openly accessible online, but it is also used as a documentation system for our reporting tasks (in particular, for the production of the yearbook). Meta-data, full texts, or links to full texts in other preprint servers of 2000 documents have been so far registered in the eDoc system. The mpi**pks** is also a pilot institute contributing to the development of a new institutional repository system called eSciDoc within the MPDL (Max Planck Digital Library). The eSciDoc system will provide a sustainable infrastructure for scientific information, communication and dissemination of research results via Open Access with persistent identifiers to make documents citable.

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 the fully equipped communal kitchen and two meeting rooms, one of them with a small library, the other one with 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 disabled 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 statutes of the Max Planck Society the mpi**pks** 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 biannual 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:

Bensimon, D. Professor Dr.	Laboratoire de Physique Statistique École Normale Supérieure 24, rue Lhomond, 75231 Paris cedex 05 Frankreich
Efetov, K. Professor Dr.	Institut für Theoretische Physik III Ruhr-Universität Bochum Universitätsstraße 150, 44801 Bochum
Frey, E. Professor Dr.	Ludwig-Maximilians-Universität Theresienstraße 37 80333 München
Haake, F. Professor Dr.	Fachbereich Physik Universität Duisburg-Essen Universitätsstraße 2, 45141 Essen
Heller, E. J. Professor Dr.	Lyman Laboratory of Physics Harvard University Cambridge, MA 02138 USA

Ketzmerick, R. Professor Dr.	Technische Universität Dresden Helmholtzstr. 10 01069 Dresden
Lhuillier, C., J. C. Professor Dr.	Physique Theoretique des Liquides Université Pierre & Marie Curie 4, Place Jussieu, 75252 Paris Cedex 05 Frankreich
Manninen, M., Professor Dr.	Nanoscience Center University of Jyväskylä, P. O. Box 35 (YFL) FIN-40014 Jyväskylä Finnland
Pietronero, L. Professor Dr.	Dipartimento di Fisica Universita degli Studi di Roma La Sapienza Piazzale Aldo Moro 2, 00185 Roma Italien
Starace, A. Professor Dr.	Department of Physics and Astronomy The University of Nebraska 116 Brace Laboratory Lincoln NE 68588-0111 USA
Stark, J. Professor Dr.	Department of Mathematics University College London Gower Street, WC1E 6BT, London Grossbritannien
Sznajd, J. Professor Dr.	Institute of Low Temperature and Structure Research Polish Academy of Sciences ul. Okolna 2, 50-422 Wroclaw Polen

3.9.2 Board of Trustees

In accord with the statutes 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 mpipks 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
Junker, F. Dr.-Ing.	Mitglied des Vorstandes König & Bauer AG Friedrich-König-Straße 4, 97080 Würzburg
Kokenge, H. Professor	Rektor der Technischen Universität Dresden Mommsenstraße 13, 01069 Dresden
Kretschmer, M. Dipl.-Ing., MdB	Mitglied des Deutschen Bundestages Wahlkreisbüro Dresdener Straße 6, 02826 Görlitz
Laubschat , C. Professor, Dr.	Prodekan der Fachrichtung Physik Fakultät für Mathematik und Naturwissenschaften Technische Universität Dresden Helmholtzstraße 10, 01069 Dresden
Orosz, H.	Oberbürgermeisterin der Landeshauptstadt Dresden, Dr.-Külz-Ring 19, 01067 Dresden
Sauerbrey, R. Professor, Dr.	Wissenschaftlicher Direktor des Forschungszentrums Dresden-Rossendorf e.V. Bautzner Landstraße 128, 01328 Dresden

Schmidt, F. Dr.-Ing.	Staatssekretär a.D. Birkenstraße 18, 01328 Dresden
Stange, E.-M. Dr.	Sächsische Staatsministerin für Wissenschaft und Kunst Wigardstraße 17, 01097 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 2008)

1. **mpipks positions** — **47**
   - Scientific personnel 17
     Scientific members *3*
     Research staff (including four junior research groups) *14*
   - Technical staff 6
   - Administration and infrastructure staff 24

2. **Externally funded research staff** — **1**

3. **PhD students** — **67**
   - PhD students with internal supervision 50
     German PhD students *28*
     Foreign PhD students *22*
   - PhD students with external supervision[a] 17
     PhD students with external funding *3*
     IMPRS PhD students with external supervision *14*

4. **Guest scientists** — **77**
   - German guest scientists 7
   - Foreign guest scientists 70

[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

2007

Aolita, L., L. Davidovich, K. Kim and H. Häffner: Universal quantum computation in decoherence-free subspaces with hot trapped ions. Physical Review A **75**, 052337 (2007).

Aolita, L., K. Kim, J. Benhelm, C.F. Roos and H. Häffner: High-fidelity ion-trap quantum computing with hyperfine clock states. Physical Review A **76**, 040303 (2007).

Baier, S., C. Ruiz, L. Plaja and A. Becker: Single and double ionization of the hydrogen molecule in an intense few-cycle laser pulse. Laser Physics **17**, 358 - 367 (2007).

Becker, A., C. Ruiz, S. Baier and L. Plaja: Few-body dynamics in ultrashort laser pulses. Journal of Physics Conference Series **88**, 012045 (2007).

Bertulani, C.A. and M.S. Hussein: Geometry of Borromean halo nuclei. Physical Review C **76**, 051602 (2007).

Ciappina, M.F.: Fully differential cross sections for ion-atom impact ionization in the presence of a laser field. Journal of Physics B **40**, 4155 - 4163 (2007).

Ciappina, M.F., A. Becker and and A. Jaro-Becker: Multislit interference patterns in high-order harmonic generation in C_{60}. Physical Review A **76**, 063406 (2007).

Ciappina, M.F., C.C. Chiril and M. Lein: Influence of Coulomb continuum wave functions in the description of high-order harmonic generation with H_2O. Physical Review A **75**, 043405 (2007).

Czasch, A., M. Schöffler, M. Hattass, S. Schössler, T. Jahnke, T. Weber, A. Staudte, J. Titze, C. Wimmer, S. Kammer, M. Weckenbrock, S. Voss, R.E. Grisenti, O. Jagutzki, L.P.H. Schmidt, H. Schmidt-Böcking, R. Dörner, J.-M. Rost, T. Schneider, C.-N. Liu, I. Bray, A.S. Kheifets and K. Bartschat: Comment on "Partial photoionization cross sections and angular distributions for double excitation of helium up to the N=13 threshold". Physical Review Letters **98**, 109302 (2007),

El-Khozondar, H.J., R. J. El-Khozondar, M.M. Shabat and A.W. Koch: Stress effect on optical nonlinear sensor. Journal of Optical Communications **28**, 175 - 179 (2007).

El-Khozondar, H.J., M.M. Shabat, G. Abu Tair and M. Abadla: Thermal-stress effects on nonlinear thin film waveguide sensors. Physics and Chemistry of Solid State **8**, 260 - 264 (2007).

Georgescu, I., U. Saalmann and J.M. Rost: Attosecond resolved charging of ions in a rare-gas cluster. Physical Review Letters **99**, 183002 (2007).

Georgescu, I., U. Saalmann and J.M. Rost: Clusters under strong VUV pulses: A quantum-classical hybrid description incorporating plasma effects. Physical Review A **76**, 043203 (2007).

Hamada, M.S., A.H. El-Astal and M.M. Shabat: Non-linear surface at a single interface of semimagnetic semiconductor - left handed materials (LHM). International Journal of Microwave and Optical Technology **2**, 112 - 118 (2007).

Hamada, M.S., A.H. El-Astal and M.M. Shabat: Non-linear surface waves in a left handed-magnetized ferrite structure. Journal of Microwaves and Optoelectronics **6**, 364 - 372 (2007).

Hamada, M.S., A.H. El-Astal and M.M. Shabat: Nonlinear te surface waves in a photosensitive semiconductor film bounded by a superconductor cover. International Journal of Modern Physics B **21**, 1817 - 1825 (2007).

He, F., C. Ruiz and A. Becker: Absorbing boundaries in numerical solutions of the time-dependent Schrödinger equation on a grid using exterior complex scaling. Physical Review A **75**, 053407 (2007).

He, F., C. Ruiz and A. Becker: Control of electron excitation and localization in the dissociation of $H_2{}^+$ and its isotopes using two sequential ultrashort laser pulses. Physical Review Letters **99**, 083002 (2007).

He, F., C. Ruiz and A. Becker: Single attosecond pulse generation with intense mid-infrared elliptically polarized laser pulses. Optics Letters **32**, 3224 - 3226 (2007).

Jaro-Becker, A., A. Becker and F.H.M. Faisal: Single-active-electron ionization of C_{60} in intense laser pulses to high charge states. Journal of Chemical Physics **126**, 124310 (2007).

Khalil, H.M., M. M. Shabat, S. A. Taya and M.M. Abadla: Nonlinear optical waveguide structure for sensor application: TM case. International Journal of Modern Physics B **21**, 5075 - 5089 (2007).

Laarmann, T., I. Shchatsinin, A. Stalmashonak, M. Boyle, N. Zhavoronkov, J. Handt, R. Schmidt, C.P. Schulz and I.V. Hertel: Control of giant breathing motion in C_{60} with temporally shaped laser pulses. Physical Review Letters **98**, 058302 (2007).

Madroñero, J., L. Hilico, B. Grémaud, D. Delande and A. Buchleitner: The driven three body Coulomb problem. Mathematical Structures in Computer Science **17**, 225 - 246 (2007).

Mikhailov, A.I., A.V. Nefiodov and G. Plunien: Single photoeffect on helium-like ions in the nonrelativistic region. Physics Letters A **368**, 391 - 395 (2007).

Mousa, H.M. and M.M. Shabat: Nonlinear te surface waves in a left-handed material and super lattices wave-guide structure. International Journal of Modern Physics B **21**, 895 - 906 (2007).

Mousa, H.M. and M.M. Shabat: Stability of nonlinear te surface waves along the boundary of linear gyrodielectric media. International Journal of Modern Physics B **21**, 4487 - 4493 (2007).

Roman, J. S., I.J. Sola, C. Mendez, C. Ruiz, J. A. Perez-Hernandez, D. Delgado , L. Plaja and L. Roso: Time domain effects during spontaneous self-channelling of light in air below the collapse threshold. Journal of Physics B **40**, 4433 - 4442 (2007).

San Roman, J., I.J. Sola, C. Mendez, C. Ruiz, J.A. Perez-Hernandez, D. Delgado, L. Plaja and L. Roso: Time domain effects during spontaneous self-channelling of light in air below the collapse threshold. Journal of Physics B **40**, 4433 - 4442 (2007).

Scully, SWJ., E.D. Emmons, M.F. Gharaibeh, R.A. Phaneuf, A.L.D. Kilcoyne, A.S. Schlachter, S. Schippers, A. Müller, H.S. Chakraborty, M.E. Madjet and J.M. Rost: Comment on "Photoexcitation of a volume plasmon in C_{60} ions". Physical Review Letterrs **98**, 179602 (2007).

Shabat, M.M., S. A. Mansour, M.S. Hamada and S.S. Yassin: Left-handed magnetostatic surface waves. In: MSMW'07: Sixth International Kharkov Symposium on Physics and Engineering of Microwaves, Millimeter and Submillimeter Waves. New York : IEEE, 2007. Vol. 1-2, S. 776 - 778.

Shatokhin, V., T. Wellens, B. Grémaud and A. Buchleitner: Spectrum of coherently backscattered light from two atoms. Physical Review A **76**, 043832 (2007).

Shatokhin, V., T. Wellens, C.A. Müller: Coherent backscattering of light from saturated atoms. European Physical Journal Special Topics **151**, 51 - 57 (2007).

Staudte, A., C. Ruiz, M. Schöffler, S. Schössler, D. Zeidler, T. Weber, M. Meckel, D. M. Villeneuve, P.B. Corkum, A. Becker and R. Dörner: Binary and recoil collisions in strong field double ionization of helium. Physical Review Letters **99**, 263002 (2007).

Théberge, F., J. Filion, N. Aközbek, Y. Chen, A. Becker and S.L. Chin: Self-stabilization of third-harmonic pulse during two-color filamentation in gases. Applied Physics B **87**, 207 - 210 (2007).

Vicencio, R.A., S. Flach, M.I. Molina and Y.S. Kivshar: Discrete surface solitons in two-dimensional anisotropic photonic lattices. Physics Letters A **364**, 274 - 276 (2007).

Vicencio, R.A., E. Smirnov, C.E. Rüter, D. Kip and M. Stepi: Saturable discrete vector solitons in one-dimensional photonic lattices. Physical Review A **76**, 033816 (2007).

2008

Al-Sahhar, Z.I. and M.M. Shabat: Floquet scattering through a heterostructure in a time-periodic potential. Journal of Applied Sciences **8**, 1325 - 1328 (2008).

Baier, S., A. Becker and L. Plaja: Nonsequential double ionization of the hydrogen molecule: Dependence on molecular alignment. Physical Review A **78**, 013409 (2008).

Bergé, L. and S. Skupin: Sub-2fs pulses generated by self-channeling in the deep ultraviolet. Optics Letters **33**, 750 - 752 (2008).

Bergé, L., S. Skupin and G. Steinmeyer: Temporal self-restoration of compressed optical filaments. Physical Review Letters **101**, 213901 (2008).

Chakraborty, H.S., M.E. Madjet, J.M. Rost and S.T. Manson: Dynamical effects of confinement on atomic valence photoionization in $Mg@C_{60}$. Physical Review A **78**, 013201 (2008).

Chin, S.L., W.Liu, F. Théberge, Q. Luo, S.A. Hosseini, V.P. Kandidov, O.G. Kosareva, N. Aközbek, A. Becker and H. Schröder: Some fundamental concepts of femtosecond laser filamentation. In : Progress in ultrafast intense laser science III. Ed. by K. Yamanouchi [u.a.] Berlin : Springer, 2008. S. 243 - 264.

Ciappina, M.F. and L.B. Madsen: Laser-assisted ion-atom collisions: Plateau, cutoff, and multiphoton peaks. Physical Review A **77**, 023412 (2008).

El-Astal, A.H., M.S. Hamada and M.M. Shabat: Characteristics of electromagnetic and magnetostatic surface waves in metal-dielectric-ferrite-left handed waveguide layered structure. Functional Materials **15**, 102 - 108 (2008).

El-Khozondor, H.J., R.J. El-Khonzondar and M.M. Shabat: Double-Negative Metamaterial Optical waveguide Behavior Subjected to Stress. The Islamic University Journal **16**, 9 - 20 (2008).

Emmanouilidou, A., P.J. Wang and J.M. Rost: Initial state dependence in multielectron threshold ionization of atoms. Physical Review Letters **100**, 063002 (2008).

Feugeas, J.L., P. Nicolai, X. Ribeyre, G. Schurtz, V. Tikhonchuk and M. Grech: Modeling of two-dimensional effects in hot spot relaxation in laser-produced plasmas. Physics of Plasmas **15**, 062701 (2008).

Georgescu, I., U. Saalmann, C. Siedschlag and J.M. Rost: Theoretical description of rare-gas clusters under intense laser pulses. In: Progress in ultrafast intense laser science.III. Ed. by K. Yamanouchi [u.a.]. Berlin : Springer, 2008. S. 149 - 169.

Gilary, I., Y. Sajeev, M.F. Ciappina, A. Croy, C.M. Goletz, S. Klaiman, M. Šindelka, M. Winter, W. Wustmann and N. Moiseyev: Suppression of Photoionization by a Static Field. Physical Review Letters **101**, 163002 (2008).

Gozman, M., I. Polishchuk and A. Burin: Light propagation in linear arrays of spherical particles. Physics Letters A **372**, 5250 - 5253 (2008).

He, F., A. Becker and U. Thumm: Strong-field modulated diffraction effects in the correlated electron-nuclear motion in dissociating $H_2{}^+$. Physical Review Letters **101**, 213002 (2008).

Hoang, A.T.: Optical properties of diluted magnetic semiconductors in coherent potential approximation. Physica B **403**, 1803 - 1807 (2008).

Madjet, M.E., H.S. Chakraborty, J.M. Rost and S.T. Manson: Photoionization of C_{60}: a model study. Journal of Physics B **41**, 105101 (2008).

Mikaberidze, A., U. Saalmann and J.M. Rost: Energy absorption of xenon clusters in helium nanodroplets under strong laser pulses. Physical Review A **77**, 041201 (2008).

Miroshnichenko, A.E., S. Flach, A. V. Gorbach, B. S. Luk'yanchuk, Y.S. Kivshar and M. I. Tribelsky: Fano resonances: A discovery that was not made 100 years ago. Optics and Photonics News **19**, 48 (2008).

Rivière, P., C. Ruiz and J.M. Rost: Attosecond light-pulse-induced photoassociation. Physical Review A **77**, 033421 (2008).

Roden, J., A. Eisfeld and J.S. Briggs: The J- and H-bands of dye aggregate spectra: Analysis of the coherent exciton scattering (CES) approximation. Chemical Physics **352**, 258 - 266 (2008).

