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. P. Fulde* as the Founding Director. The concept for the institute includes three scientific divisions and a large-scale visitors program. The incorporation of a seminar and workshop program within the visitors program was expected to become a significant part of the institute's activities. The program aims at promoting new developments in the field of the physics of complex systems. One important aspect is to provide a high-level platform for young scientists from universities to become acquainted with recent research developments much earlier than was traditionally the case. At the same time, important new research areas in the field of theoretical physics are promoted efficiently. Dresden was chosen as the location for the institute due to its favorable scientific environment and good travel connections. In July 1993, *Prof. P. Fulde* started the scientific activities of the first division *Electronic Correlations* at first in Stuttgart, as proper office space in Dresden was lacking. This was supplied in January 1994 thanks to the TU Dresden generously offering a temporary accomodation for the institute. The institute was officially inaugurated by *Prof. H. Zacher*, President of the Max Planck Society, on May 2nd, 1994. An administration was installed, headed by *Mrs. I. Auguszt*. The Visitors Program began to operate, first guests were invited, and the first workshop took place in March 1994.

1995-1998 • In 1995, *Dr. H. Kantz* joined the institute as head of an independent Junior Research Group on *Nonlinear Time Series Analysis*. Moreover, the **mpipks** decided to broaden its research spectrum considerably by installing temporary Junior Research Groups: The group *Pattern Formation in Reaction-Diffusion-Systems* headed by *Dr. M. Bär* started its activities in 1995, the group *Quantum Chaos and Mesoscopic Systems* headed by *Dr. K. Richter* in January 1996, and the group *Quantum Cheminstry* headed by *Dr. M. Dolg* soon after. At the same time, plans for the institute's building and guest houses took shape. The architecture firm Brenner und Partner (Stuttgart) with J. Wittfoth won the competitive bidding, and constructions started in September 1995. After less than two years the institute moved into the newly constructed main building and put into service the three guest houses. In the meantime the Seminar- and Visitors-Program were gaining momentum, with hundreds of scientists having visited the institute.

1999-2001 • The next, important step was the appointment of *Prof. J. M. Rost* as head of the second division of the institute. *Prof. Rost* started the activities in 1999 by setting up the division *Finite Systems*. He appointed *Dr. A. Buchleitner* as head of a research group *Nonlinear Dynamics in Quantum Systems*. After *Dr. Dolg* accepted an offer for a professorship at the University of Bonn, *Dr. U. Birkenheuer* was appointed as his successor in March 2000. Soon afterwards, *Dr. K. Richter* left for a chair of 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* was appointed as head of a new Junior Research Group *Waves in Complex Media and Mesoscopic Phenomena* in November 2000.

2001-2002 • To account for the increasing demand for building bridges between physics and biology, *Prof. F. Jülicher* 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*, and *Biological Physics of Olfaction: From Genes to Networks* headed by *Dr. M. Zapotocky* started their activities within the third division in 2002. Moreover, the division *Finite Systems* continued to broaden its research spectrum by appointing *Dr. A. Becker* as head of the new research group *Nonlinear Processes in Strong Fields*.

2003-2004 • In 2003, *Dr. S. Kümmel* started the activities of an Emmy Noether Group *Electronic Structure of Finite Systems*. One year later, the first two Junior Research Groups within the joint research program *Physics of Biological Systems* initiated together with the Max Planck Institute for Molecular Cell Biology and Genetics (MPI-CBG) in Dresden were established: *Dr. K. Kruse*, head of the group *Physics of Cell Division*, worked theoretically at the mpi**pks**; *Dr. I. M. Tolić-Nørrelykke*, head of the group *Mechanics of Cell Division*, experimentally at the MPI-CBG. The construction of an extension to the institute building was started in 2004. In the same year, *Dr. M. Bär* took up a position as a department head at the Physikalisch-Technische Bundesanstalt in Berlin.

2005-2006 • In 2005, *Dr. S. Kümmel* accepted a professorship at University of Bayreuth, and *Dr. H. Schomerus* accepted a faculty position at Lancaster University. *Dr. M. Hentschel* started the activities of an Emmy Noether group *Many Body Effects in Mesoscopic Systems*. *Dr. S. Grill* 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. The new wing of the institute was completed at the end of 2005. It provides additional office space and a new seminar room and has quickly turned into a new and vibrant focal point of meetings, poster sessions, discussions and collaborations. In 2006, *Dr. K. Kruse* and *Dr. R. Everaers* accepted professorships at the University of Saarbrücken and the École normale Supérieure in Lyon.

2007-2008 • During this period *Prof. P. Fulde* retired from his position as a director of the mpi**pks** and as head of the department *Electronic Correlations*. *Prof. R. Moessner* was appointed as new director, and started to set up his department *Condensed Matter* in early 2008. *Dr. A. Becker* accepted the offer of a JILA fellow (Joint Institute for Laboratory Astrophysics) 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 the mpi**pks** to head the Junior Research Group *Dynamics of Biological Networks*, and *Dr. B. Lindner* set up the activities of the research group *Stochastic Processes in Biophysics*. In the same year, *Dr. S. Skupin* started his Junior Research Group *Computational Nonlinear and Relativistic Optics*, with close links to the Forschungszentrum Rossendorf. In 2008, the research group *Complex Dynamics in Cold Gases* was founded and headed by *Dr. T. Pohl*, and the research group *New States of Quantum Matter* was founded and headed by *Dr. A. Läuchli*.

2009-2010 • In 2009, *Dr. S. Kirchner* joined the mpi**pks** as head of the Junior Research Group *Collective Phenomena in Solid State and Materials Physics* which is operating jointly with the neighboring Max Planck Institute for Chemical Physics of Solids (MPI-CPfS). Moreover, *Dr. K. Hornberger* arrived at the mpi**pks** to head the research group *Molecular Quantum Optics*. In the following year, *Prof. R. Ketzmerick* (TU Dresden) was appointed by the Max Planck Society as a *Max Planck Fellow* and started the activities of the Max Planck Fellow group *Chaos and Quantum Chaos* at the mpi**pks**. In winter 2010, *Dr. E. Altmann* arrived to set up the Otto Hahn Group *Dynamical Systems and Social Dynamics*. The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* was successfully renewed for a second six-year period.

2011-2012 • In 2011 and 2012, several Junior Research Group leaders left the mpi**pks** for permanent position: *Dr. K. Hornberger*, *Dr. A. Läuchli*, *Dr. B. Lindner*, and *Dr. M. Hentschel* moved to professorships at the University of Innsbruck, the University Duisburg-Essen, the Humboldt University Berlin, and the Technical University Illmenau. *Dr. T. Gross* accepted a reader position at the University in Bristol. The Junior Research Group *Computational Quantum Many-Body Physics* was concluded in August 2012 after

seven months in existence, when the group leader *Dr. E. Gull* accepted a faculty position at the University of Michigan. On the other hand, several new groups were etablished: *Dr. F. Pollmann* set up the activities of Junior Research Group *Topology and Correlation in Condensed Matter*. The group *Physics of the Cytoskeleton* headed by *Dr. G. Salbreux*, the group *Computational Biology and Evolutionary* headed by *Dr. M. Hiller*, and the group *Collective Dynamics of Cells* headed by *Dr. V. Zarbudaev* were installed to complement the activities of the *Biological Physics* division. Within the division *Finite Systems*, *Dr. A. Eisfeld* was appointed as head of the group *Quantum Aggregates*, and *Dr. N. Rohringer* as head of the group *X-Ray Quantum Optics*, which operates at the Center of Free-Electron Laser Science, Hamburg. To accomodate the increasing number of visiting scientists, a fourth guest house was build and inaugurated in November 2012. The joint research program of the mpi**pks** and the MPI-CBG was intensified and institutionalized in the form of the newly founded *Center for Systems Biology Dresden*.