Ruiz, C. and A. Becker: Time-resolved mapping of correlated electron emission from helium atom in an intense laser pulse. New Journal of Physics **10**, 025020 (2008).

Saalmann, U., I. Georgescu and J.M. Rost: Tracing non-equilibrium plasma dynamics on the attosecond timescale in small clusters. New Journal of Physics **10**, 025014 (2008).

Saalmann, U. and J.M. Rost: Rescattering for extended atomic systems. Physical Review Letters **100**, 133006 (2008).

Singh, K.P., A. Kenfack and J.M. Rost: Femtosecond photodissociation of molecules facilitated by noise. Physical Review A **77**, 022707 (2008).

Skupin, S., M. Grech and W. Krolikowski: Rotating soliton solutions in nonlocal nonlinear media. Optics Express **16**, 9118 - 9131 (2008).

Sola, I.J., V. Collados, L. Plaja, C. Méndez, J. San Román, C. Ruiz, I. Arias, A. Villamarín, J. Atencia, M. Quintanilla and L. Roso: High power vortex generation with volume phase holograms and non-linear experiments in gases. Applied Physics B **91**, 115 - 118 (2008).

Sumour, M.A., A.H. El-Astal, M.M. Shabat and M.A. Radwan: Urban segregation with cheap and expensive residences. International Journal of Modern Physics C **19**, 637 - 645 (2008).

Taya, S.A., M.M. Shabat, H.M. Khalil and D.S. Jäger: Theoretical analysis of TM nonlinear asymmetrical waveguide optical sensors. Sensors and Actuators A **147**, 137–141 (2008).

Tribelsky, M.I., S. Flach, A.E. Miroshnichenko, A.V. Gorbach and Y.S. Kivshar: Light scattering by a finite obstacle and fano resonances. Physical Review Letters **100**, 043903 (2008).

4.2 Ultracold Matter

2007

Akbari, A., D. Bodea and A. Langari: Dielectric susceptibility and heat capacity of ultra-cold glasses in magnetic fields. Journal of Physics Condensed Matter **19**, 466105 (2007).

Ates, C., T. Pohl, T. Pattard and J.M. Rost: Antiblockade in Rydberg excitation of an ultracold lattice gas. Physical Review Letters **98**, 023002 (2007).

Ates, C., T. Pohl, T. Pattard and J.M. Rost: Many-body theory of excitation dynamics in an ultracold Rydberg gas. Physical Review A **76**, 013413 (2007).

Bhattacherjee, A.B.: Bogoliubov spectrum of a cigar-shaped Fermi superfluid in an optical lattice at the BEC-BCS crossover. Journal of Physics B **40**, 4453 - 4462 (2007).

Brand, J. and A.R. Kolovsky: Emergence of superfluid transport in a dynamical system of ultra-cold atoms. European Physical Journal D **41**, 331 - 336 (2007).

Chhajlany, R.W., P. Tomczak and A. Wójcik: Topological estimator of block entanglement for Heisenberg antiferromagnets. Physical Review Letters **99**, 167204 (2007).

Dudarev, A.M., M.G. Raizen and Q. Niu: Quantum many-body culling: Production of a definite number of ground-state atoms in a Bose-Einstein condensate. Physical Review Letters **98**, 063001 (2007).

Haque, M. and H.T.C. Stoof: Trapped fermionic clouds distorted from the trap shape due to many-body effects. Physical Review Letters **98**, 260406 (2007).

Killian, T.C., T. Pattard, T. Pohl and J.M. Rost: Ultracold neutral plasmas. Physics Reports **449**, 77 - 130 (2007).

Komineas, S.: Vortex rings and solitary waves in trapped Bose-Einstein condensates. European Physical Journal Special Topics **147**, 133 - 152 (2007).

Komineas, S. and N.R. Cooper: Vortex lattices in Bose-Einstein condensates with dipolar interactions beyond the weak-interaction limit. Physical Review A **75**, 023623 (2007).

Kulič, M.L.: π-superconducting quantum interference device from ultracold fermionic atomic gases. Physical Review A **76**, 053625 (2007).

Morawetz, K., M. Männel and M. Schreiber: Phase diagram for interacting Bose gases. Physical Review B **76**, 075116 (2007).

Nguenang, J.P., R. Pinto and S. Flach: Quantum q-breathers in a finite Bose-Hubbard chain: The case of two interacting bosons. Physical Review B **75**, 214303 (2007).

Radu, T., H. Wilhelm, V. Yushankhhai, D. Kovrizhin, R. Coldea, Z. Tylczynski, T. Lühmann and F. Steglich: Comment on "Bose-Einstein condensation of magnons in Cs_2CuCl_4". Physical Review Letters **98**, 039702 (2007).

Vicencio, R.A., J. Brand and S. Flach: Fano blockade by a Bose-Einstein condensate in an optical lattice. Physical Review Letters **98**, 184102 (2007).

2008

Aolita, L., A. Buchleitner and F. Mintert: Scalable method to estimate experimentally the entanglement of multipartite systems. Physical Review A **78**, 022308 (2008).

Ates, C., A. Eisfeld and J.M. Rost: Motion of Rydberg atoms induced by resonant dipole-dipole interactions. New Journal of Physics **10**, 045030 (2008).

Bandopadhyay, S. and D. Cohen: Renormalization of the dephasing by zero point fluctuations. Physical Review B **77**, 155438 (2008).

Bhattacherjee, A.B.: Coherence properties of a Bose-Einstein condensate in an optical superlattice. European Physical Journal D **46**, 499 - 506 (2008).

Bhattacherjee, A.B.: Faraday instability in a two-component Bose-Einstein condensate. Physica Scripta **78**, 045009 (2008).

Bhattacherjee, A.B.: Superfluid properties of a Bose-Einstein condensate in an optical lattice confined in a cavity. Optics Communications **281**, 3004 - 3012 (2008).

Bhattacherjee, A.B. and M. Pietrzyk: Transport behaviour of a Bose Einstein condensate in a bichromatic optical lattice. Central European Journal of Physics **6**, 26 - 32 (2008).

Chung, M.-C. and A.B. Bhattacherjee: Dynamical structure factor and spin-density separation for a weakly interacting two-component Bose gas. Physical Review Letters **101**, 070402 (2008).

Chung, M.-C. and A.R. Kolovsky: Effect of the lattice alignment on Bloch oscillations of a Bose-Einstein condensate in a square optical lattice. European Physical Journal D **47**, 421 - 425 (2008).

Jurisch, A. and J.M. Rost: Trapping cold atoms by quantum reflection. Physical Review A **77**, 043603 (2008).

Kenfack, A., J.B. Gong and A.K. Pattanayak: Controlling the ratchet effect for cold atoms. Physical Review Letters **100**, 044104 (2008).

Li, W., M. Haque and S. Komineas: Vortex dipole in a trapped two-dimensional Bose-Einstein condensate. Physical Review A **77**, 053610 (2008).

Männel, M., K. Morawetz, M. Schreiber and P. Lipavský: Phase diagram and binding energy of interacting Bose gases. Physical Review B **78**, 054508 (2008).

Morales-Molina, L. and S. Flach: Resonant ratcheting of a Bose-Einstein condensate. New Journal of Physics **10**, 013008 (2008).

Morawetz, K., N.H. March and R.H. Squire: The chemical potential for the inhomogeneous electron liquid in terms of its kinetic and potential parts with special consideration of the surface potential step and BCS-BEC crossover. Physics Letters A **372**, 1707 - 1711 (2008).

Schmidt, K.P., J. Dorier and A.M. Läuchli: Solids and supersolids of three-body interacting polar molecules on an optical lattice. Physical Review Letters **101**, 150405 (2008).

Sen, A., P. Dutt, K. Damle and R. Moessner: Variational wave-function study of the triangular lattice supersolid. Physical Review Letters **100**, 147204 (2008).

Wüster, S.: Phonon background versus analog Hawking radiation in Bose-Einstein condensates. Physical Review A **78**, 021601 (2008).

Zozulya, O.S., M. Haque and K. Schoutens: Particle partitioning entanglement in itinerant many-particle systems. Physical Review A **78**, 042326 (2008).

4.3 Semiclassics and Chaos in Quantum Systems

2007

Beims, M.W., C. Manchein and J.M. Rost: Origin of chaos in soft interactions and signatures of nonergodicity. Physical Review E **76**, 056203 (2007).

Budiyono, A., T. Kato, K. Takatsuka and K. Nakamura: Enhancement of non-escape probability in open chaotic system due to quantum localization induced by periodic orbits. Physics Letters A **367**, 331 - 334 (2007).

de Carvalho, J.X., M. S. Hussein, M.P. Pato and A.J. Sargeant: Symmetry-breaking study with deformed ensembles. Physical Review E **76**, 066212 (2007).

Emmanouilidou, A. and J.M. Rost: Attosecond-time-scale multielectron collisions in the Coulomb four-body problem: Traces in classical probability densities. Physical Review A **75**, 022712 (2007).

Fischer, E., G. Rudolph and M. Schmidt: A lattice gauge model of singular Marsden-Weinstein reduction - Part I. Kinematics. Journal of Geometry and Physics **57**, 1193-1213 (2007).

Garcia-Mata, I., A.R.R. Carvalho, F. Mintert and A. Buchleitner: Entanglement screening by non-linear resonances. Physical Review Letters **98**, 120504 (2007).

Gorin, T., D.F. Martinez and H. Schomerus: Long-time signatures of short-time dynamics in decaying quantum-chaotic systems. Physical Review E **75**, 016217 (2007).

Kenfack, A., S.M. Sweetnam and A.K. Pattanayak: Bifurcations and sudden current change in ensembles of classically chaotic ratchets. Physical Review E **75**, 056215 (2007).

Kwon, T.Y., J. Wiersig and M. Hentschel: Directional light output from a circular microdisk laser. In: ICTON 2007: 9th International Conference on Transparent Optical Networks. New York: IEEE, Vol. 4, 2007, S. 194 - 196.

Lakshminarayan, A.: Modular multiplication operator and quantized baker's maps. Physical Review A 76, 042330 (2007).

Li, W., P.J. Song, J.B. Liu and X.X. Yang: Eigenstates and spectrum properties of a resonant field in a Kerr-like medium. Journal of Physics B **40**, 1957 - 1966 (2007).

Molina, R.A., J. Retamosa, L. Muñoz, A. Relaño and E. Faleiro: Power spectrum of nuclear spectra with missing levels and mixed symmetries. Physics Letters B **644**, 25 - 32 (2007).

Ogura, T., M. Miyamoto, A. Budiyono and K. Nakamura: Quantum mechanical analysis of fractal conductance fluctuations: a picture using self-similar periodic orbits. Journal of Physics Condensed Matter **19**, 092002 (2007).

Tanaka, T., M. Hentschel, T. Fukushima and T. Harayama: Classical phase space revealed by coherent light. Physical Review Letters **98**, 033902 (2007).

Tomsovic, S. and A. Lakshminarayan: Fluctuations of finite-time stability exponents in the standard map and the detection of small islands. Physical Review E **76**, 036207 (2007).

2008

Adamashvili, G.T.: Surface optical solitons of self-induced transparency in indefinite media. Physics Letters A **373**, 156 - 159 (2008).

Adamashvili, G.T., A. Knorr and C. Weber: Optical solitons in semiconductor quantum dot waveguides. European Physical Journal D **47**, 113 - 117 (2008).

Adhikari, S.K. and M.S. Hussein: Semiclassical scattering in two dimensions. American Journal of Physics **76**, 1108 - 1113 (2008).

Altmann, E.G., G. Del Magno and M. Hentschel: Non-Hamiltonian dynamics in optical microcavities resulting from wave-inspired corrections to geometric optics. epl **84**, 10008 (2008).

Brand, J., S. Flach, V. Fleurov, L.S. Schulman and D. Tolkunov: Localization by entanglement. epl **83**, 40002 (2008).

He, F. and A. Becker: Coherent control of electron localization in a dissociating hydrogen molecular ion. Journal of Physics B **41**, 074017 (2008).

He, F., C. Ruiz and A. Becker: Coherent control of electron wave packets in dissociating $H_2{}^+$. Journal of Physics B **41**, 081003 (2008).

Heller, E.J., L. Kaplan and F. Pollmann: Inflationary dynamics for matrix eigenvalue problems. Proceedings of the National Academy of Sciences of the United States of America **105**, 7631 - 7635 (2008).

Hussein, M.S., W.B. Li and S. Wüster: Canonical quantum potential scattering theory. Journal of Physics A **41**, 475207 (2007).

Khomeriki, R., A. Ugulava and L. Chotorlishvili: Self-chaotization in coupled opticcal waveguides. Journal of the Optical Society of America B **25**, 1265 - 1269 (2008).

Lee, S.-Y., S. Rim, J.-W. Ryu, T.-Y. Kwon, M. Choi and C.-M. Kim: Ray and wave dynamical properties of a spiral-shaped dielectric microcavity. Journal of Physics A **41**, 275102 (2008).

Lee, S.-Y., J.-W. Ryu, J.-B. Shim, S.-B. Lee, S.W. Kim and K. An: Divergent Petermann factor of interacting resonances in a stadium-shaped microcavity. Physical Review A **78**, 015805 (2008).

Madroñero, J. and A. Buchleitner: Ab initio quantum approach to planar helium under periodic driving. Physical Review A **77**, 053402 (2008).

Moon, S., J. Yang, S.-B. Lee, J.-B.Shim, S.-W. Kim, J.-H. Lee and K. An: Nondestructive high-resolution soft-boundary profiling based on forward shadow diffraction. Optics Express **16**, 11007 - 11020 (2008).

Morales-Molina, L., S. Flach and J.B. Gong: Quantum ratchet control - Harvesting on Landau-Zener transitions. epl **83**, 40005 (2008).

Ovchinnikov, Y.N., A. Barone and A.A. Varlamov: Effect of magnetic field on macroscopic quantum tunneling escape time in small Josephson junctions. Physical Review B **78**, 054521 (2008).

Santhanam, M.S., V.B. Sheorey and A. Lakshminarayan: Effect of classical bifurcations on the quantum entanglement of two coupled quartic oscillators. Physical Review E **77**, 026213 (2008).

Shim, J.-B., S.-B. Lee, S.W. Kim, S.-Y. Lee, J. Yang, S. Moon, J.-H. Lee and K. An: Uncertainty-limited turnstile transport in deformed microcavities. Physical Review Letters **100**, 174102 (2008).

Tomsovich, S., D. Ullmo and A. Bäcker: Residual coulomb interaction fluctuations in chaotic systems: The boundary, random plane waves, and semiclassical theory. Physical Review Letters **100**, 164101 (2008).

Toscano, F., A. Kenfack, A.R.R. Carvalho, J.M. Rost and A.M.Ozorio de Almeida: Husimi-Wigner representation of chaotic eigenstates. Proceedings of the Royal Society A **464**, 2094, 1503 - 1524 (2008).

Unterhinninghofen, J., J. Wiersig and M. Hentschel: Goos-Hänchen shift and localization of optical modes in deformed microcavities. Physical Review E **78**, 016201 (2008).

Wiersig, J. and M. Hentschel: Combining directional light output and ultralow loss in deformed microdisks. Physical Review Letters **100**, 033901 (2008).

Wiersig, J., S.W. Kim and M. Hentschel: Asymmetric scattering and nonorthogonal mode patterns in optical microspirals. Physical Review A **78**, 053809 (2008).

4.4 Atomic and Molecular Structure

2007

Ciappina, M.F: Assessing the role of nuclear-nuclear interaction in single ionization by ion impact. Advanced Studies in Theoretical Physics **1**, 449 - 465 (2007).

Ciappina, M.F., W.R. Cravero and M. Schulz: Post-collisional effects on single ionization in 75 keV p+He collisions. Journal of Physics B **40**, 2577 - 2586 (2007).

Dixit, G., B. K. Sahoo, R.K. Chaudhuri and S. Majumder: Ab initio calculations for forbidden transition amplitudes and lifetimes of the low-lying states in V^{4+}. Physical Review A **76**, 042505 (2007).

Dixit, G., B. K. Sahoo, P. C. Deshmukh, R.K. Chaudhuri and S. Majumdr: Accurate estimates of circumstellar and interstellar lines of quadruply ionized vanadium using the coupled cluster approach. The Astrophysical Journal Supplement Series **172**, 645 - 648 (2007).

Majumder, S., B.K. Sahoo, R.K. Chaudhuri, B.P. Das and D. Mukherjee: Many-body effects in hyperfine interactions in $^{205}Pb^{+}$. European Physical Journal D **41**, 441 - 445 (2007).

Nataraj, H.S., B.K. Sahoo, B.P. Das, R.K. Chaudhuri and D. Mukherjee: The electron electric dipole moment enhancement factors of Rubidium and Caesium atoms. Journal of Physics Conference Series **80**, 012050 (2007).