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

1.2 Research Areas and Structure of the Institute

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

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

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

- The Junior Research Group *Computational Nonlinear and Relativistic Optics* is headed by *Dr. S. Skupin* and links the work of the mpi**pks** to the Forschungszentrum Rossendorf.
- The Junior Research Group *Collective Phenomena in Solid State and Material Physics* is headed by *Dr. S. Kirchner* and connects the research pursued at the mpi**pks** and at the MPI-CPfS.
- The Max Planck Fellow Group *Chaos and Quantum Chaos* is headed by *Prof. R. Ketzmerick* (TU Dresden) and links the mpi**pks** to the Technische Universität Dresden.
- The Otto Hahn Group *Dynamical Systems and Social Dynamics* is headed by *Dr. E. Altmann*. Its research interest connects the mpi**pks** and the Technische Universität Dresden.
- The only permanent research group, headed by *Prof. H. 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.

Until mid 2012, the mpi**pks** and the MPI-CBG ran a joint research program *Physics of Biological Systems*, which comprised three closely interacting Junior Research Groups. These joint research groups built a close link between both institutes to promote collaborative work on the physics of cells:

- The Junior Research Group *Computational Biology and Evolutionary Genomics* is headed by *Dr. M. Hiller* and operates at the mpi**pks**.
- The Junior Research Group *Motor Systems* is headed by *Dr. S. Grill*. It is affiliated with both institutes and works both theoretically and experimentally.
- A third experimental Group *Interior Design of the Cell* headed by *Dr. I. M. Tolić-Nørrelykke* is located at the MPI-CBG.

In summer 2012, the joint research program of the mpi**pks** and the MPI-CBG has been expanded and institutionalized: The Center for Systems Biology Dresden was installed as a permanent research center run by both institutes. The research spectrum has been extended to Bioinformatics and Image Analysis.

1.3 Workshop and Visitors Program

Central to the mission of the institute is to conduct international *Workshops and Seminars* (p. 131), which makes the mpi**pks** an almost unique institute within the Max Planck Society, only comparable with the mathematics institute in Bonn. A small but efficient team headed by *Dr. L. Do* is responsible for the logistics and the preparation of meetings, and gives advice and support to the (usually external) scientific coordinators on the various aspects of planning and conducting the corresponding event.
The *Visitors Program* (p. 120) offers research visits ranging from a few weeks to two years in duration. Guest scientists use various ways of collaboration by joining research groups at the institute, by doing joint research with other guest scientists, or by starting collaborations with workshop and seminar participants. Further possibilities of collaboration include contacts with the TU Dresden or other local research institutions, well documented, e.g., by common publications (see p. 173).
Proposals for workshops and seminars, as well as applications for guest scientist positions, are evaluated by two different committees. Members of each committee include both external scientists and scientists of the institute.
In order to further strengthen and structure the Visitors Program, the mpi**pks** started in 2000 to annually award the *Martin Gutzwiller Fellowship* to an internationally recognized and experienced scientist. The last two awardees *Prof. B. Altshuler* (Columbia University) 2011 and *Prof. T. Nakayama* (Hokkaido University) 2012 have spent up to one academic year at the mpi**pks** (p. 121).
Moreover, the mpi**pks** annually offers one *Distinguished PKS Postdoctoral Fellowship*. It aims at excellent young researchers, shortly before accepting a tenure track position (p. 125).
In 2007, *Advanced Study Groups* were launched at the mpi**pks**. These groups consist of three to five experienced researchers, who join forces to do cutting-edge research on a topic from the field of the physics of complex systems. In 2011, we hosted the group *Towards a semiclassical Theory of Dynamical Tunneling* under the leadership of *Prof. S. Tomsovic*, in 2011 and 2012 the group *Statistical Physics of Collective Motion* coordinated by *Prof. H. Chate*. In December 2012, the group *Topological Band Structures and Their Instabilities* headed by *Prof. I. Herbut* started its activities, which will continue until summer 2013.

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. 157). 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 the mpi**pks** as well as at high schools (p. 162).
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 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. Additionally, the mpi**pks** participates in the IMPRS *Molecular Cell Biology and Bioengineering* initiated by the MPI-CBG.
Research Organization • The large-scale Workshop and Seminar Program at the mpi**pks** offers the unique possibility for young scientists to take part in the organization of meetings. Out of the 34 events during 2011-2012, young scientists of the institute took part in the coordination of 7. This has a positive educational effect for young scientists and helps the external coordinators through the permanent contact with a local scientific coordinator.

1.5 Equal Opportunities

Over the last years we were able to increase the percentage of female researchers to 10% of all postdocs and 20% of all predocs holding a contract of more than three months. In addition to the standard

measures of ensuring equal opportunities, the mpi**pks** participates in the scientific activities on the annual *Girl's Day* and invites female students from high schools to informative lectures and discussions about a career in science. In order to meet the needs of researchers with young children we have installed a *parent & child apartment* in guest house 3. In combination with day care offers, these facilities give young researchers the opportunity to participate in workshops and seminars while their children are looked after in the guest house. When not booked for workshop participants, the *parent & child apartment* is frequently used by members of the mpi**pks** who need to bring their young children during working hours.

1.6 Public Relations

The institute considers itself as a platform for the emergence, exchange, development and promotion of creative ideas in research. While mainly focusing on scientists, this also includes potential future scientists, i.e., high school students, teachers. Within our school-contact program we try to enthuse and inspire students through direct contact with young scientists.
Since 1999, the mpi**pks**, the TU Dresden, and the City of Dresden are running the lecture series *Science in the City Hall*. Well-known scientists are invited to give lectures for the broad public (p. 161). Furthermore, all workshop coordinators are encouraged to organize a public evening lecture which opens up the topic of scientific event to interested laymen. Since 2006, when Dresden was awarded the title 'Stadt der Wissenschaft 2006', the mpi**pks** has participated in numerous activities which are part of the annual program of the scientific community of Dresden.

1.7 Research Networking

Local • The mpi**pks** finds itself in the midst of a rich research environment, formed by the TU Dresden and the surrounding research institutes. The vivid scientific dialogue with the Physics Department of the TU Dresden is mirrored in the Max Planck Fellow Group *Chaos and Quantum Chaos* headed by *Prof. R. Ketzmerick*, and in the mpi**pks** participation in the cluster of excellence *Center for advancing electronics Dresden* and the graduate school *Biomedicine and Bioengineering*. The mpi**pks** has particular close contacts to the Institute of Theoretical Physics and the Institute of Biophysics at the Physics Department; Institute members are involved in various Research Focus Programs (p. 155). The division *Condensed Matter* is cooperating with the IFW (Institut für Festkörper- und Werkstoffforschung) and the neighboring Max Planck Institute for Chemical Physics of the Solid State. In particular, the two MPIs run the joint Junior Research Group *Collective Phenomena in Solid State and Material Physics* headed by *Dr. S. Kirchner*. The division *Biological Physics* has established close contact to the Max Planck Institute of Molecular Cell Biology and Genetics. The cooperation between both institutes has been institutionalized in 2012 by the foundation of the Intersectional Center for Systems Biology. There are also intense collaborations with the Biotechnological Center and the newly founded Center for Regenerative Therapies. The divisions *Finite Systems* and *Condensed Matter* cooperate closely with the Research Center Rossendorf, in particular through joint research conducted by the Junior Research Group *Computational Nonlinear and Relativistic Optics* headed by *Dr. S. Skupin*. This group is in close contact with the faculty of physics and astronomy at the Friedrich-Schiller University in Jena, where *Dr. S. Skupin* holds a *Carl Zeiss Junior Professorship for Computational Photonics* since 2009.
National and International • The numerous different national and international collaborations and contacts are listed in the research group reports (Chapters 1.8, 1.9, and p. 129).