Nataraj, H.S., B.K. Sahoo, B.P. Das, R.K. Chaudhuri and D. Mukherjee: Theoretical studies of the atomic transitions in boron-like ions: Mg VIII, Si X and S XII. Journal of Physics B **40**, 3153 - 3162 (2007).

Sahoo, B.K.: An *ab initio* relativistic coupled-cluster theory of dipole and quadrupole polarizabilities: Applications to a few alkali atoms and alkaline earth ions. Chemical Physics Letters **448**, 144 - 149 (2007).

Sahoo, B.K., B.P. Das, R.K. Chaudhuri and D. Mukherjee: A coupled-cluster approach to polarizabilities: Computational aspects. Journal of Computational Methods in Science and Engineering **7**, 57 - 74 (2007).

Sahoo, B.K., B.P. Das, R.K. Chaudhuri and D. Mukherjee: Theoretical studies of the $6s^2S_{1/2}$ $5d^2D_{3/2}$ parity-nonconserving transition amplitude in Ba^{+} and associated properties. Physical Review A **75**, 032507 (2007).

Sahoo, B.K., B.P. Das, R.K. Chaudhuri and D. Mukherjee, R.G.E. Timmermans and K. Jungmann: Investigations of Ra^+ properties to test possibilities for new optical-frequency standards. Physical Review A **76**, 040504 (2007).

2008

Alexander, J.S., A.C. Laforge, A. Hasan, Z.S. Machavariani, M.F. Ciappina, R.D. Rivarola, D. H. Madison and M. Schulz: Interference effects due to projectile target nucleus scattering in single ionization of H_2 by 75-keV proton impact. Physical Review A **78**, 060701 (2008).

Bhattacharyya, S., A.N. Sil, S. Fritzsche and P.K. Mukherjee: Effect of strongly coupled plasma on the spectra of hydrogenlike carbon, aluminium and argon. European Physical Journal D **46**, 1 - 8 (2008).

Brisker, D., I. Cherkes, C. Gnodtke, D. Jarukanont, S. Klaiman, W. Koch, S. Weissmann, R. Volkovich, M.C. Toroker and U. Peskin: Controlled electronic transport through branched molecular conductors. Molecular Physics **106**, 281 - 287 (2008).

Ciappina, M.F. and W.R. Cravero: Fully differential cross sections in single ionization of helium by ion impact: Assessing the role of correlated wave functions. Nuclear Instruments and Methods in Physics Research B **266**, 555 - 560 (2008).

Ciappina, M.F. and R.D. Rivarola: Interference pattern signatures in fully differential cross sections for single ionization of H_2 molecules by fast protons. Journal of Physics B **41**, 015203 (2008).

Ciappina, M.F., M. Schulz, T. Kirchner, D. Fischer, R. Moshammer and J. Ullrich: Double ionization of helium by ion impact analyzed using four-body Dalitz plots. Physical Review A **77**, 062706 (2008).

de Carvalho, J.X., M. S. Hussein and W.B. Li: Quantum reflection: The invisible quantum barrier. Physical Review A **78**, 032906 (2008).

Dixit, G., H.S. Nataraj, B.K. Sahoo, R.K. Chaudhuri and S. Majumder: Relativistic calculations in the lifetimes and hyperfine structure constants in $^{67}Zn^+$. Journal of Physics B **41**, 025001 (2008).

Eisfeld, A., J. Seibt and V. Engel: On the inversion of geometric parameters from absorption and circular dichroism spectroscopy of molecular dimers. Chemical Physics Letters **467**, 186 - 190 (2008).

Grimaldi, C.: Energy levels of a two-dimensional hydrogen atom with spin-orbit Rashba interaction. Physical Review B **77**, 113308 (2008).

Grimaldi, C.: Weak-and strong-coupling limits of the two-dimensional Fröhlich polaron with spin-orbit Rashba interaction. Physical Review B **77**, 024306 (2008).

Kamieniarz, G., P. Kozlowski, G. Musia, W. Florek, M. Antkowiak, M. Haglauer, A. Caramico D'Auria and F. Esposito: Phenomenological modeling of molecular-based rings beyond the strong exchange limit: Bond alternation and single-ion anisotropy effects. Inorganica Chimica Acta **361**, 3690 - 3696 (2008).

Kenfack, A., J.M. Rost and F. Großmann: Dissociation and ionization of small molecules steered by external noise. New Journal of Physics **10**, 013020 (2008).

Kozhedub, Y.S., O.V. Andreev, V.M. Shabaev, I.I. Tupitsyn, C. Brandau, C. Kozhuharov, G. Plunien and T. Stöhlker: Nuclear deformation effect on the binding energies in heavy ions. Physical Review A **77**, 032501 (2008).

Mandal, S., G. Dixit, B.K. Sahoo, R. K. Chaudhuri and S. Majumder: Theoretical spectroscopic studies of the atomic transitions and lifetimes of low-lying states in Ti IV. Journal of Physics B **41**, 055701 (2008).

Oh, S., Z. Huang, U. Peskin and S. Kais: Entanglement, Berry phases, and level crossings for the atomic Breit-Rabi Hamiltonian. Physical Review A **78**, 062106 (2008).

Sil, A.N., M. Pawlak, P.K. Mukheriee and M. Bylicki: The influence of Debye plasma on the ground state energies of exotic systems. Journal of Quantitative Spectroscopy Radiative Transfer **109**, 873 - 880 (2008).

Wynveen, A., D.J. Lee, A.A. Kornyshev and S. Leikin: Helical coherence of DNA in crystals and solution. Nucleic Acids Research **36**, 5540 - 5551 (2008).

4.5 Electronic Structure

2007

Antonov, V.N., B.N. Harmon, A.N. Yaresko and A.P. Shpak: Electronic structure, noncollinear magnetism, and x-ray magnetic circular dichroism in the Mn_3ZnC perovskite. Physical Review B **75**, 165114 (2007).

Antonov, V.N., B.N. Harmon, A.N. Yaresko and A.P. Shpak: X-ray magnetic circular dichroism in UGe_2: first-principles calculations. Journal of Physics Condensed Matter **19**, 186222 (2007).

Bekenov, L.V., V.N. Antonov, N.A. Plotnikov, A.P. Shpak and A.N. Yaresko: Electronic structure and optical properties of Co_2TiAl and Co_2VAl from ab initio calculations. Metallofizika i Noveishie Tekhnologii **29**, 57 - 65 (2007).

Buth, C.: A priori Wannier functions from modified Hartree-Fock and Kohn-Sham equations. Physical Review B **75**, 125121 (2007).

Cappelluti, E., C. Grimaldi and F. Marsiglio: Electron-phonon effects on spin-orbit split bands of two-dimensional systems. Physical Review B **76**, 085334 (2007).

Craco, L., S. Leoni, M.S. Laad and H. Rosner: Orbital-selective charge dynamics in $YTiO_3$ across the magnetic transition: Combined local-density approximation and dynamical mean-field theory. Physical Review B **76**, 115128 (2007).

Danzenbächer, S., Y. Kucherenko, D.V. Vyalikh, M. Holder, C. Laubschat, A.N. Yaresko, C. Krellner, Z. Hossain, C. Geibel, X.J. Zhou, W.L. Yang, N. Mannella, Z. Hussain, Z.X. Shen, M. Shi, L. Patthey and S.L. Molodtsov: Momentum dependence of $4f$ hybridization in heavy-fermion compounds: Angle-resolved photoemission study of $YbIr_2Si_2$ and $YbRh_2Si_2$. Physical Review B **75**, 045109 (2007).

De Menech, M., U. Saalmann and M.E. Garcia: Recovering hidden electronic states using energy-resolved imaging of metal clusters at surfaces. New Journal of Physics **9**, 340 (2007).

de Wijn, A.S., S. Kümmel and M. Lein: Numerical aspects of real-space approaches to strong-field electron dynamics. Journal of Computational Physics **226**, 89 - 103 (2007).

Ejima, S., F. Gebhard and S. Nishimoto: Luttinger-liquid exponent in the vicinity of charge-density wave instabilities. Journal of Magnetism and Magnetic Materials **310**, 996 - 998 (2007).

Ejima, S., F. Gebhard and S. Nishimoto: Phase diagram of the one-dimensional extended Hubbard model with hopping dimerization. Physica C **460**, 1079 - 1080 (2007).

Ejima, S. and S. Nishimoto: Phase diagram of the one-dimensional half-filled extended Hubbard model. Physical Review Letters **99**, 216403 (2007).

Gaston, N., I. Opahle, H.W. Gäggeler and P. Schwerdtfeger: Is eka-mercury (Element 112) a group 12 metal? Angewandte Chemie (Intern. Ed.) **46**, 1663 - 1666 (2007).

Gaston, N. and B. Paulus: Ab initio correlation calculations for the ground-state properties of group-12 metals Zn and Cd. Physical Review B **76**, 214116 (2007).

Gvozdikov, V.M.: Incoherence, metal-to-insulator transition, and magnetic quantum oscillations of interlayer resistance in an organic conductor. Physical Review B **76**, 235125 (2007).

Gvozdikov, V.M.: Magnetoresistance oscillations in a periodically modulated two-dimensional electron gas: The magnetic-breakdown approach. Physical Review B **75**, 115106 (2007).

Gvozdikov, V.M. and M. Taut: Magnetic quantum oscillations of electrons on a two-dimensional lattice: Numerical simulations and the magnetic breakdown approach. Physical Review B **75**, 155436 (2007).

Hövel, H., M. De Menech, M. Bödecker, C. Rettig, U. Saalmann and M.E. Garcia: Tip-induced distortions in STM imaging of carbon nanotubes. European Physical Journal D **45**, 459 - 463 (2007).

Hozoi, L., U. Birkenheuer, P. Fulde, A. Mitrushchenko and H. Stoll: Ab initio wave function-based methods for excited states in solids: Correlation corrections to the band structure of ionic oxides. Physical Review B **76**, 085109 (2007).

Kulič, M.L. and O.V. Dolgov: Angle-resolved photoemission spectra of $Bi_2Sr_2CaCu_2O_8$ show a Coulomb coupling 1 and an electron-phonon coupling of 2-3. Physical Review B **76**, 132511 (2007).

Leonov, I. and A.N. Yaresko: On the Verwey charge nordering in magnetite. Journal of Physics Condensed Matter **19**, 021001 (2007).

Matysiak, R., G. Kamieniarz, P. Gegenwart, H. Aoki and A. Ochiai: Field-dependent specific-heat of the pure and diluted 4f electron system Yb_4As_3. Inorganica Chimica Acta **360**, 3955 - 3958 (2007).

Sereda, Y., I.Y. Polishchuk and A.L. Burin: Resonant susceptibility of dielectric glasses in magnetic field. Physical Review B **75**, 024207 (2007).

Tuan, H.A. and L.D. Anh: Optical conductivity of (III, Mn)V diluted magnetic semiconductors. Modern Physics Letters B **21**, 69 - 77 (2007).

Uba, L., S. Uba, A. Polewko-Klim, E. Miniuk, T. Lucinski, P. Wandziuk, A. N. Yaresko and V.N. Antonov: Optical and magneto-optical study of Fe/Si multilayers. Materials Science **25**, 383 - 389 (2007).

Voloshina, E., N. Gaston and B. Paulus: Embedding procedure for ab initio correlation calculations in group II metals. Journal of Chemical Physics **126**, 134115 (2007).

Voloshina, E. and B. Paulus: Correlation energies for small magnesium clusters in comparison with bulk magnesium. Molecular Physics **105**, 2849 - 2855 (2007).

Voloshina, E. and B. Paulus: Electron-correlation effects in metals from first principles: a multi-reference incremental scheme. AIP Conference Proceedings **963**, 274 - 277 (2007).

Voloshina, E. and B. Paulus: Wave-function-based ab initio method for metals: Application of the incremental scheme to magnesium. Physical Review B **75**, 245117 (2007).

Wedig, U., M. Jansen, B. Paulus, K. Rosciszewski and P. Sony: Structural and electronic properties of Mg, Zn, and Cd from Hartree-Fock and density functional calculations including hybrid functionals. Physical Review B **75**, 205123 (2007).

Yushankhai, V., A. Yaresko, P. Fulde and P. Thalmeier: Dynamic spin susceptibility of paramagnetic spinel LiV_2O_4. Physical Review B **76**, 085111 (2007).

2008

Antonov, V.N., A. Ernst, I.V. Maznichenko, A.N. Yaresko and A.P. Shpak: Electronic structure and x-ray magnetic circular dichroism in Heusler-type $Fe_{2-x}V_{1+x}Al$: First-principles calculations. Physical Review B **77**, 134444 (2008).

Baltazar, S.E., M. De Menech, U. Saalmann, A.H. Romero and M. E. Garcia: Quantum electronic transport through supported $Si_{29}H_{24}$ clusters on an ideal Si[111] surface. Journal of Applied Physics **103**, 023714 (2008).

Bezugly, V., M. Albrecht and U. Birkenheuer: Comparison of three quantum chemical *ab initio* methods for band structure calculations: the hydrogen fluoride chain. Journal of Physics Conference Series **117**, 012006 (2008).

Cárdenas, W.H.Z., M.S. Hussein, L.S. Canto and J. Lubian: Local approximations for polarization potentials. Physical Review C **77**, 034609 (2008).

Craco, L., M.S. Laad, S. Leoni and H. Rosner: Normal-state correlated electronic structure of iron pnictides from first principles. Physical Review B **78**, 134511 (2008).

Craco, L., M.S. Laad, S. Leoni and H. Rosner: Theory of the orbital-selective Mott transition in ferromagnetic $YTiO_3$ under high pressure. Physical Review B **77**, 075108 (2008).

Dedkov, Y.S., S.L. Molodtsov, C. Laubschat, M. Fonin, U. Rüdiger, E.N. Voloshina and Y. Kucherenko: Spin-resolved photoelectron spectroscopy of rare-earth overlayers on rare-earth and d-metal substrates. Journal of Magnetism and Magnetic Materials **320**, E231 - E234 (2008).

Dixit, G., H.S. Nataraj, B.K. Sahoo, R.K. Chaudhuri and S. Majumder: Ab initio relativistic many-body calculation of hyperfine splittings of $^{113}Cd^+$. Physical Review A **77**, 012718 (2008).

Ejima, S. and S. Nishimoto: Ground-state properties of the one-dimensional extended Hubbard model at half filling. Journal of Physics and Chemistry of Solids **69**, 3293 - 3296 (2008).

Farberovich, O.V., A. Yaresko, K. Kikoin and V. Fleurov: Electronic structure of transition-metal impurities in semiconductors: Cu in GaP. Physical Review B **78**, 085206 (2008).

Gaston, N., B. Paulus, U. Wedig and M. Jansen: Multiple minima on the energy landscape of elemental zinc: A wave function based *ab initio* study. Physical Review Letters **100**, 226404 (2008).

Ghosh, H.: Ground and excited state nonlinear optical properties of poly(-para phenylene vinylene). Synthetic Metals **158**, 320 - 329 (2008).

Grigoriev, P.D., A.M. Dyugaev and E.V. Lebedeva: Electron mobility on the surface of liquid Helium: influence of surface level atoms and depopulation of lowest subbands. Journal of Experimental and Theoretical Physics **106**, 316 - 325 (2008).

Grigor'ev, P.D., A.M. Dyugaev and E.V. Lebedeva: Temperature dependence of the spectrum of electrons levitating above solid hydrogen. JETP Letters **87**, 106 - 110 (2008).

Hozoi, L., M.S. Laad and P. Fulde: Fermiology of cuprates from first principles: From small pockets to the Luttinger Fermi surface. Physical Review B **78**, 165107 (2008).

Kamieniarz, G. and P. Sobczak: Ground-State Configurations of 2D Clusters of Classical Charged Particles. Acta Physica Polonica A **113**, 477 - 480 (2008).

Kolorenč, P., V. Averbukh, K. Gokberg and L. S. Cederbaum: Ab initio calculation of interatomic decay rates of excited doubly ionized states in clusters. Journal of Chemical Physics **129**, 244102 (2008).

Majumdar, S.N., O. Bohhigas and A. Lakshminarayan: Exact minimum eigenvalue distribution of an entangled random pure state. Journal of Statistical Physics **131**, 33 - 49 (2008).

Mazumdar, C., M. Rotter, M. Frontzek, H. Michor, M. Doerr, A. Kreyssig, M. Koza, A. Hiess, J. Voigt, G. Behr, L.C. Gupta, M. Prager and M. Loewenhaupt: Crystalline electric field effects in $PrNi_2B_2C$: Inelastic neutron scattering. Physical Review B **78**, 14422 (2008).

Mikhailov, A.I., A.V. Nefiodov and G. Plunien: Ionization of K-shell electrons by electron impact. Physics Letters A **372**, 4451 - 4461 (2008).

Mikhailov, A.I., A.V. Nefiodov and G. Plunien: Ionization of K-shell electrons by positron impact. Physics Letters A **372**, 5171 - 5176 (2008).