1.8 Departments and Research Groups

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

In condensed matter physics, complex behaviour arises due to the interactions between a large number of microscopic degrees of freedom; these degrees of freedom can themselves be very simple. The resulting behaviour is fascinating in its richness: many different phases exist as distinct 'vacua', each with its

own characteristic properties such as ground-state correlations, excitations, and dynamics in and out of equilibrium. The *Condensed Matter* division studies such collective behaviour. One aim is to connect the macroscopic behaviour of matter with the microscopic properties of its constituent particles. Another one is not only to discover and understand novel behaviour, but also to identify the principles according to which we can understand how the physical world is organised.

The search for such organising principles aims at extending the reach of universality in physics, a concept already well-entrenched in the context of phase transitions and critical phenomena. Its role in the more 'modern' context of topological condensed matter physics is yet to be determined. At the current stage, much effort is being invested in building up a comprehensive phenomenology which can serve as a basis for identifying these organising principles.

Development in the field is driven by a combination of analytical, numerical and experimental advances. In particular on the numerical front, the continous development of novel computer algorithms, which goes along with and utilises the ever-increasing availability of computing power, is playing an increasingly important role. In addition to this, we work on utilising field theories and developing more intuitive 'heuristic' approaches to advance our understanding of the new field. Experimentally, a central challenge continues to be the identification of topological physics – featureless to many conventional probes – in laboratory settings and our theoretical effort is aimed at guiding this search.

Research Topics

New settings for topological physics in electronic and optical systems: a family of studies on topics as disparate as the excitation spectrum of Skyrmion lattices in the quantum Hall effect away from commensurate fillings; design strategies for optical flux lattices; as well as interacting lattice models with bands with non-zero Chern number, has unearthed a wealth of connections rooted in common mathematical underpinnings. On the level of phenomenology, for the latter topic we have not only established the presence of a hierarchy of fractional Chern insulating states (the analogue of quantum Hall hierarchies) but also the existence of compressible states and we have identified a lattice-based mechanism for their competition.

Extended and itinerant degrees of freedom in magnets: We have investigated non-local correlations in unconventional magnets, as well as their role in the physics of itinerant electrons, whose paths can be sensitive to them. We have found that in magnetic Coulomb phases, extended one-dimensional degrees of freedom ('strings') arise naturally independently of spatial dimensionality. Their length distribution is characteristically power-law in nature. Intriguingly, such a distribution occurs also in a class of trial wavefunctions for spin liquids, where they turn out to herald the presence of magnetic Néel order!

Fluctuation-induced ordering: order by disorder describes the genesis of order when degeneracies are lifted by thermal or quantum fluctuations. For both cases, we have made contributions to long-standing open questions. Firstly, we have established that thermal order by disorder in the kagome Heisenberg antiferromagnet leads to spin order with a tripled unit cell and a tiny ordered moment, thus answering a question that had been open for a couple of decades. Secondly, our analysis of the behaviour of $Er_2Ti_2O_7$ has provided the best example yet of quantum order by disorder in a magnetic compound in experiment.

Magnetic monopoles and frustrated spin systems: our analysis of the fundamentally novel properties of spin ice, as well as their manifestations in experiment, has continued. This has included analyses of the internal field distribution in spin ice and its signatures in NMR and μSR experiments; a detailed development of Debye-Hückel theory for the low-energy thermodynamics; as well as analyses of out-of-equilibrium behaviour.

Superconductivity and materials phenomenology: our work especially on the pnictide superconductors and their intricate order parameters and concomitant excitations is ongoing, much of it in collaboration with local experimental groups.

Adiabatic quantum computing: We have established (the absence of) a connection between the thermodynamic order of a phase transition and the scaling of the many-body gap near it, explicitly proving that first-order transitions can have gaps which are only algebraically small and which are therefore not fatal for a quantum adiabatic computer. In addition, we have provided a new 'topological' mechanism for generating exponentially small gaps, which adds a new "failure mode" for adiabatic quantum computation protocols.

Perspectives

The condensed matter division at the mpi**pks** was constituted in late 2007 with the arrival of Roderich Moessner as director. The first group leader to join, in the course of the year 2008, was Andreas Läuchli, a computational physicist who has left for a professorship at the University of Innsbruck in Austria. Frank Pollmann arrived in 2011 to head a group working on "Topology and correlations in condensed matter". His interests lie in the study of strongly correlated phases in low dimension, in particular in the development of new algorithms for their investigation. Emmanuel Gull joined at the beginning of 2012 to head the group "Computational quantum many-body physics", and was quickly offered a Professorship in Michigan which he took up later that year.

Among the research directions we plan to pursue in the future, we would like to highlight the following.

Glassiness and topology: the combined appearance of spin liquidity and glassiness has been one of the mainstays of the study of exotic magnets since its very inception. Few are the examples where the interplay between these two phenomena is well understood. In particular, it is generally not even known whether one typically encounters a relatively trivial (e.g. spatially segregated) coexistence, or whether the spin liquid intrinsically functions as the matrix for the glass. With the understanding of defects and their interactions in spin liquids that we have built up over the past few years, we are now in a position to address this complex of questions.

The study of excitations and dynamics is a very active and rapidly growing field, combining many facets such as the genesis of novel excitations in topological phases; real-time dynamics under (periodic) driving or after a quench and the approach to a (generalised) equilibrium; or non-linear transport phenomena. This set of questions will be a focal point of our research over the next few years.

Complexity and quantum information theory: The study of computational complexity classifies the hardness of families of problems according to the scaling of the runtime of instances according to their size. A natural complementary question is how hard it is, in the absence of an efficient solution strategy, to find an *approximate* solution of the problem at hand. This requires developing an understanding of how quantum entanglement influences our ability to design approximation strategies. This we plan to study in the context of *quantum* complexity thoery, for k-QSAT, an ensemble of random quantum optimisation problems, the worst-case instances of which are known to be in the complexity class QMA_1, a generalisation of the venerable classical complexity class NP.

Cooperations

- *Joint group with Max Planck Institute for the Chemical Physics of Solids:* At the beginning of 2009, a joint research group in the field of quantum condensed matter was set up between the mpi**pks** and the MPI-CPfS. This group on "Collective phenomena in solid state and materials physics" has a research activity centred on the field of quantum phase transitions, which substantively complements the research undertaken in the condensed matter division. It is headed by Stefan Kirchner.

- *Manifold collaborations with theory groups internationally, e.g.:*
  - England: Oxford University (John Chalker); University of Cambridge (Claudio Castelnovo; Nigel Cooper)
  - France: École Normale Supérieure Lyon (Peter Holdsworth); Université Paris VI (Jussieu) (Benoit Douçot); Université Paul Sabatier Toulouse (F. Alet); CEA Grenoble (M. Zhitomirsky)
  - Hungary: Budapest University of Technology and Economics (Balazs Dora)
  - India: Tata Institute for Fundamental Research (Kedar Damle)
  - Italy: ICTP Trieste (Antonello Scardiccio)
  - Ukraine: National Academy of Sciences (Oleg Derzkho)
  - United States: Harvard University (Chris Laumann); Princeton University (Shivaji Sondhi); University of Wisconsin at Madison (Andrey Chubukov)

- *Collaborations with experimental groups, e.g.:*
  - Argentina: UNLP-Conicet La Plata – Santiago Grigera (non-equilibrium behaviour in spin ice)

- Germany:
  - Helmholtz-Zentrum Berlin – Alan Tennant (Magnetic materials with Coulomb phases)
  - High magnetic field laboratory, Helmholtz Zentrum Dresden-Rossendorf – Sergei Zherlitsyn, Jochen Wosnitza (ultrasound studies on frustrated magnets)
  - IFW Dresden – Bernd Büchner (novel superconductors)
  - TU Dresden – Hans-Henning Klauss (novel superconductors)
  - Universität Köln – Markus Braden (novel superconductors)
- Japan: RIKEN – Masashi Takigawa (NMR on frustrated magnets)

Research Group: Computational Many-Body Physics
(Head: Dr. Emanuel Gull)

Strongly correlated quantum many-body systems show a wealth of collective phenomena and appear in condensed matter physics in topics ranging from quantum criticality in heavy fermion systems to the Kondo screening of impurities, high temperature superconductivity, or anomalous metallic phases. Similar correlated quantum behavior is also visible in experiments probing strongly interacting quark/gluon matter, among them relativistic heavy ion collisions. Our understanding of correlated quantum many-body systems is severely limited as none of the established analytical approaches are able to provide reliable and generally valid results. Perturbation theory, for example, does not work away from the weak coupling limit. Unbiased numerical methods for strongly correlated systems have proven to be a reliable alternative. The design, development, and implementation of such methods was the task of the computational quantum many-body physics group at the mpi**pks**.