Morawetz, K., S. Gemming, R. Luschtinetz, L.M. Eng, G. Seifert and A. Kenfack: Current without external bias and diode effect in shuttling transport and nanoshafts. New Journal of Physics **10**, 103014 (2008).

Morawetz, K., P. Lipavský, J. Koláek and E. H. Brandt: Surface energy and magnetocapacitance of superconductors under electric field bias. Physical Review B **78**, 054525 (2008).

Nguyen, V.H., B.H. Nguyen, V.P. Gerdt, O. Chuluunbaatar, A.A. Gusev, Y.G. Palii and V.H. Nguyen: Analytical Asymptotic Expressions for the Green's Function of the Electron in a Single-Level Quantum Dot at the Kondo and the Fano Resonances. Journal of the Korean Physical Society **53**, 3645 - 3649 (2008).

Nishimoto, S. and M. Arikawa: Low-lying excitations of the three-leg spin tube: A density-matrix renormalization group study. Physical Review B **78**, 054421 (2008).

Nishimoto, S., M. Shingai and Y. Ohta: Coexistence of distinct charge fluctuations in -(BEDT-TTF)$_2$X. Physical Review B **52**, 035113 (2008).

Siurakshina, L., B. Paulus and V. Yushankhai: Ab initio cluster caluclations of Co^{3+} spin states in $RBaCo_2O_{5.5.}$ (R= Ho,Gd). European Physical Journal B **63**, 445 - 450 (2008).

Sur, C., R.K. Chaudhuri, B.K. Sahoo, B.P. Das and D. Mukherjee: Relativistic unitary coupled cluster theory and applications. Journal of Physics B **41**, 065001 (2008).

Vetere, V., A. Monari, G.L. Bendazzoli, S. Evangelisti and B. Paulus: Full configuration interaction study of the metal-insulator transition in model systems: Li_N linear chains (N=2,4,6,8). Journal of Chemical Physics **128**, 024701 (2008).

Voloshina, E. and B. Paulus: Cohesive properties of CeN and LaN from first principles. Journal of Computational Chemistry **29**, 2107 - 2112 (2008).

Voloshina, E., B. Paulus and H. Stoll: Quantum-chemical approach to cohesive properties of metallic beryllium. Journal of Physics Conference Series **117**, 12029 (2008).

Vyalikh, D.V., S. Danzenbächer, A. Yaresko, M. Holder, Y. Kucherenko, C. Laubschat, C. Krellner, Z. Hossain, C. Geibel, M. Shi, L. Pathey and S.L. Molodtsov: Photoemission Insight into Heavy-Fermion Behavior in $YbRh_2Si_2$. Physical Review Letters **100**, 056402 (2008).

Wosnitza, J., V.M. Gvozdikov, J. Hagel O. Ignatchik, B. Bergk, P.J. Meeson, J.A. Schlueter, H. Davis, R.W. Winter and G.L. Gard: Spin-zero anomaly in the magnetic quantum oscillations of a two-dimensional metal. New Journal of Physics **10**, 083032 (2008).

Yaresko, A.N.: Electronic band structure and exchange coupling constants in ACr_2X_4 spinels (A=Zn, Cd, Hg; X=O, S, Se). Physical Review B **77**, 115106 (2008).

Ziesche, P.: Wichtige Formeln für die sphärischen Bessel-Funktionen. In: Taschenbuch der Mathematik. Eds. I.N. Bronstejn [u.a.] Frankfurt: Deutsch, 2008. S. 568 - 569.

4.6 Superconductivity and Magnetism

2007

Antonov, V.N., B.N. Harmon, A.N. Yaresko and A.P. Shpak: X-ray magnetic circular dichroism in GdN: first-principles calculations. Physical Review B **75**, 184422 (2007).

Ass'ad, A.I., H.S. Ashour and M.M. Shabat: Magnetostatic surface waves in ferrite-nonlinear non-magnetic negative permittivity material structure. International Journal of Modern Physics B **21**, 1951 - 1960 (2007).

Basleti, M., B. Korin-Hamzi, K. Maki and S. Tomic.: Unconventional spin-density wave in Bechgaard salt $(TMTSF)_2NO_3$. Physical Review B **75**, 052409 (2007).

Burdin, S., D.R. Grempel and M. Grilli: Disorder effects in the quantum Heisenberg model: Extended dynamical mean-field theory analysis. Physical Review B **75**, 224423 (2007).

Chang, J., I. Eremin, P. Thalmeier and P. Fulde: Eliashberg theory of superconductivity and inelastic rare-earth impurity scattering in the filled skutterudite $La_{1-x}Pr_xOs_4Sb_{12}$. Physical Review B **76**, 220510 (2007).

Chang, J., I. Eremin, P. Thalmeier and P. Fulde: Theory of magnetic excitons in the heavy-fermion superconductor UPd_2Al_3. Physical Review B **75**, 024503 (2007).

Eremin, I., D.K. Morr, A. V. Chubukov and K. Bennemann: Spin susceptibility in bilayered cuprates: Resonant magnetic excitations. Physical Review B **75**, 184534 (2007).

Eremin, M.V., A.I. Andreev and I.M. Eremin: On the theory of inelastic neutron scattering in the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ superconductor. JETP Letters **86**, 333 - 336 (2007).

Inosov, D.S., S.V. Borisenko, I. Eremin, A.A. Kordyuk, V.B. Zabolotnyy, J. Geck, A. Koitzsch, J. Fink, M. Knupfer and B. Büchner: About the relation between the quasiparticle Green's function in cuprates obtained from ARPES data and the magnetic susceptibility. Physica C **460**, 939 - 940 (2007).

Inosov, D.S., S.V. Borisenko, I. Eremin, A.A. Kordyuk, V.B. Zabolotnyy, J. Geck, A. Koitzsch, J. Fink, M. Knupfer, B. Büchner, H. Berger and R. Follath: Relation between the one-particle spectral function and dynamic spin susceptibility of superconducting $Bi_2Sr_2CaCu_2O_8$-δ. Physical Review B **75**, 172505 (2007).

Ismer, J.P., I. Eremin and D.K. Morr: Dynamical spin susceptibility in the underdoped cuprate superconductors: DDW state and influence of orthorhombicity. In: Electron correlation in new materials and nanosystems. Ed. by K. Scharnberg and S. Kruchinin. Dordrecht : Springer, 2007. S. 187 - 197.

Ismer, J.P., I. Eremin and D.K. Morr: Resonant spin excitations in high-T_c cuprates: Influence of the pseudogap. Physica C **460**, 1133 - 1134 (2007).

Ismer, J.P., I. Eremin, E. Rossi and D.K. Morr: Magnetic resonance in the spin excitation spectrum of electron-doped cuprate superconductors. Physical Review Letters **99**, 047005 (2007).

Kamieniarz, G., M. Haglauer, G. Musial, A.C. D'Auria, F. Esposito and D. Gatteschi: Single-ion anisotropy effects on the energy spectra of spin S=1 Heisenberg ring. Inorganica Chimica Acta **360**, 3941 - 3944 (2007).

Kishimoto, Y., Y. Kawasaki, M. Tanabe, T. Tanaka, T. Ohno, G. Ghosh, A.K. Tyagi and L.C. Gupta: ^{11}B NMR study of superconductivity in $YRuB_2$ and $LuRuB_2$. Journal of Magnetism and Magnetic Materials **310**, 581 - 583 (2007).

Lipavský, P., K. Morawetz, J. Koláek and E. H. Brandt: Vortex-induced deformation of the superconductor crystal lattice. Physical Review B **76**, 052502 (2007).

Manske, D. and I. Eremin: Anisotropic resonance peak in orthorhombic superconductors. In: Electron correlation in new materials and nanosystems. Eds. K. Scharnberg and S.P. Kruchinin. Dordrecht: Springer, 2007. S. 175 - 186.

Mayer, T., M. Eremin, I. Ermenin and P.F. Meier: Spin dynamics of itinerant holes in HTSC cuprates: the singlet-correlated band model and its applications. Journal of Physics Condensed Matter **19**, 116209 (2007).

Nishimoto, S., T. Shirakawa and Y. Ohta: Phase separation, spin polarization, and triplet superconductivity in the Hubbard chains coupled with ferromagnetic zigzag bonds. Journal of Magnetism and Magnetic Materials **310**, 669 - 671 (2007).

Nishimoto, S., T. Shirakawa and Y. Ohta: Spin-triplet superconductivity in the Hubbard chains coupled with ferromagnetic exchange interaction. Physica C **460**, 1059 - 1060 (2007).

Ohta, Y., S. Nishimoto and T. Shirakawa: Spin-triplet f-wave pairing in the one-dimensional triangular-lattice Hubbard model: Possible relevance to superconductivity in Bechgaard salts. Physica C **460**, 246 - 247 (2007).

Ohta, Y., S. Nishimoto and T. Shirakawa: Spin-triplet f-wave superconductivity in one-dimensional triangular-lattice Hubbard models. Journal of Magnetism and Magnetic Materials **310**, 578 - 580 (2007).

Ovchinnikov, Y.N.: Conductivity of granular metallic films. Journal of Experimental and Theoretical Physics **104**, 254 - 257 (2007).

Ovchinnikov, Y.N., A. Barone and A.A. Varlamov: Macroscopic quantum tunneling in "Small" Josephson junctions in a magnetic field. Physical Review Letters **99**, 037004 (2007).

Pandey, S. and A. Singh: Ferromagnetism in the t-t' Hubbard model: Interplay of lattice, band dispersion, and interaction effects studied within a Goldstone-mode preserving scheme. Physical Review B **75**, 064412 (2007).

Parker, D.: Enhanced superconducting and spin-density-wave ordering temperatures of gated quasi-one-dimensional organic superconductors. Physical Review B **76**, 224518 (2007).

Parker, D. and S. Haas: T_1^{-1} peak near T_c in unconventional Bardeen-Cooper-Schrieffer superconductors. Physical Review B **75**, 052501 (2007).

Parker, D., S. Haas and A.V. Balatsky: Generalized cuprate gap symmetry and higher d-wave harmonics: Effects of correlation length, doping, temperature, and impurity scattering. Physical Review B **76**, 104503 (2007).

Parker, D. and P. Thalmeier: Graphite-superconductor junctions as a probe of order-parameter symmetry. Physical Review B **76**, 064525 (2007).

Parker, D. and P. Thalmeier: Theory of tunneling spectroscopy in UPd_2Al_3. Physical Review B **75**, 184502 (2007).

Parker, D., H. Won and K. Maki: Upper critical field H_{c2} in $PrOs_4Sb_{12}$. physica status solidi b **244**, 1347 - 1353 (2007).

Pinto, R.A. and S. Flach: Quantum localized modes in capacitively coupled Josephson junctions. epl **79**, 66002 (2007).

Plakida, N.M. and V.S. Oudovenko: Electron spectrum in high-temperature cuprate superconductors. Journal of Experimental and Theoretical Physics **104**, 230 - 244 (2007).

Plakida, N.M. and V.S. Oudovenko: Electronic spectrum in cuprates within *p-d* Hubbard model. Physica C **460**, 993 - 994 (2007).

Shirakawa, T., Y. Ohta and S. Nishimoto: Spin-triplet superconductivity in the double-chain Hubbard model with ferromagnetic exchange interaction. Journal of Magnetism and Magnetic Materials **310**, 663 - 665 (2007).

Singh, A.: Clustering induced suppression of ferromagnetism in diluted magnets. Physical Review B **75**, 035206 (2007).

Sumour, M.A., A.H. El-Astal, F.W.S. Lima, M.M. Shabat and H.M. Khalil: Comparison of ising magnet on directed versus undirected Erdös-Rényi and scale-free networks. International Journal of Modern Physics C **18**, 53 - 60 (2007).

Tkachov, G.: Fine structure of the local pseudogap and Fano effect for superconducting electrons near a zigzag graphene edge. Physical Review B **76**, 235409 (2007).

Tkachov, G. and K. Richter: Effect of magnetic pair breaking on Andreev bound states and resonant supercurrent in quantum dot Josephson junctions. Physical Review B **75**, 134517 (2007).

Uzunov, D.I.: New magnetic effects on the phase transitions in unconventional superconductors. epl **77**, 20008 (2007).

Wrobel, P. and W. Suleja: Nonfrustrated antiferromagnet in a frustrated lattice due to charge ordering: A scenario for pairing in layered. Acta Physica Polonica **111**, 563 - 572 (2007).

Wrobel, P. and W. Suleja: Unconventional pairing in a weakly doped antiferromagnet on the honeycomb lattice: Mechanism of symmetry selection. Physical Review B **75**, 174522 (2007).

Yaresko, A. and V. Antonov: Magnetic interactions in Cr spinels. Journal of Magnetism and Magnetic Materials **310**, 1672 - 1674 (2007).

2008

Annett, J.F., B.L. Györffy, G. Litak and K. Wysokiski: Magnetic field induced rotation of the d-vector in the spin-triplet superconductor Sr_2RuO_4. Physical Review B **78**, 054511 (2008).

Antonov, V.N., A.P. Shpak and A.N. Yaresko: X-ray magnetic circular dichroism in d and f ferromagnetic materials: recent theoretical progress. Part I. Low Temperature Physics **34**, 1 - 36 (2008).

Antonov, V.N., A.P. Shpak and A.N. Yaresko: X-ray magnetic circular dichroism in d and f ferromagnetic materials: recent theoretical progress. Part II. Low Temperature Physics **34**, 79 - 112 (2008).

Castelnovo, C., R. Moessner and S.L. Sondhi: Magnetic monopoles in spin ice. Nature **451**, 42 - 45 (2008).

Chern, G.W., R. Moessner and O. Tchernyshyov: Partial order from disorder in a classical pyrochlore antiferromagnet. Physical Review B **78**, 144418 (2008).

Chiatti, O., A. Sytcheva, J. Wosnitza, S. Zherlitsyn, A.A. Zvyagin, V.S. Zapf, M. Jaime and A. Paduan-Filho: Character of magnetic excitations in a quasi-one-dimensional antiferromagnet near the quantum critical points: Impact on magnetoacoustic properties. Physical Review B **78**, 094406 (2008).

Chubukov, A., D.V. Efremov and I. Eremin: Magnetism, superconductivity, and pairing symmetry in iron-based superconductors. Physical Review B **78**, 134512 (2008).

Chubukov, A. and I. Eremin: Strong-coupling theory of the universal linear temperature dependence of the nodal Fermi velocity in layered cuprates. Physical Review B **78**, 060509 (2008).

Crisan, M., D. Bodea, I. Grosu and I. Tifrea: Metallic glass in two dimensional disordered bose systems; A renormalization group approach. Journal of Superconductivity and Novel Magnetism **21**, 51 - 55 (2008).

Eremin, I., E. Tsoncheva and A.V. Chubukov: Signature of the nonmonotonic d-wave gap in electron-doped cuprates. Physical Review B **77**, 024508 (2008).

Eremin, I., G. Zwicknagl, P. Thalmeier and P. Fulde: Feedback spin resonance in superconducting $CeCu_2Si_2$ and $CeCoin_5$. Physical Review Letters **101**, 187001 (2008).

Eremin, M.V., A.A. Aleev and I.M. Eremin: Dynamic spin susceptibility of hole-doped high-temperature superconductors in a singlet-correlated conduction band model. Journal of Experimental and Theoretical Physics **106**, 752 - 764 (2008).

Gnezdilov, V., P.Lemmens, A.A. Zvyagin, V.O. Cheranovskii, K. Lamonova, Y. G. Pashkevich, R.K. Kremer and H. Berger: Magnetic crossover and complex excitation spectrum of the ferromagnetic/antiferromagnetic spin-1/2 chain system -$TeVO_4$. Physical Review B **78**, 184407 (2008).

Jaubert, L.D.C., J.T. Chalker, P.C.W. Holdsworth and R. Moessner: Three-dimensional kasteleyn transition: Spin ice in a [100] field. Physical Review Letters **100**, 067207 (2008).

Kishimoto, Y., Y. Kawasaki, M. Tanabe, Y. Ideta, T. Ohno, G. Ghosh, A.K. Tyagi and L.C. Gupta: ^{11}B NMR relaxation in superconductors: $YRuB_2$ and $LuRuB_2$. Journal of Physics and Chemistry of Solids **69**, 3153 - 3155 (2008).

Klauss, H.-H., H. Luetkens, R. Klingeler, C. Hess, F.J. Litterst, M. Kraken, M.M. Korshunov, I. Eremin, S.-L. Drechsler, R. Khasanov, A. Amato, J. Hamann-Borrero, N. Leps, A. Kondrat, G. Behr, J. Werner and B. Buchner: Commensurate spin density wave in LaFeAsO: A local probe study. Physical Review Letters **101**, 077005 (2008).

Korshunov, M.M. and I. Eremin: Doping evolution of itinerant magnetic fluctuations in Fe-based pnictides. epl **83**, 67003 (2008).