Physics of lattice systems in the thermodynamic limit Can numerical methods provide numerically exact solutions of interesting fermionic lattice systems in the correlated regime? Can all approximations (finite size approximations, systematic errors, stochastic errors) be controlled and encapsulated in an error bar that can be made arbitrarily small? Can finite size scaling be done to the standards that are commonly employed in classical statistical mechanics, such that accurate phase boundary and equations of state for, e.g., the Hubbard model on a two-dimensional square lattice (relevant to high temperature superconductivity and cold atomic gas experiments) can be extracted? These are among the core questions that our group addressed when simulating large systems using the cluster dynamical mean field approach.

Physics of lattice systems at low temperature Numerically exact solutions are not always obtainable, especially at low temperature. Numerical methods nevertheless can provide insight into quantum many-body physics and test theoretical proposals based on uncontrolled approximations. The physics of lattice systems at very low temperature, especially in ordered (e.g. superconducting) phases, was another topic of this group.

Physics of correlated impurity systems in non-equilibrium at low T Equilibrium physics is relatively well understood, and a large set of tools for solving the equations of equilibrium quantum statistical mechanics exists. The generalization of these tools to non-equilibrium situations, and in particular correlated non-equilibrium situations, was another focus area of this group. We investigated quantum quenches, Kondo resonances, and the initial transients and short time behavior of correlated quantum impurities.

Algorithm design and development Numerical simulations require reliable numerical methods. The design, development, and implementation of these methods were a core activity of this group and one of the main prerequisites for obtaining results for interesting physics systems. Our algorithms are published and our implementations eventually become open source and are provided to the physics community free of charge. Our open source implementations for quantum impurity systems, for example, are rapidly becoming popular in the materials simulation community in the context of the so-called 'dynamical mean field' approximation, where they are used to investigate the physics of a wide range of correlated materials.

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

The research group "New states of quantum matter" started its activity at the mpi**pks** in September 2008. During the report period it hosted three postdocs (D. Charrier from 2009 to 2011, I. Rousochatzakis from 2009 to 2011 and V. Alba from 2010 to 2012), as well as shorter term visitors.

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

Ground state phases of $SU(N)$-symmetric quantum magnetism Quantum magnetism in condensed matter originates from the spin of the electron and is ideally $SU(2)$-invariant. Recently it was suggested that ultracold alkaline-earth atoms are particularly well suited as potential quantum simulators for $SU(N)$ quantum magnetism in optical lattices, where the N is encoded in the size of the nuclear spin and can be as large as $N = 10$. In condensed matter $SU(N)$ quantum magnetism has mostly been studied out of theoretical curiosity so far, but now a quantitative understanding of phase diagrams of simple $SU(N)$ symmetric quantum spin Hamiltonians is needed. In collaboration with P. Corboz (ETH Zürich), K. Penc (Budapest) and F. Mila (EPF Lausanne) we have started to investigate several models with $N = 3$ and 4 on different lattices. The resulting zoo of phases is very rich and ranges from $SU(N)$ analogues of valence bond solids and magnetic order to exotic emergent degrees of freedom, which then order in a second step and culminates in the discovery of an algebraic spin liquid for the $SU(4)$ Heisenberg model on the honeycomb lattice.

Entanglement spectra of gapped and continuous symmetry breaking wave functions In recent years the cross fertilization between quantum information and condensed matter has led to new insights into the physics of quantum many body systems. In particular the concept of *entanglement spectrum* (the negative logarithm of the eigenvalues of a reduced density matrix) has established itself as an informative and intriguing theme. Many results are now available for the entanglement spectrum and entanglement entropies of one-dimensional (1D) systems. In contrast, higher dimensions are far less explored. We performed a thorough analysis of the ES of the 2D Bose-Hubbard model, in particular highlighting very different structures of the ES in the Mott and superfluid phases. In the Mott phase, the ES can be understood perturbatively starting from the $U \to \infty$ product state limit. The ES is organized in a perturbative hierarchy and within each group there are dispersion structures reflecting the freedom of excitations to move along the boundary while retaining the same perturbation order. In the superfluid regime, the ES reflects the spontaneous symmetry breaking of the underlying state, and is related to the tower of states known from finite-size studies of energy spectra. The emergence of tower of states structures in the entanglement spectrum of ground state wave functions is likely to become a useful diagnostic in DMRG studies of systems undergoing continuous symmetry breaking in various forms.

Cooperations

- Theory groups
  - Lausanne, École Polytechnique Fédérale de Lausanne, collaboration with the group of F. Mila on topics in frustrated quantum magnetism and $SU(N)$ quantum magnetism
  - Dortmund, TU Dortmund, collaboration with the group of K.P. Schmidt on magnetic systems close to the Mott transition.
- Experimental groups
  - Collaborations with neutron scattering group at the University College London (Ch. Rüegg) on the modelling and interpretation of inelastic neutron scattering experiments performed on low-dimensional quantum magnets.
  - Dresden, MPI-CPfS, collaboration with the group of H. Rosner on the experimental characterization of magnetic insulators.

Research Group: Topology and Correlations in Condensed Matter
(Head: Dr. Frank Pollmann)

The research group "Topology and Correlations in Condensed Matter" has been established at the mpi**pks** in January 2011. It has now grown to have four postdocs (Luis Seabra, Shijie Hu, Jonas Kjäll, and Ching-Yu Huang) and three PhD students (Johannes Motruk, Krishanu Roy Chowdhury, and Siddhardh Chandra). We also hosted a number of summer students who worked in our group for one to two months each (Vivek Lohani, Richard Winkelmann, Sangmin Lee, and Mike Zaletel).

Our group is interested in a variety of problems in condensed matter physics. The focus mainly lies on the study of phenomena which arise due to quantum mechanical effects in systems of correlated electrons. Areas of research include the study of topological phases of matter, dynamical properties of quantum-many body systems, charge and spin degrees of freedom on geometrically frustrated lattices, and the applications of quantum-information concepts to strongly correlated systems. Over the past two years, our group worked particularly on the following topics:

Symmetry protected topological phases in one-dimensional systems. A topological phase is a phase of matter which cannot be characterized by a local order parameter. The lack of a local order parameter makes it impossible to understand these phases using the well established Landau-Ginzburg theory. Thus, new frameworks need to be developed to characterize this class of phases. We showed in a number of works that topological phases in one-dimensional systems can be completely characterized using tools related to projective representations of the symmetry groups. This gives us a theoretical background which allows us to tell which kinds of topological phases can be realized given a certain set of symmetries in a physical system. Based on these insights, we derived non-local order parameters that can be use to detect topological phases. The non-local order parameters can be seen as a generalization of the string order which is used to detect the Haldane phase in integer spin chains. Using these tools, we found a number of realizations of symmetry protected topological phases in simple, one-dimensional model systems.

Characterization of fractional quantum Hall systems: A matrix-product state approach. A prominent example of a topologically ordered phase is the fractional quantum Hall (FQH) effect which occurs due to electron-electron interactions in a Landau level of fractional filling. Topologically ordered phases have unusual properties such as excitations which carry fractions of the elementary charge and have exotic exchange statistics (i.e., they are neither fermions nor bosons). We introduced a numerical approach which allows us to efficiently simulate microscopic Hamiltonians and to extract many of their characterizing properties. In particular, we employ the infinite density matrix renormalization group (iDMRG) method, based on the matrix-product state (MPS) representation of FQH states on an infinite cylinder, to find a complete set of ground states. From the MPS representation, we can then directly extract the topological entanglement, the entanglement spectra and the quantum dimension of the quasiparticle excitations. Most interestingly, we could show that the wave function obtained on the infinite cylinder geometry can be adapted to a torus of arbitrary modular parameter, which allows us to explicitly calculate the non-Abelian Berry connection associated with the modular T-transformation. As a result, the topological spins, chiral central charge, and Hall viscosity of the phase can be obtained using data contained entirely in the entanglement of an infinite cylinder.

Dynamical properties and quantum systems out of equilibrium. While it is difficult to study genuine non-equilibrium dynamics in solid state systems due to the presence of many relaxation channels (phonons, impurities, interactions etc.), cold atoms in optical lattices provide an ideal laboratory for non-equilibrium investigations due to the high degree of control over various dissipation mechanisms. Cold-atom experiments in the past decade have explored a wide variety of non-equilibrium quantum dynamics in previously inaccessible regimes. We studied a number of different model systems which are motivated by optical lattice experiments: (i) An important and incompletely answered question is whether a closed quantum system of many interacting particles can be localized by disorder. We have studied the time evolution of a quench (i.e., a change of the Hamiltonian) in a disordered system. It turned out that interactions induce a dramatic change in the propagation of entanglement and a smaller change in the propagation of particles. (ii) We considered variable-rate linear quenches of the anisotropy in the Heisenberg chain, starting at the non-interacting (i.e., XX) point. An excellent agreement between exact numerics and analytical results from bosonization was found. (iii) We explored the dynamical properties of a one-dimensional Bose-Hubbard model where two different bosonic species interact via Feshbach resonance. In a particular parameter regime, we observed the celebrated E_8 mass spectrum in the excited states.

Frustrated systems: Quantum ice. Ice states, in which frustrated interactions lead to a macroscopic ground-state degeneracy, occur in water ice, in problems of frustrated charge order on the pyrochlore lattice, and in the family of rare-earth magnets collectively known as spin ices. Of particular interest at the moment are "quantum spin-ice" materials, where large quantum fluctuations may permit tunnelling between a macroscopic number of different classical ground states. Here we use zero-temperature quantum Monte Carlo simulations to show how such tunnelling can lift the degeneracy of a spin or charge ice, stabilizing a unique "quantum-ice" ground state; a quantum liquid with excitations described

by the Maxwell action of (3+1)-dimensional quantum electrodynamics. In real spin ice materials, the ice states are not perfectly degenerate because of the long-range dipolar interaction. We studied the stability of the quantum-ice ground state when exposed to these perturbations.

Cooperations

- *University of California, Berkeley, USA*: Collaboration with Joel Moore and several members of his group on problems related to many-body localization and fractional-quantum Hall effect
- *University of California, Riverside, USA*: Collaboration with Kirill Shtengel on frustrated spin- and fermionic systems
- *The Institute for Solid State Physics, Kashiwa, Japan*: Collaboration with Masaki Oshikawa on topological phases
- *National Taiwan University, Taipei, Taiwan*: Collaboration with Kao Ying-Jer and several members of his group on the development of tensor-product state based numerical methods
- *University of Amsterdam, The Netherlands*: Collaboration with Ari Turner on the classification of topological phases and one-dimensional systems
- *Weizmann Insitute, Rehovot, Israel*: Collaboration with Erez Berg on topological phases
- *Research Institute for Solid State Physics and Optics, Budapest, Hungary*: Collaboration with Karlo Penc on the study of frustrated magnets
- *Budapest University of Technology and Economics, Hungary*: Collaboration with Balazs Dora on quenches in one-dimensional systems
- *Okinawa Institute of Science and Technology, Japan*: Collaboration with Nic Shannon on the study of frustrated magnets

Division: Finite Systems
(Head: Prof. Dr. Jan Michael Rost)

The department *Finite Systems* is concerned with few- and many-particle dynamics of finite microscopic systems. An important role is played by the environment of those finite systems. It can consist of similar entities as the atom or molecule under consideration (e.g., clusters, quantum aggregates, ultracold Rydberg gases). Intense light pulses provide another, quite universal kind of environment. Thirdly, noise forms an important class of environment, also studied at the **mpipks** outside the *Finite Systems* department in various contexts, from breathers over chaotic dynamics to biological systems.

The research group *Finite Systems* within the department concentrates on clusters (project leader *Ulf Saalmann*), quantum aggregates (project leader *Alexander Eisfeld* and *Sebastian Wüster*) and the interaction of finite systems with strong and short light pulses, inspired by rapid technological development towards ultrashort pulses (attosecond science) and short X-ray pulses (X-ray Free Electron Lasers). Fruitful synergy emerges from the relation between exciton dynamics in traditional quantum aggregates and their counterpart in the context of ultracold Rydberg complexes. This connection will be pursued even more intensely with Alexander Eisfeld having established his own research group *Quantum aggregates* in the fall of 2012 after his return from Harvard University. The second research group in the Finite Systems department, *Complex Dynamics in Ultracold Gases*, headed by *Thomas Pohl* focuses on many-body aspects of interacting ultracold Rydberg systems and light.

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

Dominant interaction hamiltonians Systems of many degrees of freedom are notoriously difficult to handle, especially in the context of time-dependent external interaction (e.g. a laser field) which lasts long on the natural (electronic) time scale of the system. We have explored a novel approach by partitioning the phase space into regions of different approximate but dominant interaction hamiltonians (DIH). This leads to a simplification of the numerical treatment and, at the same time, to insight into the system dynamics through the specific sequences of DIH.

Low-energy electrons Ionization of an atomic or molecular system leading to the escape of very low-energy electrons constitutes a universal phenomenon which is akin to phase transition phenomena with the

ionization threshold as the critical point. Motivated by recent experimental observations of a surprisingly rich structure in the low energy photo electron spectrum of strong field ionization, we have established so called "soft recollisions" driven by the laser field as the origin of the most prominent of these low energy features.

In a different context it has become possible to probe multi-electron escape near threshold in extended systems such as fullerenes through a comparison of the neutral and the negatively charged ion where the latter serves as a sensitive probe of low energy phenomena owing to its small binding energy.

Studying low energy electron escape builds an obvious bridge to ultra cold Rydberg dynamics, a major activity in the department.

Ultracold Rydberg dynamics and quantum aggregates An ultracold environment harmonizes perfectly with Rydberg dynamics and its inherently small energy scales. Consequently, this field has gained enormous momentum recently, holding hopes for information science and offering flexible means to design and investigate condensed matter like systems of very variable character. In most applications the focus is on electron dynamics ("frozen gas") with the atomic motion as an annoying but unavoidable fact. In our research we incorporate atomic motion explicitly and focus on its interplay we with electronic dynamics akin to chemical dynamics.

In fact, we have formulated dynamical situations with the goal to preserve maximum coherence. This can be achieved by letting the atoms move according to the forces exerted by the electronic (Rydberg) excitations. Examples so far include a Rydberg version of Newton's cradle permitting mesoscopic transport of entanglement, controlled conical intersections and a mesoscopic Schrödingier cat state on the micrometer scale represented by an entangled pair of atom clouds, mesoscopically separated through internal electronic forces.

We also actively investigate schemes to extend the flexibility of ultracold Rydberg systems with the goal of experimental implementations, in particular through Rydberg dressing.