Korshunov, M.M. and I. Eremin: Dynamical magnetic susceptibility in the lamellar cobaltate superconductor Na_xCoO_2 .yH_2O. Physical Review B **77**, 064510 (2008).

Korshunov, M.M. and I. Eremin: Theory of magnetic excitations in iron-based layered superconductors. Physical Review B **78**, 140509 (2008).

Kresin, V.Z. and Y.N. Ovchinnikov: 'Giant' strengthening of superconducting pairing in metallic nanoclusters: large enhancement of T_c and potential for room-temperature superconductivity. Physics Uspekhi **51**, 427 - 435 (2008).

Kutuzov, A.S., A.M. Skvortsova, S.I. Belov, J. Sichelschmidt, J. Wykhoff, I. Eremin, C. Krellner, C. Geibel and B.I. Kochelaev: Magnetic susceptibility of $YbRh_2Si_2$ and $YbIr_2Si_2$ on the basis of a localized 4f electron approach. Journal of Physics Condensed Matter **20**, 455208 (2008).

Lipavský, P., J. Koláek, K. Morawetz, E. H. Brandt and T.-J. Yang: Bernoulli potential in superconductors. Berlin: Springer, 2008. XV, 268 S.

Lipavský, P., K. Morawetz, J. Koláek and E. H. Brandt: Nonlinear theory of deformable superconductors: Ginzburg-Landau description. Physical Review B **78**, 174516 (2008).

Lipavský, P., K. Morawetz, J. Koláek and E. H. Brandt: Surface deformation caused by the Abrikosov vortex lattice. Physical Review B **77**, 184509 (2008).

Lipavský, P., K. Morawetz, J. Koláek, E. H. Brandt and M. Schreiber: Contribution of the dipole to deformation of superconductors. Physical Review B **77**, 014506 (2008).

Liu, B. and I. Eremin: Impurity resonance states in noncentrosymmetric superconductor $CePt_3Si$: A probe for Cooper-pairing symmetry. Physical Review B **78**, 014518 (2008).

Parker, D. and A.V. Balatsky: Quantitative evidence for spin-fluctuation-mediated higher-harmonic d-wave components: Hole- and electron-doped cuprates. Physical Review B **78**, 214502 (2008).

Parker, D., O.V. Dolgov, M.M. Korshunov, A.A. Golubov and I.I. Mazin: Extended s± scenario for the nuclear spin-lattice relaxation rate in superconducting pnictides. Physical Review B **78**, 134524 (2008).

Parker, D. and P. Thalmeier: Inelastic quasiparticle scattering and T_1^{-1} NQR relaxation rate in $Pr_{1-x}La_xOs_4Sb_{12}$. Physical Review B **77**, 184503 (2008).

Pinto, R.A. and S. Flach: Quantum breathers in capacitively coupled Josephson junctions: Correlation, number conservation, and entanglement. Physical Review B **77**, 024308 (2008).

Plakida, N.M. and V.S. Oudovenko: Electronic spectrum and superconductivity in Hubbard model. Condensed Matter Physics **11**, 495 - 507 (2008).

Reznik, D., J.P. Ismer, I. Eremin, L. Pintschovius, T. Wolf, M. Arai, Y. Endoh, T. Masui and S. Tajima: Local-moment fluctuations in the optimally doped high-T_c superconductor $YBa_2Cu_3O_{6.95}$. Physical Review B **78**, 132503 (2008).

Shopova, D.V. and D.I. Uzunov: Large Fluctuation and Gauge Effects on the Critical Behavior of Superconductors. In: Progress in superconductivity research. Ed. O.A. Chang. New York : Nova Science Publ., 2008. S. 13 - 53.

Thalmeier, P., T. Takimoto, J. Chang and I. Eremin: Multipolar order and superconductivity in f-electron compounds. Journal of Physical Society of Japan **77**, Suppl. A, 43 - 47 (2008).

Tkachov, G. and K. Richter: Spin-polarized tunneling through randomly transparent magnetic junctions: Reentrant magnetoresistance approaching the Jullière limit. Physical Review B **77**, 184427 (2008).

Wilhelm, F., P. Poulopoulos, V. Kapaklis, J.P. Kappler, N. Jaouen, A. Rogalev, A.N. Yaresko and C. Politis: Au and Fe magnetic moments in disordered Au-Fe alloys. Physical Review B **77**, 224414 (2008).

Zvyagin, A.A. and S.-L. Drechsler: Magnetic ordering of weakly coupled frustrated quantum spin chains. Physical Review B **78**, 014429 (2008).

4.7 Phase Transitions and Critical Phenomena

2007

Ainane, A., I. Essaoudi and M. Saber: Ferroelectric/antiferroelectric bilayer superlattice described by a transverse spin-1/2 Ising model. Journal of Magnetism and Magnetic Materials **315**, 132 - 136 (2007).

Ainane, A., P. Häussler, K. Htoutou and M. Saber: Magnetic properties of the site-diluted spin-1/2 Ising bilayer system. Surface Science **601**, 4256 - 4260 (2007).

Ares, S. and G. Sánchez: Modelling disorder: the case of DNA denaturation. European Physical Journal B **56**, 253 - 258 (2007).

Bodea, D., M. Crisan, I. Grosu and I. Tifrea: Large n-expansion limit of the three-dimensional ferromagnetic quantum phase transition. Journal of Low Temperature Physics **146**, 315 - 327 (2007).

Boughrara, M., M. Kerouad, M. Saber and D. Baldomir: The phase diagram of the biaxial spin-1 Ising system. Chinese Journal of Physics **45**, 75 - 83 (2007).

Essaoudi, I., A. Ainane, M. Saber and J.J. de Miguel: Hysteresis loops of a bilayer superlattice. physica status solidi b **244**, 3398 - 3407 (2007).

Essaoudi, I., K. Bärner, A. Ainane and M. Saber: Hysteresis loops of a ferroelectric superlattice with an antiferroelectric interfacial coupling. Physica Scripta **75**, 500 - 505 (2007).

Essaoudi, I., K. Bärner, A. Ainane and M. Saber: Magnetic properties and hysteresis loops of the S=1/2 and S=3/2 bilayer ising model. Physica A **385**, 208 - 220 (2007).

Madani, M., A. Ainane, K. Bärner and M. Saber: Phase transitions in a transverse spin-1/2 ising ferroelectric superlattice. Chinese Journal of Physics **45**, 544 - 553 (2007).

Mukherjee, P.K.: Structural phase transitions in pentacosane $C_{25}H_{52}$. Journal of Chemical Physics **126**, 114501 (2007).

Mukherjee, P.K. and J. Bhattacharya: Phenomenological theory of the nematic to lamellar phase transition in lyotropic liquid crystals. Journal of Chemical Physics **126**, 024901 (2007).

Saber, M., A. Ainane and K. Bärner: Phase transitions in an alternating superlattice. Surface Science **601**, 4274 - 4278 (2007).

Saber, M., A. Ainane, K. Bärner and I. Essaoudi: Dielectric properties of the $Ba_xSr_{1-x}TiO_3$ system. Physica Scripta **76**, 475 - 479 (2007).

Saber, M., I. Lukyanchuk, M. Madani, A. Tabyaoui and A. Ainane: The dielectric properties of the $KH_2PO_4/KD_2H_2PO_4$ superlattice. Chinese Journal of Physics **45**, 58 - 74 (2007).

Saber, M., I. Lukyanchuk, M. Madani, A. Tabyaoui and A. Ainane: The transverse spin-1/2 Ising order-disorder superlattice. Physica A **374**, 127 - 138 (2007).

Tabyaoui, A., M. Saber, K. Bärner and A. Ainane: Critical properties of a ferroelectric superlattice described by a transverse spin-1/2 Ising model. Physica Scripta **75**, 94 - 102 (2007).

2008

Barbero, C., A.P. Galeão, M.S. Hussein and F. Krmpoti: Kinetic energy sum spectra in nonmesonic weak decay of hypernuclei. Physical Review C **78**, 044312 (2008).

Chaudhuri, D. and S. Sengupta: Anomalous structural and mechanical properties of solids confined in quasi-one-dimensional strips. Journal of Chemical Physics **128**, 194702 (2008).

Essaoudi, I., M. Saber and A. Ainane: Effects of surface on the critical temperature of ferroelectric films. Ferroelectrics **372**, 22 - 30 (2008).

Giuliano, D. and P. Sodano: Frustration of decoherence in Y-shaped superconducting Josephson networks. New Journal of Physics **10**, 093023 (2008).

Johner, N., C. Grimaldi, I. Balberg and P. Ryser: Transport exponent in a three-dimensional continuum tunneling-percolation model. Physical Review B **77**, 174204 (2008).

Luigi, M., A. Protogenov and V. Verbus: Where do braid statistics and discrete motion meet each other? Journal of Nonlinear Mathematical Physics **15**, 353 - 361 (2008).

Madani, M., A. Ainane, M. Saber and J.J. de Miguel: The critical temperature for an alternating magnetic superlattice. Physica A **387**, 449 - 456 (2008).

Mitra, B., S. Ghose, N. Canculy and F. Peruani: Stability analysis of peer-to-peer networks against churn. Pramana **71**, 263 - 273 (2008).

Müller, M. and I. Rotter: Exceptional points in open quantum systems. Journal of Physics A **41**, 244018 (2008).

Nazario, Z. and D.I. Santiago: Heavy fermion quantum criticality. Physical Review Letters **101**, 136408 (2008).

4.8 Strongly Correlated Electrons

2007

Burdin, S. and P. Fulde: Random Kondo alloys investigated with the coherent potential approximation. Physical Review B **76**, 104425 (2007).

Cioslowski, J. and P. Ziesche: Ring-diagram summations and the self-energy of the homogeneous electron gas at its weak-correlation limit. Physical Review B **75**, 085103 (2007).

Daoud, M. and A. Jellal: Effective Wess-Zumino-Witten action for edge states of quantum Hall systems on Bergman ball. Nuclear Physics B **764**, 109 - 127 (2007).

Daoud, M. and A. Jellal: Quantum hall droplets on disc and effective Wess-Zumino-Witten action for edge states. International Journal of Geometric Methods in Modern Physics **4**, 1187 - 1204 (2007).

Derzhko, O., J. Richter, A. Honecker and H.J. Schmidt: Universal properties of highly frustrated quantum magnets in strong magnetic fields. Low Temperature Physics **33**, 745 - 756 (2007).

Dickmann, S., V. Fleurov and K. Kikoin: Collective excitations in a magnetically doped quantized Hall ferromagnet. Physical Review B **76**, 205309 (2007).

Donkov, A. and A.V. Chubukov: Spin-wave spectra of a Kagome stripe. epl **80**, 67005 (2007).

Dóra, B.: Local phonon mode in a fermionic bath and its relation to the Kondo effect. Physical Review B **75**, 245113 (2007).

Dóra, B., M. Gulácsi, F. Simon and H. Kuzmany: Spin gap and Luttinger liquid description of the NMR relaxation in carbon nanotubes. Physical Review Letters **99**, 166402 (2007).

Dóra, B., K. Maki, A. Virosztek and A. Ványolos: Pseudogap enhancement due to magnetic impurities in d-density waves. Physical Review B **75**, 132504 (2007).

Dóra, B. and P. Thalmeier: Magnetotransport and thermoelectricity in Landau-quantized disordered graphene. Physical Review B **76**, 035402 (2007).

Dóra, B. and P. Thalmeier: Reentrant Kondo effect in Landau-quantized graphene: Influence of the chemical potential. Physical Review B **76**, 115435 (2007).

Ghosh, H.: Excited state nonlinear optics of quasi-one-dimensional Mott-Hubbard insulators. Physical Review B **75**, 235127 (2007).

Hamada, M.S., A.H. El-Astal and M.M. Shabat: Characteristic of surface waves in nonlinear left handed - photosensitive semiconductor waveguide structure. International Journal of Modern Physics B **21**, 5319 - 5329 (2007).

Hentschel, M. and F. Guinea: Orthogonality catastrophe and Kondo effect in graphene. Physical Review B **76**, 115407 (2007).

Hoang, A.T. and D.A. Le: Optical conductivity of (III,Mn)V diluted magnetic semiconductors. Modern Physics Letters B **21**, 69 - 77 (2007).

Hozoi, L. and M.S. Laad: Quasiparticle bands in cuprates by quantum-chemical methods: Towards an ab initio description of strong electron correlations. Physical Review Letters **99**, 256404 (2007).

Hozoi, L., S. Nishimoto and C. de Graaf: Renormalization of quasiparticle hopping integrals by spin interactions in layered copper oxides. Physical Review B **75**, 174505 (2007).

Hozoi, L., S. Nishimoto, G. Kalosakas, D.B. Bodea and S. Burdin: Nonlocal interactions in doped cuprates: Correlated motion of Zhang-Rice polarons. Physical Review B **75**, 024517 (2007).

Kakehashi, Y. and P. Fulde: Marginal Fermi liquid and kink structure of quasiparticles in cuprates. Journal of Magnetism and Magnetic Materials **310**, 489 - 491 (2007).

Kakehashi, Y. and P. Fulde: Nonlocal excitation spectra in two-dimensional doped Hubbard model. Journal of the Physical Society of Japan **76**, 074702 (2007).

Korshunov, M.M., I. Eremin, A. Shorikov and V.I. Anisimov: Electronic theory for itinerant in-plane magnetic fluctuations in Na_xCoO_2. JETP Letters **84**, 650 - 655 (2007).

Korshunov, M.M., I. Eremin, A. Shorikov, V.I. Anisimov, M. Renner and W. Brenig: Itinerant in-plane magnetic fluctuations and many-body correlations in Na_xCoO_2. Physical Review B **75**, 094511 (2007).

Korshunov, M.M., V.A. Gavrichkov, S.G. Ovchinnikov, I.A. Nekrasov, E.E. Kokorina and Z.V. Pchelkina: Dominance of many-body effects over the one-electron mechanism for band structure doping dependence in $Nd_{2-x}Ce_xCuO_4$: the LDA + GTB approach. Journal of Physics Condensed Matter **19**, 486203 (2007).

Korshunov, M.M. and S.G. Ovchinnikov: Doping-dependent evolution of low-energy excitations and quantum phase transitions within an effective model for high-T_c copper oxides. European Physical Journal B **57**, 271 - 278 (2007).

Korshunov, M.M. and S.G. Ovchinnikov: LDA+GTB (Generalized Tight-Binding) method for the electronic structure calculations of strongly correlated electron systems: application for the band structure calculations of p-type cuprates. Physica C **460-462**, 1018 - 1019 (2007).

Morawetz, K., P. Lipavský, J. Koláek, E. H. Brandt and M. Schreiber: The concept of correlated density and its application. In: Condensed matter thories. Vol. 22. Ed. by H. Reinholz [u.a.] Singapore : World Scientific, 2007, S. 314 - 327.

Morawetz, K., P. Lipavský, J. Koláek, E. H. Brandt and M. Schreiber: The concept of correlated density and its application. International Journal of Modern Physics B **21**, 2348 - 2361 (2007).

Moyano, G.E., P. Schwerdtfeger and K. Rosciszewski: Lattice dynamics for fcc rare gas solids Ne, Ar, and Kr from *ab initio* potentials. Physical Review B **75**, 024101 (2007).

Nishimoto, S. and P. Fulde: Single magnetic impurity in a correlated electron system: Density-matrix renormalization group study. Physical Review B **76**, 035112 (2007).

Paulus, B.: The method of increments – a wavefunction-based correlation method for solids. In: Condensed matter theories. Vol. 22. Ed. by H. Reinholz [u.a.] Singapore : World Scientific, 2007, S. 166 - 176.

Paulus, B.: The method of increments – a wavefunction-based correlation method for solids. International Journal of Modern Physics B **21**, 2204 - 2214 (2007).

Perkins, N.B. and O. Sikora: Magnetic excitations in vanadium spinels. Physical Review B **76**, 214434 (2007).

Pollmann, F., J.J. Betouras, E. Runge and P. Fulde: Charge degrees in the quarter-filled checkerboard lattice. Journal of Magnetism and Magnetic Materials **310**, 966 - 968 (2007).

Rueff, J.P., S. Raymond, A. Yaresko, D. Braithwaite, P. Leininger, G. Vankó, A. Huxley, J. Rebizant and N. Sato: Pressure-induced f-electron delocalization in the U-based strongly correlated compounds UPd_3 and UPd_2Al_3: Resonant inelastic x-ray scattering and first-principles calculations. Physical Review B **76**, 085113 (2007).

Runge, E. F. Pollmann and P. Fulde: Fractionally charged excitations on frustrated lattices. In: Condensed matter thories. Vol. 22. Ed. by H. Reinholz [u.a.] Singapore : World Scientific, 2007, S. 177 - 193.

Runge, E. F. Pollmann and P. Fulde: Fractionally charged excitations on frustrated lattices. International Journal of Modern Physics B **21**, 2215 - 2231 (2007).

Singh, A., S.K. Das, A. Sharma and W. Nolting: Spin dynamics in the diluted ferromagnetic Kondo lattice model. Journal of Physics Condensed Matter **19**, 236213 (2007).

Ványolos, A., B. Dóra, K. Maki and A. Virosztek: Impurity scattering in unconventional density waves: non-crossing approximation for arbitrary scattering rate. New Journal of Physics **9**, 216 (2007).

Ványolos, A., B. Dóra and A. Virosztek: Local density of states and Friedel oscillations around a nonmagnetic impurity in unconventional density waves. Physical Review B **75**, 193101 (2007).

Ványolos, A., B. Dóra and A. Virosztek: Unconventional charge density wave arising from electron-phonon interaction. Journal of Superconductivity and Novel Magnetism **20**, 643 - 645 (2007).

Wang, Y.X. and B. Paulus: A comparative electron correlation treatment in H_2S-benzene dimer with DFT and wavefunction-based *ab initio* methods. Chemical Physics Letters **441**, 187 - 193 (2007).

Ziesche, P.: The on-shell self-energy of the uniform electron gas in its weak-correlation limit. physica status solidi b **244**, 2022 - 2036 (2007).

Ziesche, P.: The self-energy of the uniform electron gas in the second order of exchange. Annalen der Physik **16**, 45 - 56 (2007).

Zozulya, O.S., M. Haque, K. Schoutens and E.H. Rezayi: Bipartite entanglement entropy in fractional quantum Hall states. Physical Review B 76, 125310 (2007).

2008

Akbari, A.: Quadrupole effect on the heat conductivity of cold glasses. Physica B **403**, 3942-3945 (2008).

Akpojotor, G.E.: Possible Propagation of the Zhang-Rice singlet as a probable Cooper channel in the CuO_2 planes. Physics Letters A **372**, 6992 - 6995 (2008).

Borisenko, S.V., A.A. Kordyuk, A.N. Yaresko, V.B. Zabolotnyy, D.S. Inosov, R. Schuster, B. Büchner, R. Weber, R. Follath, L. Patthey and H. Berger: Pseudogap and charge density waves in two dimensions. Physical Review Letters **100**, 196402 (2008).

Daoud, M. and A. Hamama: Chiral bosons on Bargmann space associated with A_r statistics. Journal of Physics A **41**, 205205 (2008).

Daoud, M. and A. Hamama: Symplectic deformations, noncommutative scalar fields and fractional quantum hall effect. International Journal of Modern Physics A **23**, 2591 - 2612 (2008).

Daoud, M. and A. Jellal: Quantum Hall effect on the flag manifold F_2. International Journal of Modern Physics A **23**, 3129 - 3154 (2008).

Domański, T. A. Donabidowicz and K. Wysokiński: Meservey-Tedrow-Fulde effect in a quantum dot embedded between metallic and superconducting electrodes. Physical Review B **78**, 144515 (2008).

Donkov, A., M.M. Korshunov, I. Eremin, P. Lemmens, V. Gnezdilov, F.C. Chou und C.T. Lin: Electron-phonon interaction in the lamellar cobaltate Na_xCoO_2. Physical Review B **77**, 100504 (2008).

Dóra, B.: Disorder effect on the density of states in Landau quantized graphene. Low Temperature Physics **34**, 801 - 804 (2008).

Dóra, B. and M. Gulácsi: Ineastic scattering from local vibrational modes. Physical Review B **78**, 165111 (2008).

Dóra, B., M. Gulácsi, J. Koltai, V. Zólyomi, J. Kürti and F. Simon: Electron spin resonance signal of Luttinger liquids and single-wall carbon nanotubes. Physical Review Letters **101**, 106408 (2008).

Dóra, B., M. Gulácsi, F. Simon, P. Wzietek and H. Kuzmany: Luther-Emery liquid in the NMR relaxation rate of carbon nanotubes. physica status solidi b **245**, 2159 - 2163 (2008).

Dóra, B., K. Ziegler and P. Thalmeier: Effect of weak disorder on the density of states in graphene. Physical Review B **77**, 115422 (2008).

Doucot, B., M.O. Goerbig, P. Lederer and R. Moessner: Entanglement skyrmions in multicomponent quantum Hall systems. Physical Review B **78**, 195327 (2008).

Fulde, P. and F. Pollmann: Strings in strongly correlated electron systems. Annalen der Physik **17**, 441 - 449 (2008).

Fulde, P., F. Pollmann and E. Runge: Strongly correlated electrons on frustrated lattices. Iranian Journal of Physics Research **8**, 13 - 24 (2008).

Ghosh, H.: Gigantic excited state optical nonlinearities in one-dimensional Mott-Hubbard insulators. AIP Conference Proceedings **1014**, 260 - 264 (2008).

Hotta, C. and F. Pollmann: Dimensional tuning of electronic states under strong and frustrated interactions. Physical Review Letters **100**, 186404 (2008).

Kashuba, A.B.: Conductivity of defectless graphene. Physical Review B **78**, 085415 (2008).

Lal, S. and M.S. Laad: From frustrated insulators to correlated anisotropic metals: charge-ordering and quantum criticality in coupled chain systems. Journal of Physics Condensed Matter **20**, 235213 (2008).

Liu, B. and Y. Liang: Density of states and nonmagnetic impurity effects in electron-doped cuprates. Physical Review B **77**, 245121 (2008).

Mahdavifar, S. and A. Akbari: Heat capacity of Schottky type in low-dimensional spin systems. Journal of Physics Condensed Matter **20**, 215213 (2008).

Nakamura, M., L. Hirasawa and K.-I. Imura: Quantum Hall effect in bilayer and multilayer graphene with finite Fermi energy. Physical Review B **78**, 033403 (2008).

Nishimoto, S., K. Sano and Y. Ohta: Phase diagram of the one-dimensional Hubbard model with next-nearest-neighbor hopping. Physical Review B **77**, 085119 (2008).

Nishimoto, S.,T. Shirakawa and Y. Ohta: Charge and spin excitation spectra in the one-dimensional Hubbard model with next-nearest-neighbor hopping. Physical Review B **77**, 115102 (2008).

Ovchinnikov, S.G., M.M. Korshunov and E.V. Zakharova: Temperature evolution of spin-polaron in-gap states in undoped antiferromagnetic cuprates. Physics of the Solid State **50**, 1401 - 1406 (2008).

Pollmann, F., J.J. Betouras, E. Runge and P. Fulde: Erratum to: "Charge degrees of freedom in the quarter-filled checkerboard lattice" [JMMM 310 (2007) 966]. Journal of Magnetism and Magnetic Materials **320**, 1802 (2008).

Pollmann, F., P. Fulde and K. Shtengel: Kinetic ferromagnetism on a kagome lattice. Physical Review Letters **100**, 136404 (2008).

Quintanilla, J., M. Haque and A.J. Schofield: Symmetry-breaking Fermi surface deformations from central interactions in two dimensions. Physical Review B **78**, 035131 (2008).

Quintanilla, J., C. Hooley, B.J. Powell, A.J. Schofield and M. Haque: Pomeranchuk instability: Symmetry-breaking and experimental signatures. Physica B **403**, 1279 - 1281 (2008).

Ralko, A., D. Poilblanc and R. Moessner: Generic mixed columnar-plaquette phases in Rokhsar-Kivelson models. Physical Review Letters **100**, 037201 (2008).

Raman, K.S., E. Fradkin, R. Moessner, S. Papanikolaou and S.L. Sondhi: Quantum dimer models and exotic orders. In: Quantum Magnetism. Ed. by B. Barbara. Berlin: Springer Science and Business, 2008. S. 139 - 150.

Shingai, M., S. Nishimoto and Y. Ohta: Numerical study on the anisotropic triangular-lattice Hubbard model at quarter filling: Charge fluctuations with three-fold periodicity. Journal of Physics and Chemistry of Solids **69**, 3382 - 3384 (2008).

Simon, F., B. Dóra, F, Murányi, A. Jánossy, S, Garaj, L. Forró, S. Bud'ko, C. Petrovic and P.C. Canfield: Generalized Elliott-Yafet theory of electron spin relaxation in metals: origin of the anomalous electron spin lifetime in MgB_2 . Physical Review Letters **101**, 177003 (2008).

Taraphder, A., M.S. Laad, L. Craco and A.N. Yaresko: GdI_2: A New Ferromagnetic Excitonic Solid? Physical Review Letters **101**, 136410 (2008).

Trousselet, F., D. Poilblanc and R. Moessner: Mixed columnar-plaquette crystal of correlated fermions on the two-dimensional pyrochlore lattice at fractional filling. Physical Review B **78**, 195101 (2008).

4.9 Time Dependent Processes

2007

Blaustein, G.S., M.I. Gozman, O. Samoylova, I.Y. Polishchuk and A. L. Burin: Guiding optical modes in chains of dielectric particles. Optics Express **15**, 17380 - 17391 (2007).

Carvalho, A.R.R., F. Mintert, S. Palzer and A. Buchleitner: Entanglement dynamics under decoherence: from qubits to qudits. European Physical Journal D **41**, 425 - 432 (2007).

Denisov, S., L. Morales-Molina and S. Flach: Quantum resonances and rectification in ac-driven ratchets. epl **79**, 10007 (2007).

Denisov, S., L. Morales-Molina, S. Flach and P. Hänggi: Periodically driven quantum ratchets: Symmetries and resonances. Physical Review A **75**, 063424 (2007).

Facchini, A. and H. Kantz: Curved structures in recurrence plots: The role of the sampling time. Physical Review E **75**, 036215 (2007).

Garcia, S.P., L.B. DeLancey, J.S. Almeida and R.W. Chapman: Ecoforecasting in real time for commercial fisheries: the Atlantic white shrimp as a case study. Marine Biology **152**, 15 - 24 (2007).

Morawetz, K.: Fluctuations due to the nonlocal character of collisions. New Journal of Physics **9**, 313 (2007).

Morisset, S., L. Pichl, A.E. Orel and I. F. Schneider: Wave-packet approach to Rydberg resonances in dissociative recombination. Physical Review A **76**, 042702 (2007).

Pindzola, M.S., F. Robicheaux, S.D. Loch, J.C. Berengut, T. Topcu, J. Colgan, M. Foster, D.C. Griffin, C.P. Ballance, D.R. Schultz, T. Minami, N.R. Badnell, M.C. Witthoeft, D.R. Plante, D.M. Mitnik, J.A. Ludlow and U. Kleiman: The time-dependent close-coupling method for atomic and molecular collision processes. Journal of Physics B **40**, R39 - R60 (2007).

Schulman, L.S.: Decoherence induced equilibration. Foundations of Physics **37**, 1716 - 1726 (2007).

Urbanowicz, K. and H. Kantz: Improvement of speech recognition by nonlinear noise reduction. Chaos **17**, 023121 (2007).

2008

Aquino, G. and F. Giraldi: Entanglement entropy and determination of an unknown quantum state. Physical Review A **78**, 062115 (2008).

Baptista, M.S., C. Bohn, R. Kliegl, R. Engbert and J. Kurths: Reconstruction of eye movements during blinks. Chaos **18**, 013126 (2008).

de Wijn, A.S., M. Lein and S. Kümmel: Strong-field ionization in time-dependent density functional theory. epl **84**, 43001 (2008).

Denisov, S., Y. Zolotaryuk, S. Flach and O. Yevtushenko: Vortex and translational currents due to broken time-space symmetries. Physical Review Letters **100**, 224102 (2008).

Helbing, D., J. Jost and H. Kantz: Nonlinear physics everywhere: from molecules to cities. European Physical Journal B **63**, 283 (2008).

Hussein, M.S.: Absorption-fluctuation theorem for nuclear reactions: Brink-Axel, incomplete fusion and all that. AIP Conference Proceedings **1005**, 129 - 134 (2008).

Hussein, M.S. and R. Lichtenthäler: Exit doorway model for nuclear elastic breakup of weakly bound projectiles. Physical Review C **77**, 054609 (2008).

Iqbal, S. and F. Saif: Quantum computing with particle in a driven square well. Journal of Russian Laser Research **29**, 466 - 473 (2008).

Khomeriki, R. and J. Leon: Tristability in the pendula chain. Physical Review E **78**, 057202 (2008).

Marwan, N., A. Facchini, M. Thiel, J.P. Zbilut and H. Kantz: 20 Years of Recurrence Plots: Perspectives for a Multi-purpose Tool of Nonlinear Data Analysis. European Physical Journal Special Topics **164**, 1 -2 (2008).

Nistazakis, H.E., Z. Rapti, D.J. Frantzeskakis, P.G. Kevrekidis, P. Sodano and A. Trombettoni: Rabi switch of condensate wave functions in a multicomponent Bose gas. Physical Review A **78**, 023635 (2008).

Oh, S.: Quantum computational method of finding the ground-state energy and expectation values. Physical Review A **77**, 012326 (2008).

Sahoo, B.K., H.S. Nataraj, B.P. Das, R. K. Chaudhuri and D. Mukherjee: Theoretical estimation of lifetimes of the lowest metastable states in Sc III and Y III. Journal of Physics B **41**, 055702 (2008).

4.10 Living Matter

2007

Ares, S. and G. Kalosakas: Distribution of bubble lengths in DNA. Nano Letters **7**, 307 - 311 (2007).

Becker, N.B. and R. Everaers: From rigid base pairs to semiflexible polymers: Coarse-graining DNA. Physical Review E **76**, 021923 (2007).

Bollenbach, T., K. Kruse, P. Pantazis, M. González-Gaitán and F. Jülicher: Morphogen transport in epithelia. Physical Review E **75**, 011901 (2007).

Cherstvy, A.G.: Electrostatics of DNA complexes with cationic lipid membranes. Journal of Physical Chemistry B **111**, 7914 - 7927 (2007).

Cherstvy, A.G.: Effect of a low-dielectric interior on DNA electrostatic response to twisting and bending. Journal of Physical Chemistry B **111**, 12933 - 12937 (2007).

Doubrovinski, K. and K. Kruse: Self-organization of treadmilling filaments. Physical Review Letters **99**, 228104 (2007).

Everaers, R., S. Kumar and C. Simm: Unified description of poly- and oligonucleotide DNA melting: Nearest-neighbor, Poland-Sheraga, and lattice models. Physical Review E **75**, 041918 (2007).

Farhadifar, R., J.C. Röper, B. Algouy, S. Eaton and F. Jülicher: The influence of cell mechanics, cell-cell interactions and proliferation on epithelial packing. Current Biology **17**, 2095 - 2104 (2007.

Friedrich, B.M. and F. Jülicher: Chemotaxis of sperm cells. Proceedings of the National Academy of Sciences of the United States of America **104**, 13256 - 13261 (2007).

Galburt, E.A., S.W. Grill, A. Wiedmann, L. Lubkowska, J. Choy, E. Nogales, M. Kashlev and C. Bustamante: Backtracking determines the force sensitivity of RNAP II in a factor-dependent manner. Nature **446**, 820 - 823 (2007).

Graupner, M. and N. Brunel: STDP in a bistable synapse model based on CaMKII and associated signaling pathways. PLoS Computational Biology **3**, e221 (2007).

Greulich, P., A. Garai, K. Nishinari, A. Schadschneider and D. Chowdhury: Intracellular transport by single-headed kinesin KIF1A: Effects of single-motor mechanochemistry and steric interactions. Physical Review E **75**, 041905 (2007).

Grill, S.W.: The mechanics of asymmetric cell division. European Journal of Cell Biology **86 S1**, 40-40 (2007).

Günther, U. and K. Kruse: Spontaneous waves in muscle fibres. New Journal of Physics **9**, 417 (2007).

Joanny, J.F., F. Jülicher, K. Kruse and J. Prost: Hydrodynamic theory for multi-component active polar gels. New Journal of Physics **9**, 422 (2007).

Jülicher, F., K. Kruse, J. Prost and J.F. Joanny: Active behavior of the Cytoskeleton. Physics Reports **449**, 3 - 28 (2007).

Kicheva, A., P. Pantazis, T. Bollenbach, Y. Kalaidzidis, T. Bittig, F. Jülicher and M. González-Gaitán: Kinetics of morphogen gradient formation. Science **315** (5811), 521–525 (2007).

Mohanty, P.K. and K. Kruse: Driven diffusive systems of active filament bundles. Journal of Statistical Physics **128**, 95 - 110 (2007).

Morelli, L.G. and F. Jülicher: Precision of genetic oscillators and clocks. Physical Review Letters **98**, 228101 (2007).

Riedel-Kruse, I.H., A. Hilfinger, J. Howard and F. Jülicher: How molecular motors shape the flagellar beat. HFSP Journal **1**, 192 - 208 (2007).

Sibona, G.J., C.A. Condat and S.C. Isasi: Relevance of intracellular replication to the evolution of Chagas' disease. In: Mathematical modeling of biological systems. Ed. by A. Deutsch [u.a.]. Boston: Springer, 2007. S. 289 - 297.