Perspectives for the future

With additional FEL sources coming on line and more groups getting interested, the general emphasis in theoretical research shifts towards simulation of specific situations and experiments. In contrast to this trend, we will continue to concentrate on general principles of interaction and their simple formulation for light-matter interaction in the attosecond- and XUV- as well as X-ray-short pulse parameter regime, including the development of simplified models for a better understanding, such as the concept of Coulomb complexes. We will study, e.g., cooperative (not collective!) many particle effects leading in particular for finite systems to unusual transient surface phenomena upon massively parallel ionization of many constituents almost at the same time.

Our increasing understanding of the principles ruling exciton dynamics coupled to atomic motion in the context of ultracold Rydberg aggregates opens the perspective to design ultra cold Rydberg networks with specific properties in the future. This may also have implications on the understanding of fundamental molecular networks such as light harvesting complexes.

Cooperations

We have collaborations with

- Prof. Stienkemeier (Freiburg) regarding clusters embedded in helium nano-droplets,
- Prof. Berrah (Kalamazou, USA) regarding photo ionization of fullerenes and fullerene negative ions,
- Prof. Davis (Brisbane, Australia) on nonlinear effects in dynamical tunneling of BECs,
- Prof. Keller (Zürich, Switzerland) on ultrafast non-linear light-matter coupling,
- Prof. Möller (Berlin) regarding imaging of highly excited clusters at X-FELs,
- on semiclassical theory with Prof. A. Ozorio de Almeida (Rio, Brazil).
- Through the two European ITN networks CORINF in the area of intense light-matter interactions and COHERENCE in the field of ultra cold Rydberg physics, we are closely connected to international groups active in those fields. In particular we have a collaboration with
- Prof. Pfau (Stuttgart) regarding ultra cold long range molecules (COHERENCE) and
- Prof. Suraud (Toulouse) regarding the exposure of rare gas clusters to VUV, IR and long-wavelength light (CORINF).

Local cooperations
The interaction with Prof. Schmidt's group from the TU Dresden within our IMPRS has been continued concerning a quantum-classical mixed description in all degrees of freedom of small systems (atoms and molecules) in strong laser fields. With Dr. Großmann from the TU Dresden we enjoy a productive collaboration on *semiclassical propagation techniques* which has led to the concept of dominant interaction hamiltonians. Together with Prof. Strunz, TU Dresden, we develop approaches based on stochastic Schrödinger equations to study quantum aggregates.

Research Group: Quantum Aggregates
(Head: Dr. Alexander Eisfeld)

The group was established in October 2012 and currently hosts two PhD students (Sebastian Möbius, Gerhard Ritschel) and three postdoctoral guest scientists (Ramy El-Ganainy, Sebastiaan Vlaming, Xiaoqing Wang). A third PhD student will start in the middle of April.

The main focus of our research is the emergence of collective quantum effects in mesoscopic assemblies of atoms and molecules (so called aggregates), where the individual atoms/molecules interact via long range forces. In particular we are interested in the interplay between electronic and nuclear dynamics and its influence on optical and transport properties. Below are examples of topics that we are currently investigating.

Self-assembled organic-dye aggregates Certain organic molecules can self-assemble into supra-molecular structures. These molecular aggregates can consist of up to several thousands of individual molecules. The geometrical arrangement depends sensitively on the type of molecule and the environment. The Coulomb interaction between the molecules leads to collective electronic dynamics which manifests itself for example in extreme changes of the optical properties. Application of aggregates ranges from sensitizers in photography to the measurement of membrane potentials, cancer therapy and organic solar cells. When the concentration of organic dye molecules in solution exceeds a critical value, these individual molecules (monomers) start to self-assemble into weakly bound supra-molecular structures of usually unknown arrangement. We develop methods to infer the geometry from linear and non-linear spectroscopy. Dielectric materials like KCl or NaCl can be used as templates to induce specific arrangements of adsorbed molecules. Together with the experimental group of Prof. Sokolowski (University of Bonn) we investigate monolayers of the organic semiconductor PTCDA on a KCl surface. Of particular interest is the temperature dependence of the observed superradiance.

Energy transfer in photosynthesis The ability of photosynthetic plants, algae and bacteria to efficiently harvest sunlight has attracted researchers for decades and a fairly clear picture of photosynthesis has emerged: Sunlight is absorbed by assemblies of chromophores, e.g. chlorophylls. These assemblies, termed light harvesting complexes, transfer the excitation energy with high efficiency to so-called reaction centers, where the excitation energy is converted into a trans-membrane chemical potential. Our particular interest is the interaction of the chormophores with the protein environment and its role for the transport. We demonstrated the importance of vibrations on the energy transport efficiency and discovered an important suppression of quantum oscillations in the Fenna-Matthews-Olson (FMO) complex when one takes the newly discovered 8th bacteriochlorophyll into account. These results where obtained using an open quantum system approach. Recently we have started to develop suitable mixed molecular dynamics and quantum chemical simulations to obtain the influence of the protein environment on the chlorophylls from a detailed microscopic model.

Stochastic Schrödinger equations Open quantum system approaches are widely used in the description of physical, chemical and biological systems to describe the coupling of electronic degrees of freedom to vibrations. This structured vibrational environment leads to long-lasting non-Markovian dynamics, which makes numerical simulations quite demanding. Instead of using a master equation, we tackle the problem by solving a stochastic Schrödinger equation of the diffusion type which gives the exact reduced density operator. Although this approach is formally exact, it is difficult to solve, due to the appearance of a functional derivative with respect to a stochastic process. In collaboration with Prof. Strunz from the TU Dresden we develop an efficient numerical method.

Quantum simulators for open quantum systems Quantum simulators are well controlled quantum systems that can be used to simulate quantum Hamiltonians. Such an approach will be particularly fruitful, if the corresponding numerical simulation on a classical computer is intractable. Here we focus on finite

dimensional systems interacting with a structured environment. *Ultra-cold Rydberg aggregates:* Laser dressing of ground state atoms with Rydberg states allows us to create potentials which are different for different electronic states. This is similar to the Born-Oppenheimer potentials of small molecules. Upon electronic excitation/de-excitation nuclear dynamics is induced such that each Rydberg atom behaves like an artificial molecule. The resonant dipole-dipole interaction between the dressed Rydberg atoms then leads to polaron dynamics similar to that in molecular crystals, for which we know how to map it onto an open system model. *Superconducting circuits:* The diagonal elements of the system Hamiltonian are described by superconducting qubits and the off-diagonal ones by strongly detuned coupler qubits. Engineering of the non-Markovian environment is achieved by coupling quantum mechanical inductor-resistor-capacitor oscillators to the qubits. We know how to simulate the full time dependent density matrix for time independent Hamiltonians. The next step is to consider the time dependent case, which is important, e.g., to treat pump probe spectroscopy. *Quantum Hamiltonian vs. classical coupled oscillators:* We have shown that the quantum dynamics of open systems that can be described by a Lindblad master equation can be reproduced by a set of coupled Kubo oscillators. In particular we have shown under which circumstances quantum coherences can be adequately described in purely classical terms. This in turn is relevant in the context of the question if there are quantum effects in biological light harvesting.

Cooperations

- Prof. Aspuru-Guzik (Harvard University, Cambridge, USA): Light-harvesting-systems.
- Dr. Croy (Chalmers University, Göteborg, Sweden): Nano-electro mechanical devices.
- Prof. Engel (University of Wŕuzburg, Germany): Molecular dimers.
- Prof. Knoester (University of Groningen, The Netherlands): Unconventional disorder and localization.
- Prof. Sokolowski (University of Bonn, Germany): PTCDA monolayers on dielectric surfaces.
- Prof. Stienkemeier (University of Freiburg, Germany): Spectroscopy in helium nano-droplets.
- Prof. Strunz (TU Dresden, Germany): Stochastic Schrödinger equations.
- Dr. Wüster, Prof. Rost (mpi**pks**): Flexible Rydberg aggregates.

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

The group was established in September 2008, and currently hosts five PhD students (Nils Henkel, Rick Mukherjee, Laura Gil, Belinda Kapidani, Wildan Abdusallam) and four postdoctoral guest scientists (Georg Bannasch, Fabio Cinti, Tommaso Macri, Gunes Soyler). The focus of our research lies at the interface of light and ultracold ensembles of particles with strong controllable interactions. Specific settings range from ultracold highly-excited atoms and polar molecules to laser-cooled ions, where the interaction between particles can depend strongly on their internal quantum states. As a consequence, the coupling of classical or quantum light fields to such systems gives rise to a rich spectrum of many-body phenomena, driven by the intricate interplay between strong light-matter and various kinds of matter-matter interactions. Understanding the resulting *complex dynamics of such cold gases* and how salient effects may be turned into useful scientific and technological applications presents the core of our research interests. This involves diverse problems, ranging from elementary atomic and molecular interactions of laser-driven particles, over light propagation in nonlinear media to classical and quantum simulations of many-body systems. Specific topics of current interest in our group include:

Ultracold plasmas produced via photoionization of laser-cooled atoms, open up an exotic regime of plasma physics. Their extremely low temperature enables applications in nano-technology and permits to reach strong coupling conditions where the potential energy greatly exceeds the thermal energy of the charges. Strongly coupled plasmas are of fundamental and technological interest, since they occur in dense astrophysical environments such as Jovian planets and form under extreme conditions, e.g., in inertial confinement fusion experiments. In ultracold plasma, on the other hand, one can realize strong coupling conditions already at very low densities, which presents unique opportunities for studying non-equlibrium processes and dynamics. Exploiting this property we recently studied velocity relaxation processes of ions in an ultracold plasma, which in collaboration with the experimental group of Prof. Thomas C. Killian (Rice University, USA) led to the first measurement of the corresponding relaxation rates in the strong coupling domain. Up to now the range of achievable coupling strength has been restricted to moderate values due to intrinsic heating mechanisms. More recently, we could devise a

new scheme that overcomes this fundamental limitation by exploiting long-range atomic correlations that can be imprinted onto the gas via coherent laser excitation to strongly interacting internal states. This method dramatically expands the scope of current ultracold plasma experiments and can boost the performance of the aforementioned nano-technological applications. Currently we are working on possible extensions of this idea to open up a new regime of crystalline ultracold plasmas and on possible variations to aid an experimental realization in collaboration with the Killian group at Rice.

Quantum liquids and solids of long-range interacting ultracold atoms or molecules represent another focus of our research interests. Here, we are studying the few-body physics of particles driven by static and dynamic electromagnetic fields in various different configurations. Based on such calculations, we recently discovered a particular setting of microwave fields that permits to control and even turn off the van der Waals interaction between highly excited Rydberg atoms and showed how optical driving of such atoms or polar molecules can be used to induce a peculiar type of soft-core interaction in an ultracold gas. The latter gives rise to a number of remarkable phenomena. For example, soft-core repulsion can promote the formation of so-called cluster crystals and, as we showed recently, leads to the emergence of supersolidity due to zero-point defects in the ground state of a quantum cluster crystal. A supersolid combines the seemingly antithetic properties of crystalline rigidity and dissipation-less superfluid flow of particles. This enigmatic phase of matter has been actively pursued in pressurized Helium for several decades but so far eluded experimental and theoretical verification. In fact, the described system of soft-core particles constitutes the first setting to unambiguously display defect-induced supersolidity and a range of further interesting phenomena, such as quantum glass phases, which are among the questions we are currently investigating.

Optical lattices formed by superimposed standing wave light fields provide a versatile approach to control the motion of ultracold atoms and molecules. In recent years, these systems have attracted enormous interest owing to their great potential as quantum simulators for important lattice models in condensed matter physics. Much of this success stems from the ability to tune short range collisional atomic interactions via external magnetic fields. In our group we are working on extending the scope of such settings towards long-range interacting quantum systems. On the one hand, this concerns the dynamics of strongly interacting internal states of stationary atoms pinned to the sites of an optical lattice. Here we study the ground state phases and laser driven dynamics of the resulting effective spin systems, partly in collaboration with the experimental group of Prof. Immanuel Bloch at the MPQ in Garching. In addition, we are exploring approaches for designing new types of interactions in more-complex multi-electron atoms via optical dressing to Rydberg states, where we recently discovered a viable route to spin squeezing in Strontium lattice clocks. On the other hand, we are building on these insights to study situations in which atoms are free to move, i.e. can tunnel between adjacent lattice sites. Here, we are currently investigating the physics of dressed Strontium atoms in magic-wavelength lattices with long-range spin dependent interactions and the prospects for realizing extended Bose-Hubbard models with coherent and dissipative interactions via controlled photo-association of exotic ultralong-range molecules.

Open quantum systems are realized naturally in the aforementioned setting due to dissipation arising, e.g., from spontaneous photon emission of atoms and molecules or coupling to phonon excitations in laser-cooled ion crystals. The resulting interplay between coherent interactions, leading to strong many-body entanglement, and de-coherence, corresponding to progressive projective measurements, gives rise to a rich spectrum of phenomena which we are currently investigating. Besides fundamental interest, one of our aims is to explore possible applications of such systems as non-classical light sources and all-optical switches.

Hybrid quantum interfaces present a promising approach to quantum computing, where different quantum systems with distinct properties are coupled in order to simultaneously provide fast processing of quantum information, long coherence times for information storage and scalability via coherent links between different units. Within an EU-funded STREP project together with the University of Nottingham and the University of Vienna we are working on such a hybrid-architecture in which single photons controlled via small-scale waveguides will be interfaced with a lattice of ultracold atoms on a so-called atom chip. The goal is to achieve strong atom-light coupling for long-time storage and manipulation of photons on a robust integrated quantum device that will, thereby, provide a universal building block for scalable quantum networks. Along another line of research, we are theoretically exploring different schemes for exploiting the strong dipole-dipole interaction between Rydberg atoms for noise-resistant interfacing of cold atomic ensembles and solid state devices such as superconducting microwave cavities.

Nonlinear quantum optics is typically based on local effective photon interactions. Prominent examples are the optical Kerr in atomic ensembles or the photon blockade effect in an optical cavity, which on a few photon level arises from the simultaneous interaction of several photons with one and the same quantum system (atom). Over the past two years, we have been working on a different approach, where optical nonlinearities instead arise from strong interactions between the atoms, inducing effective photon-photon interactions for light fields propagating through the highly correlated optical medium. As we have shown this yields nonlocal single-photon nonlinearities of unprecedented strength, promising a new approach for optical quantum information processing. First steps towards an experimental realization have been undertaken in collaboration with MIT and Harvard, where we demonstrated the generation of single photons from classical light traversing a strongly interacting Rydberg gas. Despite considerable efforts from several groups, a complete theory for quantum light propagation in long-range correlated ensembles has not emerged so far. We are currently working on such a theoretical description, which potentially will lay the basis for new generations of nonlinear quantum-optical devices and may open up new routes for studying many-body physics entirely with photons.