Théry, M., A. Jiménez-Dalmaroni, V. Racine, M. Bornens and F. Jülicher: Experimental and theoretical study of mitotic spindle orientation. Nature **447**, (7143) 493 - 496 (2007).

Tinevez, J.-Y., F. Jülicher and P. Martin: Unifying the various incarnations of active hairbundle motility by the vertebrate hair cell. Biophysical Journal **93**, 4053 - 4067 (2007).

Zumdieck, A., K. Kruse, H. Bringmann, A.A. Hyman and F. Jülicher: Stress generation and filament turnover during actin ring constriction. PLoS ONE **2(8)**, e696 (2007).

2008

Basu, A., J.F. Johanny, F. Jülicher and J. Prost: Thermal and non-thermal fluctuations in active polar gels. European Physical Journal E **27**, 149 - 160 (2008).

Bittig, T., O. Wartlick, A. Kicheva, M. González-Gaitán and F. Jülicher: Dynamics of anisotropic tissue growth. New Journal of Physics **10**, 063001 (2008).

Bollenbach, T., P. Pantazis, A. Kicheva, C. Bökel, M. González-Gaitán and F. Jülicher: Precision of the Dpp gradient. Development (Company of Biologists) **135**, 1137 - 1146 (2008).

Cherstvy, A.G.: DNA cholesteric phases: The role of DNA molecular chirality and DNA - DNA electrostatic interactions. Journal of Physical Chemistry B **112**, 12585 - 12595 (2008).

Cherstvy, A.G., A.B. Kolomeisky, A.A. Kornyshev: Protein-DNA interactions: Reaching and recognizing the targets. Journal of Physical Chemistry B **112**, 4741 - 4750 (2008).

Dierkes, K., B. Lindner and F. Jülicher: Enhancement of sensitivity gain and frequency tuning by coupling of active hair bundles. Proceedings of the National Academy of Sciences of the United States of America **105**, 18669 - 18674 (2008).

Duke, T.A.J. and F. Jülicher: Critical oscillators as active elements in hearing. In: Active processes and otoacoustic emissions. Ed. by G. A. Manley [u.a.]. Berlin: Springer, 2008. S. 63 - 92.

Foret, L. and P. Sens: Kinetic regulation of coated vesicle secretion. Proceedings of the National Academy of Sciences of the United States of America **105**, 14763 - 14768 (2008).

Friedrich, B.M.: Search along persistent random walks. Physical Biology **5**, 026007 (2008).

Friedrich, B.M. and F. Jülicher: The stochastic dance of circling sperm cells: sperm chemotaxis in the plane. New Journal of Physics **10**, 123025 (2008).

Garai, A., D. Chowdhury and M.D. Betterton: Two-state model for helicase translocation and unwinding of nucleic acids. Physical Review E **77**, 061910 (2008).

Hilfinger, A. and F. Jülicher: The chirality of ciliary beats. Physical Biology **5**, 016003 (2008).

Jülicher, F.: Biophysik der Zellbewegungen. Von molekularen Motoren zu zellulärem Transport. Nova Acta Leopoldina NF **97**, Nr. 358, 103 - 114 (2008).

Kruse, K. and A. Iomin: Superdiffusion of morphogens by receptor-mediated transport. New Journal of Physics **10**, 023019 (2008).

Kücken, M., J. Soriano, P.A. Pullarkat, A. Ott and E.M. Nicola: An osmoregulatory basis for shape oscillations in regenerating *Hydra*. Biophysical Journal **95**, 978 - 985 (2008).

Loose, M., E. Fischer-Friedrich, J. Ries, K. Kruse and P. Schwille: Spatial regulators for bacterial cell division self-organize into surface waves in vitro. Science **320**, 5877, 789 - 792 (2008).

Paar, V., N. Pavin, I. Basar, M. Rosandić, M. Glunčić and N. Paar: Hierarchical structure of cascade of primary and secondary periodicities in Fourier power spectrum of alphoid higher order repeats. BMC Bioinformatics **9**, 466 (2008).

Rosa, A. and R. Everaers: Structure and Dynamics of Interphase Chromosomes. PLoS Computational Biology **4**, e100153 (2008).

Schötz, E.-M., R.D. Burdine, F. Jülicher, M.S. Steinberg, C.-P. Heisenberg and R.A. Foty: Quantitative differences in tissues surface tension influence zebrafish germ layer positioning. HFSP Journal **2**, 42 - 56 (2008).

Selmeczi, D., L. Li, L.I.I. Pedersen, S.F. Nrrelykke, P.H. Hagedorn, S. Mosler, N.B. Larsen, E.C. Cox and H. Flyvbjerg: Cell motility as random motion: A review. European Physical Journal Special Topics **157**, 1 - 15 (2008).

Tripathi, T. and D. Chowdhury: Interacting RNA polymerase motors on a DNA track: Effects of traffic congestion and intrinsic noise on RNA synthesis. Physical Review E **77**, 011921 (2008).

Uchida, N., G.S. Grest and R. Everaers: Viscoelasticity and primitive path analysis of entangled polymer liquids: From F-actin to polyethylene. Journal of Chemical Physics **128**, 044902 (2008).

Ullner, E., A. Koseska, J. Kurths, E. Volkov, H. Kantz and J. Garcia-Ojalvo: Multistability of synthetic genetic networks with repressive cell-to-cell communication. Physical Review E **78**, 031904 (2008).

4.11 Stochastic Processes

2007

Aquino, G., P. Grigolini and B.J. West: Linear response and fluctuation-dissipation theorem for non-poissonian renewal processes. epl **80**, 10002 (2007).

Bandyopadhyay, J.N. and S. Jalan: Universality in complex networks: Random matrix analysis. Physical Review E **76**, 026109 (2007).

Buchleitner, A., A.R.R. Carvalho and F. Mintert: Entanglement in Open Quantum Systems. Acta Physica Polonica **112**, 575 - 588 (2007).

Carvalho, A.R.R., M. Busse, O. Brodier, C. Viviescas and A. Buchleitner: Optimal dynamical characterization of entanglement. Physical Review Letters **98**, 190501 (2007).

Chacron, M.J., B. Lindner and A. Longtin: Threshold fatigue and information transfer. Journal of Computational Neuroscience **23**, 301 - 311 (2007).

Farahpour, F., Z. Eskandari, A. Bahraminasab, G.R. Jafari, F. Ghasemi, M. Sahimi and M. Reza Rahimi Tabar: A Langevin equation for the rates of currency exchange based on the Markov analysis. Physica A **385**, 601 - 608 (2007).

Ghasemi, F., M. Sahimi, J. Peinke, R. Friedrich, G.R. Jafari and M. Reza Rahimi Tabar: Markov analysis and Kramers-Moyal expansion of nonstationary stochastic processes with application to the fluctuations in the oil price. Physical Review E **75**, 060102 (2007).

Gopalakrishnan, M., P. Borowski, F. Jülicher and M. Zapotocky: Response and fluctuations of a two-state signaling module with feedback. Physical Review E **76**, 021904 (2007).

Hallerberg, S., E.G. Altmann, D. Holstein and H. Kantz: Precursors of extreme increments. Physical Review E **75**, 016706 (2007).

Hamacher, K.: Adaptive extremal optimization by detrended fluctuation analysis. Journal of Computational Physics **227**, 1500 - 1509 (2007).

Hamacher, K.: Energy landscape paving as a perfect optimization approach under detrended fluctuation analysis. Physica A **378**, 307 - 314 (2007).

Hamacher, K.: Information theoretical measures to analyze trajectories in rational molecular design. Journal of Computational Chemistry **28**, 2576 - 2580 (2007).

Jafari, G.R., M. Sadegh Movahed, P. Norouzzadeh, A. Bahraminasab, M. Sahimi, F. Ghasemi and M. Reza Rahimi Tabar: Uncertainty in the fluctuations of the price of stocks. International Journal of Modern Physics C **18**, 1689 - 1697 (2007).

Kantz, H., D. Holstein, M. Ragwitz and N.K. Vitanov: Short time prediction of wind speeds from local measurements. In: Wind Energy. Ed. by J. Peinke [u.a.]. Berlin : Springer, 2007., S. 93-98.

Lewis, J.E., B. Lindner, B. Laliberté and S. Groothuis: Control of neuronal firing by dynamic parallel fiber feedback: implications for electrosensory reafference suppression. Journal of Experimental Biology **210**, 4437 - 4447 (2007).

Lindner, B.: The diffusion coefficient of nonlinear Brownian motion. New Journal of Physics **9**, 136 (2007).

Lindner, B. and T. Schwalger: Correlations in the sequence of residence times. Physical Review Letters **98**, 210603 (2007).

Mintert, F. and A. Buchleitner: Observable entanglement measure for mixed quantum states. Physical Review Letters **98**, 140505 (2007).

Peruani, F., M. Choudhury, A. Mukherjee and N. Ganguly: Emergence of a non-scaling degree distribution in bipartite networks: A numerical and analytical study. epl **79**, 28001 (2007).

Peruani, F. and L.G. Morelli: Self-propelled particles with fluctuating speed and direction of motion in two dimensions. Physical Review Letters **99**, 010602 (2007).

Schäffer, E., S.F. Nørrelykke and J. Howard: Surface forces and drag coefficients of microspheres near a plane surface measured with optical tweezers. Langmuir **23**, 3654 - 3665 (2007).

Selmeczi, D., S.F. Toli-Nørrelykke, R. Schäffer, P. H. Hagedorn, S. Mosler, K. Berg-Sørenson, N. B. Larsen and H. Flyvbjerg: Brownian Motion after Einstein: Some New Applications and New Experiments. In: Controlled nanoscale motion. Ed. by H. Linke and A. Mansson. Berlin : Springer, 2007. S. 181 - 199.

Selmeczi, D., S.F. Toli-Nørrelykke, R. Schäffer, P. H. Hagedorn, S. Mosler, K. Berg-Sørenson, N. B. Larsen and H. Flyvbjerg: Brownian Motion after Einstein and Smoluchowski: Some New Applications and New Experiments. Acta Physica Polonica B **38**, 2407 - 2431 (2007).

Singh, K.P. and J.M. Rost: Femtosecond photoionization of atoms under noise. Physical Review A **76**, 063403 (2007).

Singh, K.P. and J.M. Rost: Optimal stochastic enhancement of photoionization. Physical Review Letters **98**, 160201 (2007).

Urbanowicz, K., J.J. Źebrowski, R. Baranowski and J. A. Hoyst: How random is your heart beat? Physica A **384**, 439 - 447 (2007).

Varn, D.P., G.S. Canright and J.P. Crutchfield: Inferring planar disorder in close-packed structures via epsilon-machine spectral reconstruction theory: structure and intrinsic computation in zinc sulfide. Acta Crystallographica B **63**, 169 - 182 (2007).

Walborn, S.P., P.H. Souto Ribeiro, L. Davidovich, F. Mintert and A. Buchleitner: Experimental determination of entanglement by a projective measurement. Physical Review A **75**, 032338 (2007).

2008

Adamashvili, G.T., D. J. Kaup, A. Knorr and C. Weber: Influence of non-Markovian relaxation processes on self-induced transparency: Memory function theory for optical solitons. Physical Review A **78**, 013840 (2008).

Bohigas, O., J.X. de Carvalho and M.P. Pato: Disordered ensembles of random matrices. Physical Review E **77**, 011122 (2008).

Bröcker, J.: Some Remarks on the Reliability of Categorical Probability Forecasts. Monthly Weather Review **136**, 4488 - 4502 (2008).

Bröcker, J. and L. A. Smith: From ensemble forecasts to predictive distribution functions. Tellus A **60**, 663 - 678 (2008).

Clausznitzer, D., B. Lindner, F. Jülicher and P. Martin: Two-state approach to stochastic hair bundle dynamics. Physical Review E **77**, 041901 (2008).

de Carvalho, J.X., M. S. Hussein, M.P. Pato and A.J. Sargeant: Perturbation treatment of symmetry breaking within random matrix theory. Physics Letters A **372**, 4898 - 4901 (2008).

Denisov, S.I., W. Horsthemke and P. Hänggi: Steady-state Lévy flights in a confined domain. Physical Review E **77**, 061112 (2008).

Hallerberg, S., J. Bröcker and H. Kantz: Prediction of extreme events. In: Nonlinear time series analysis in the geosciences. Eds. R.V. Donner, S.M. Barbosa. Berlin : Springer, 2008. S. 35 - 60.

Hallerberg, S. and H. Kantz: How does the quality of a prediction depend on the magnitude of the events under study? Nonlinear Processes in Geophysics **15**, 321 - 331 (2008).

Hallerberg, S. and H. Kantz: Influence of the event magnitude on the predictability of an extreme event. Physical Review E **77**, 011108 (2008).

Hussein, M.S., J.X. de Carvalho, M.P. Pato and A.J. Sargeant: Symmetry breaking study with random matrix ensembles. AIP Conference Proceedings **995**, 212 - 220 (2008).

Ihle, T.: Transport coefficients of multi-particle collision algorithms with velocity-dependent collision rules. Journal of Physics Condensed Matter **20**, 235224 (2008).

Jalan, S. and J.N. Bandyopadhyay: Random matrix analysis of network Laplacians. Physica A **387**, 667 - 674 (2008).

Konrad, T., F. de Melo, M. Tiersch, C. Kasztelan, A. Aragão and A. Buchleitner: Evolution equation for quantum entanglement. Nature Physics **4**, 99 - 102 (2008).

Lakshminarayan, A., S. Tomsovic , O. Bohigas and S.N. Majumdar: Extreme statistics of complex random and quantum chaotic states. Physical Review Letters **100**, 044103 (2008).

Lindner, B.: Diffusion coefficient of a Brownian particle with a friction function given by a power law. Journal of Statistical Physics **130**, 523 - 533 (2008).

Lindner, B. and E.M. Nicola: Critical asymmetry for giant diffusion of active Brownian particles. Physical Review Letters **101**, 190603 (2008).

Lindner, B. and E.M. Nicola: Diffusion in different models of active Brownian motion. European Physical Journal Special Topics **157**, 43 - 52 (2008).

Mohanty, P.K. and S. Jalan: Analytical results for stochastically growing networks: Connection to the zero-range process. Physical Review E **77**, 045102 (2008).

Müller, M., G. Baier, C. Rummel and K. Schindler: Estimating the strength of genuine and random correlations in non-stationary multivariate time series. epl **84**, 10009 (2008).

Niemann, M. and H. Kantz: Joint probability distributions and multipoint correlations of the continuous-time random walk. Physical Review E **78**, 051104 (2008).

Niemann, M., T. Laubrich, E. Olbrich and H. Kantz: Usage of the Mori-Zwanzig method in time series analysis. Physical Review E **77**, 011117 (2008).

Rummel, C., M. Müller and K. Schindler: Data-driven estimates of the number of clusters in multivariate time series. Physical Review E **78**, 066703 (2008).

Santhanam, M.S. and H. Kantz: Return interval distribution of extreme events and long-term memory. Physical Review E **78**, 051113 (2008).

Schwalger, T. and B. Lindner: Higher-order statistics of a bistable system driven by dichotomous colored noise. Physical Review E **78**, 021121 (2008).

Wolff, L. and B. Lindner: Method to calculate the moments of the membrane voltage in a model neuron driven by multiplicative filtered shot noise. Physical Review E **77**, 041913 (2008).

Yamano, T., K. Sato, T. Kaizoji, J.M. Rost and L. Pichl: Symbolic analysis of indicator time series by quantitative sequence alignment. Computational Statistics and Data Analysis **53**, 486 - 495 (2008).

4.12 Deterministic Dynamics

2007

Altmann, E.G. and H. Kantz: Hypothesis of strong chaos and anomalous diffusion in coupled symplectic maps. epl **78**, 10008 (2007).

Benczik, I.J., T. Tél and Z. Köllö: Modulated point-vortex couples on a beta-plane: dynamics and chaotic advection. Journal of Fluid Mechanics **582**, 1 - 22 (2007).

Chong, G.S. and W.H. Hai: Dynamical evolutions of matter-wave bright solitons in an inverted parabolic potential. Journal of Physics B **40**, 211 - 220 (2007).

de Wijn, A.S. and H. Kantz: Vertical chaos and horizontal diffusion in the bouncing-ball billiard. Physical Review E **75**, 046214 (2007).

Flach, S., O.I. Kanakov, K.G. Mishagin and M. V. Ivanchenko: q-breathers in FPU-lattices - scaling and properties for large systems. International Journal of Modern Physics B **21**, 3925 - 3932 (2007).

Gelfert, K. and H. Kantz: Dynamical quantities and their numerical analysis by saddle periodic orbits. Physica D **232**, 166 - 172 (2007).

Kanakov, O.I., S. Flach, M.V. Ivanchenko and K.G. Mishagin: Scaling properties of q-breathers in nonlinear acoustic lattices. Physics Letters A **365**, 416 - 420 (2007).

Lissouck, D. and J.P. Nguenang: Solitary magnon excitations in a one-dimensional antiferromagnet with Dzyaloshinsky-Moriya interactions. Journal of Physics Condensed Matter **19**, 096202 (2007).

Penati, T. and S. Flach: Tail resonances of Fermi-Pasta-Ulam q-breathers and their impact on the pathway to equipartition. Chaos **17**, 023102 (2007).

Riecke, H., A. Roxin, S. Madruga and S.A. Solla: Multiple attractors, long chaotic transients, and failure in small-world networks of excitable neurons. Chaos **17**, 026110 (2007).

Riegert, A., W. Just, N. Baba and H. Kantz: Fast Hamiltonian chaos: Heat bath without thermodynamic limit. Physical Review E **76**, 066211 (2007).

Vilela, R.D. and A. E. Motter: Can Aerosols Be Trapped in Open Flows?. Physical Review Letters **99**, 264101 (2007).

Vilela, R.D., T. Tél, de Moura, A.P.S. and C. Grebogi: Signatures of fractal clustering of aerosols advected under gravity. Physical Review E **75**, 065203 (2007).

2008

Altmann, E.G., T. Friedrich, A.E. Motter, H. Kantz and A. Richter: Prevalence of marginally unstable periodic orbits in chaotic billiards. Physical Review E **77**, 016205 (2008).

Altmann, E.G. and T. Tél: Poincaré recurrences from the perspective of transient chaos. Physical Review Letters **100**, 174101 (2008).

Bahraminasab, A., F. Ghasemi, A. Stefanovska, P.V.E. McClintock and H. Kantz: Direction of coupling from phases of interacting oscillators: A permutation information approach. Physical Review Letters **100**, 084101 (2008).

Bahraminasab, A., D. Kenwright, A. Stefanovska, F. Ghasemi and McClintock: Phase coupling in the cardiorespiratory interaction. IET Systems Biology **2**, 48 - 54 (2008).

Baptista, M.S., J. X. de Carvalho and M.S. Hussein: Finding quasi-optimal network topologies for information transmission in active networks. PLoS ONE **3**, e3479 (2008).

Baptista, M.S., S.P. Garcia, S.K. Dana and J. Kurths: Transmission of information and synchronization in a pair of coupled chaotic circuits: An experimental overview. European Physical Journal Special Topics **165**, 119 - 128 (2008).

Baptista, M.S. and J. Kurths: Transmission of information in active networks. Physical Review E **77**, 026205 (2008).

Bröcker, J.: On reliability analysis of multi-categorical forecasts. Nonlinear Processes in Geophysics **15**, 661 - 673 (2008).

Bunimovich, L.A. and G. Del Magno: Semi-focusing billiards: ergodicity. Ergodic Theory and Dynamical Systems **28**, 1377 - 1417 (2008).

Cristadoro, G. and R. Ketzmerick: Universality of algebraic decays in Hamiltonian systems. Physical Review Letters **100**, 184101 (2008).

De Menech, M., P. Garstecki, F. Jousse and H.A. Stone: Transition from squeezing to dripping in a microfluidic T-shaped junction. Journal of Fluid Mechanics **595**, 141 - 161 (2008).

Eleftheriou, M. and S. Flach: Interaction of discrete breathers with thermal fluctuations. Low Temperature Physics **34**, 554 - 558 (2008).

Flach, S. and A.V. Gorbach: Discrete breathers - Advances in theory and applications. Physics Reports **467**, 1 - 116 (2008).

Flach, S. and A.V. Gorbach: Discrete breathers with dissipation. In: Dissipative solitons: from optics to biology and medicine. Ed. by N. Akhmediev. Berlin : Springer, 2008. S. 289 - 320.

Flach, S., M.V. Ivanchenko, O.I. Kanakov and K.G. Mishagin: Periodic orbits, localization in normal mode space, and the Fermi-Pasta-Ulam problem. American Journal of Physics **76**, 453 - 459 (2008).

Flach, S. and A. Ponno: The Fermi-Pasta-Ulam problem: Periodic orbits, normal forms and resonance overlap criteria. Physica D **237**, 908 - 917 (2008).

Gelfert, K. and C. Wolf: Topological pressure via saddle points. Transactions of the American Mathematical Society **360**, 545 - 561 (2008).

Javaloyes, J., M. Perrin and A. Politi: Collective atomic recoil laser as a synchronization transition. Physical Review E **78**, 011108 (2008) .

Kopidakis, G., S. Komineas, S. Flach and S. Aubry: Absence of wave packet diffusion in disordered nonlinear systems. Physical Review Letters **100**, 084103 (2008).

Maranhão, D.M., M.S. Baptista, J.C. Sartorelli and I.L. Caldas: Experimental observation of a complex periodic window. Physical Review E **77**, 037202 (2008).

Mishagin, K.G., S. Flach, O.I. Kanakov and M.V. Ivanchenko: q-breathers in discrete nonlinear Schrödinger lattices. New Journal of Physics **10**, 073034 (2008).

Moukam Kakmeni, F.M. and M.S. Baptista: Synchronization and information transmission in spatiotemporal networks of deformable units. Pramana **70**, 1063 - 1076 (2008).

Pasichnyk, I., R. Everaers and A.C. Maggs: Simulating Van der Waals interactions in water/hydrocarbon-based complex fluids. Journal of Physical Chemistry B **112**, 1761-1764 (2008).

Pereira, T., M. Thiel, M.S. Baptista and J. Kurths: Network mutual information and synchronization under time transformations. New Journal of Physics **10**, 083003 (2008).

Schulman, L.S. and E. Mihóková: Torus doubling resonances and breather stability. Physical Review E **78**, 026212 (2008).

Vincent, U.E. and A. Kenfack: Synchronization and bifurcation structures in coupled periodically forced non-identical Duffing oscillators. Physica Scripta **77**, 045005 (2008),

Zahnow, J.C., R.D. Vilela, U. Feudel and T. Tél: Aggregation and fragmentation dynamics of inertial particles in chaotic flows. Physical Review E **77**, 055301 (2008).

Ziesche, P.: Nichtlineare partielle Differentialgleichungen: Solitonen, periodische Muster und Chaos. In: Taschenbuch der Mathematik. Eds. I.N. Bronstejn [u.a.] Frankfurt: Deutsch, 2008. S. 608 - 614.

4.13 Structure Formation and Active Systems

2007

Chaudhuri, D.: Semiflexible polymers: Dependence on ensemble and boundary orientations. Physical Review E **75**, 021803 (2007).

Emmerich, H., R. Siquieri, M. Jurgk, J. Rezende and J. Hubert: A sharp interface model for the morphological evolution of precipitates in Al cast alloys. Philosophical Magazine Letters **87**, 863 - 869 (2007).

Fischer-Friedrich, E., R.N. van Yen and K. Kruse: Surface waves of Min-proteins. Physical Biology **4**, 38 - 47 (2007).

Jalan, S. and J.N. Bandyopadhyay; Random matrix analysis of complex networks. Physical Review E **76**, 046107 (2007).

John, K. and U. Thiele: Liquid transport generated by a flashing field-induced wettability ratchet. Applied Physics Letters **90**, 264102 (2007).

Kruse, K., M. Howard and W. Margolin: An experimentalist's guide to computational modelling of the Min system. Molecular Microbiology **63**, 1279 - 1284 (2007).

Li, W. and X. Cai: Empirical analysis of a scale-free railway network in China. Physica A **382**, 693 - 703 (2007).

Madruga, S. and H. Riecke: Hexagons and spiral defect chaos in non-Boussinesq convection at low Prandtl numbers. Physical Review E **75**, 026210 (2007).

Madruga, S. and H. Riecke: Reentrant and whirling hexagons in non-Boussinesq convection. European Physical Journal Special Topics **146**, 279 - 290 (2007).

Martin, C.P., M.O. Blunt, E. Paulic-Vaujour, A. Stannard, P. Moriarty, I. Vancea and U. Thiele: Controlling pattern formation in nanoparticle assemblies via directed solvent dewetting. Physical Review Letters **99**, 116103 (2007).

Pereira, A., P.M.J. Trevelyan, U. Thiele and S. Kalliadasis: Dynamics of a horizontal thin liquid film in the presence of reactive surfactants. Physics of Fluids **19**, 112102 (2007).

Pereira, A., P.M.J. Trevelyan, U. Thiele and S. Kalliadasis: Interfacial hydrodynamic waves driven by chemical reactions. Journal of Engineering Mathematics **59**, 207 - 220 (2007).

Rüdiger, S., E.M. Nicola, J. Casademunt and L. Kramer: Theory of pattern forming systems under traveling-wave forcing. Physics Reports **447**, 73 - 111 (2007).

Siepmann, P., C.P. Martin, I. Vancea, P.J. Moriarty and N. Krasnogor: A genetic algorithm approach to probing the evolution of self-organized nanostructured systems. Nano Letters **7**, 1985 - 1990 (2007).

Siquieri, R., H. Emmerich and M. Jurgk: Computation of solidification problems with hydrodynamic convection resolving energetic anisotropies at the microscale quantitatively. European Physical Journal Special Topics **149**, 27 - 41 (2007).

Thiele, U.: Structure formation in thin liquid films. In: Tin films of soft matter. Ed. by S. Kalliadasis and U. Thiele. Wien, New York: Springer, 2007. S. 25 - 93.

Thiele, U., S. Madruga and L. Frastia: Decomposition driven interface evolution for layers of binary mixtures. I. Model derivation and stratified base states. Physics of Fluids **19**, 122106 (2007).

Winkler, R.G. and A.G. Cherstvy: Adsorption of weakly charged polyelectrolytes onto oppositely charged spherical colloids. Journal of Physical Chemistry B **111**, 8486 - 8493 (2007).

2008

Aquino, G., A. Allahverdyan and T.M. Nieuwenhuizen: Memory effects in the two-level model for glasses. Physical Review Letters **101**, 015901 (2008).

Gross, T. and B. Blasius: Adaptive coevolutionary networks: a review. Journal of the Royal Society Interface **5**, 259 - 271 (2008).

Gross, T. and I.G. Kevrekidis: Robust oscillations in SIS epidemics on adaptive networks: Coarse graining by automated moment closure. epl **82**, 38004 (2008).

Günther, S. and K. Kruse: A simple self-organized swimmer driven by molecular. epl **84**, 68002 (2008).

John, K., P. Hänggi and U. Thiele: Ratchet-driven fluid transport in bounded two-layer films of immiscible liquids. Soft Matter **4**, 1183 - 1195 (2008).

Pazó, D. and E.M. Nicola: Breaking chirality in nonequilibrium systems on the lattice. epl **81**, 10009 (2008).

Peruani, F., A. Deutsch and M. Bär: A mean-field theory for self-propelled particles interacting by velocity alignment mechanisms. European Physical Journal Special Topics **157**, 111 - 122 (2008).

Peruani, F. and G.J. Sibona: Dynamics and steady states in excitable mobile agent systems. Physical Review Letters **100**, 168103 (2008).

Stannard, A., C.P. Martin, E. Pauliac-Vaujour, P. Moriarty and U. Thiele: Dual-scale pattern formation in nanoparticle assemblies. Journal of Physical Chemistry C **112**, 15195 - 15203 (2008).

Vancea, I., U. Thiele, E. Pauliac-Vaujour, A. Stannard, C.P. Martin, M.O. Blunt and P.J. Moriarty: Front instabilities in evaporatively dewetting nanofluids. Physical Review E **78**, 041601 (2008).

4.14 Dynamics in Nanoscale Systems

2007

Bandopadhyay, S. and A.M. Jayannavar: Phase time for a tunneling particle. International Journal of Modern Physics B **21**, 1681 - 1704 (2007).

Bulgakov, E.N., I. Rotter and A.F. Sadreev: Comment on "Bound-state eigenenergy outside and inside the continuum for unstable multilevel systems". Physical Review A **75**, 067401 (2007).

Bulgakov, E.N., I. Rotter and A.F. Sadreev: Correlated behavior of conductance and phase rigidity in the transition from the weak-coupling to the strong-coupling regime. Physical Review B **76**, 214302 (2007).

Chakrabarti, A.: Fano resonance in discrete lattice models: Controlling lineshapes with impurities. Physics Letters A **366**, 507 - 512 (2007).

Chaudhuri, D., A. Chaudhuri and S. Sengupta: Fluctuations at a constrained liquid-solid interface. Physical Review Letters E **76**, 021603 (2007).

Chaudhuri, D., A. Chaudhuri and S. Sengupta: Heat conduction through a trapped solid: the effect of structural changes on the thermal conductance. Journal of Physics Condensed Matter **19**, 152201 (2007).

Günther, U., I. Rotter and B. F. Samsonov: Projective Hilbert space structures at exceptional points. Journal of Physics A **40**, 8815 - 8833 (2007).

Hentschel, M., G. Röder and D. Ullmo: Many-body effects in the mesoscopic x-ray edge problem. Progress of Theoretical Physical Supplement **166**, 143 - 151 (2007).

Hentschel, M., D. Ullmo and H.U. Baranger: Fermi-edge singularities in the mesoscopic regime: Photo-absorbtion spectra. Physical Review B **76**, 245419 (2007).

Hentschel, M., D.C.B. Valente, E.R. Mucciolo and H.U. Baranger: Improving intrinsic decoherence in multi-quantum-dot charge qubits. Physical Review B **76**, 235309 (2007).

Komineas, S.: Rotating vortex dipoles in ferromagnets. Physical Review Letters **99**, 117202 (2007).

Moutafis, C., S. Komineas, C.A.F. Vaz, J.A.C. Bland, T. Shima, T. Seki and K. Takanashi: Magnetic bubbles in FePt nanodots with perpendicular anisotropy. Physical Review B **76**, 104426 (2007).

Rotter, I.: The brachistochrone problem in open quantum systems. Journal of Physics A **40**, 14515 - 14526 (2007).

Rotter, I. and A.F. Sadreev: Singularities caused by coalesced complex eigenvalues of an effective hamilton operator. International Journal of Theoretical Physics **46**, 1914 - 1928 (2007).

Sandalov, I. and R.G. Nazmitdinov: Shell effects in nonlinear magnetotransport through small quantum dots. Physical Review B **75**, 075315 (2007).

Shabat, M.M., H. Khalil, S.A. Taya and M.M. Abadla: Analysis of the sensitivity of self-focused nonlinear optical evanescent waveguide sensors. International Journal of Optomechatronics **1**, 284 - 296 (2007).

2008

Bertulani, C.A., M.S. Hussein and G. Verde: Blurred femtoscopy in two-proton decay. Physics Letters B **666**, 86 - 90 (2008).

Buchleitner, A., A.R.R. Carvalho and F. Mintert: Measures and dynamics of entanglement. European Physical Journal Special Topics **159**, 47 - 56 (2008).

Ciappina, M.F., A. Becker and A. Jaro-Becker: High-order harmonic generation in fullerenes with icosahedral symmetry. Physical Review A **78**, 063405 (2008).

Komineas, S. and N. Papanicolaou: Transmutation of momentum into position in magnetic vortices. New Journal of Physics **10**, 043021 (2008).

Licata, N.A. and A.V. Tkachenko: How to build nanoblocks using DNA scaffolds. epl **84**, 20010 (2008).

Morawetz, K., C. Olbrich and S. Gemming: Reduction of surface coverage of finite systems due to geometrical steps. European Physical Journal B **62**, 311 - 317 (2008).

Müller, C., B. Herschend, K. Hermansson and B. Paulus: Application of the method of increments to the adsorption of CO on the $CeO_2(110)$ surface. Journal of Chemical Physics **128**, 214701 (2008).

Pauliac-Vaujour, E., A. Stannard, C.P. Martin, M.O. Blunt, I. Notingher, P.J. Morianty, I. Vancea and U. Thiele: Fingering Instabilities in Dewetting Nanofluids. Physical Review Letters **100**, 176102 (2008).

Rotter, I. and A. F. Sadreev: Unified Description of Resonance and Decay Phenomena in Quantum Dots. In: Quantum Dots: Research, Technology and Applications. Ed. by R. W. Knoss. New York : Nova Science Publ., 2008. S. 429 - 492.

Sadreev, A.F., E. N. Bulgakov, K. N. Pichugin, I. Rotter and T. V. Babushkina: Transmission through Quantum Dots with Variable Shape. Bound States in the Continuum. In: Quantum Dots: Research, Technology and Applications. Ed. by R. W. Knoss. New York : Nova Science Publ., 2008. S. 547 - 577.

Scholak, T., F. Mintert and C.A. Müller: Entanglement witnesses from single-particle interference. epl **83**, 60006 (2008).

Shamshutdinova, V.V., K.N. Pichugin, I. Rotter and B.F. Samsonov: Feshbach projection-operator formalism applied to resonance scattering on Bargmann-type potentials. Physical Review A **78**, 062712 (2008).

Wiersig, J., S. Flach and K.-H. Ahn: Discrete breathers in ac-driven nanoelectromechanical shuttle arrays. Applied Physics Letters **93**, 222110 (2008).