Cooperations

- Collaborations with experimental groups:
  - Prof. Immanuel Bloch (MPQ, Germany), [Rydberg atoms in optical lattices]
  - Prof. Vladan Vuletic (MIT, USA), [nonlinear quantum optics]
  - Prof. Thomas C. Killian (Rice University, USA), [ultracold neutral plasmas]
  - Dr. Matthew Jones (Durham University, UK), [spin squeezing in Strontium gases]
  - Prof. Philip Walther (University of Vienna, Austria) and Prof. Lucia Hackermüller (University of Nottingham, UK), [light coupling to atom chips]

- Collaborations with theory groups:
  - Prof. Mikhail D. Lukin (Harvard, USA), [nonlinear quantum optics]
  - Prof. Andreas Läuchli (University of Innsbruck, Austria), [quantum spin lattices]
  - Prof. Guido Pupillo (University of Strassbourg, France), [supersolidity with cold soft-core Bosons]
  - Prof. Igor Lesanovsky (University of Nottingham, UK) [light coupling to atom chips]

Research Group: Quantum Optics with X-rays
(Head: Dr. Nina Rohringer)

The group was established in February 2011 and currently consists of two PhD students (Clemens Weninger and Jhih-An You) and two postdoctoral scholars (Victor Kimberg and Song-Bin Zhang). Our group is located at the Center for Free-Electron Laser Science (CFEL) at the DESY campus in Hamburg, to strengthen the institute's connection to one of the world-leading centers in X-ray science. We focus on theoretical studies on quantum optical and nonlinear X-ray processes in atoms and molecules and are also actively involved in planning and performing experiments at X-ray free-electron laser (XFEL) sources in the USA (LCLS at the SLAC National Accelerator Laboratory) and the FLASH facility in Hamburg (FLASH XUV Free-Electron Laser at DESY). With the advent of short-wavelength free-electron lasers, delivering femtosecond X-ray pulses of unprecedented high intensity, exceeding brilliances of the brightest synchrotron sources by nine orders of magnitude, new opportunities in the field of nonlinear quantum optics with X-rays arise, a field which so far is virtually unexplored. Still, most of the science drivers in the condensed phase, structural biology, correlation spectroscopy etc. are based on a sequence of essentially linear, single-photon interactions with matter. Among those processes are coherent diffractive imaging of biological molecules, X-ray diffraction of nano-crystals, time resolved photo absorption spectroscopy, resonant inelastic X-ray scattering and Thomson scattering. The core activity of the group centers around the development of quantum mechanical methods to describe the interaction of ultrafast high-intensity X-ray interaction with matter beyond the linear, single photon response. Especially, we are interested to explore nonlinear quantum optical processes in the X-ray regime, to ultimately develop new powerful nonlinear X-ray spectroscopy techniques, for application in energy research and catalysis.

Photoionization X-ray lasers in atomic and molecular gases A main focus of our research is the combined theoretical and experimental study of amplification of X-rays on atomic inner-shell transitions in optically

dense targets. By focusing ultrashort high-intensity X-ray radiation from XFELs into a gas target, initially neutral atoms are core-ionized on ultrafast timescales. Thereby a transient population inversion of the atomic system is achieved, which can be exploited for an X-ray lasing process. This process, predicted in 1967, was recently demonstrated experimentally for the first time, in a collaboration with Colorado State University, SLAC National Accelerator Laboratory and Lawrence Livermore National Laboratory. Our group develops quantitative theoretical models, to predict and characterize the X-ray laser output. Specifically , we develop generalized Maxwell-Bloch codes to simulate the propagation, wavelength conversion and amplification of high-intensity X-ray radiation in atomic and molecular gases. In molecules with relatively light constituents, the nuclear dynamics can happen on the time scale of typical inverse X-ray ionization rates and core-hole lifetimes. To treat the interplay of nuclear and electronic dynamics in these dynamically complex systems, electronic and nuclear degrees of freedom have to be treated on the same footing. In the strongly nonlinear coupling regime, also rotational degrees of freedom have to be taken into account, especially for impulsively aligned gas samples. Our theoretical estimates are the basis of feasibility studies to guide new X-ray amplification schemes in molecules.

Stimulated Electronic X-ray Raman Scattering XFELs open the pathway to nonlinear X-ray spectroscopy. Powerful methods such as multidimensional IR spectroscopy, or coherent femtosecond stimulated Raman spectroscopy could be transferred from the optical to the X-ray domain of the spectrum, thereby getting access to study the coherent interplay of electronic and nuclear degrees of freedom. A promising way to initiate and probe electronic and nuclear dynamics in matter is based on stimulated electronic X-ray Raman scattering, or inelastic X-ray scattering. In a recent experiment at the LCLS XFEL, our group managed to achieve stimulated resonance Raman scattering in atomic neon, the first step towards sophisticated nonlinear all X-ray pump probe schemes. We focus on feasibility studies of stimulated Raman processes at present-day XFEL sources. Since the currently operating XFEL sources are inherently incoherent, we develop statistical approaches to obtain both high temporal and spectral resolution of the scattering process. Multivariate statistical analysis and covariance mapping are applied, to unravel coherent electronic und nuclear dynamics in XFEL stimulated processes. The methods are tested on simulated inelastic X-ray scattering spectra. Our findings are crucial to guide future stimulated X-ray Raman scattering experiments at XFEL sources. Our current studies deal with atomic and molecular systems in the gas phase. In future research, we will extend our studies to stimulated X-ray scattering in liquid droplets, clusters and solids. The current one-dimensional Maxwell Bloch approach will be extended to two spatial dimensions, to capture transverse propagation effects and diffraction in dense samples. Collective effects, such as superfluorescence and collective inelastic X-ray scattering will be theoretically explored. For solids, a kinematic inelastic X-ray scattering theory will be developed for high X-ray intensity. A focus will be to study resonant X-ray diffraction at high X-ray intensity, where resonance and Bragg conditions are simultaneously satisfied. Effects, such as the Borrmann effect - X-ray induced transparency at Bragg conditions - will be studied in the nonlinear regime and soliton like wave-propagation schemes will be studied. So far, nonlinear X-ray effects in solids are uncharted territory, but in principle accessible with XFEL sources. Our theoretical studies are aimed to inspiring new experiments along these lines.

Optical and X-ray wave mixing techniques in the linear X-ray regime are accessible at accelerator based XFEL sources and table-top laser experiments, combing attosecond XUV pulses from high-harmonic sources with optical lasers. The latter has the advantage of well-characterized, transform-limited pulses of unprecedented, subfemtosecond timing control, which allows manipulation of electron dynamics at its inherent attosecond time scale. One method to achieve optical X-ray wave mixing is by combining the high-harmonic generation (HHG) process initiated by strong optical fields with subfemtosecond XUV pulses. Thereby, the HHG can be enhanced by attosecond XUV assisted tunnel ionization. Moreover, transient absorption of precisely timed XUV pulses by inner valence states during the HHG process can induce coherent electronic wave packets in the residual ion. These wave packets have an imprint on the emitted HHG spectrum. An extension of the HHG plateau is predicted and different spectral regions can be assigned to specific coherent processes. Theoretical methods are developed to describe these processes on different levels of sophistication, starting from semiclassical strong-field approximation for electronic wave packets including transient interaction with the XUV field by time-dependent perturbation theory, as well as time-dependent configuration-interaction methods. The ultimate goal is to extend this method to molecules, to develop the theoretical foundation of a combined attosecond transient absorption and HHG spectroscopy tool. In molecular samples, it is expected, that resonant transient absorption of a short XUV pulses during the HHG process will additionally induce nuclear wave packets, which can be coherently probed by the HHG rescattering process. Another wave-mixing process to be studied in the

future is parametric X-ray optical sum frequency and difference frequency generation in solids. Although the stationary description of this process is more or less well understood, dynamical effects induced by ultrashort optical pulses are unfathomed. By understanding these fundamental processes, new insight into the dynamical response of matter-light interaction can be gained and can spur new X-ray probing techniques.

Cooperations

- Prof. Jorge J. Rocca (Colorado State University, Fort Collins, CO, USA) on inner-shell atomic X-ray lasers
- Dr. Richard A. London and Dr. Gregory Brown (Lawrence Livermore National Laboratory, Livermore, CA, USA) on X-ray lasers and X-ray spectroscopy
- Dr. John D. Bozek and Dr. Christoph Bostedt (SLAC National Accelerator laboratory, Menlo Park, CA, USA) on X-ray lasers and stimulated Raman scattering
- Prof. Alexander Föhlisch und Dr. Philippe Wernet (Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, Helmholz-Zentrum Berlin für Materialien und Energie. Berlin, Germany) on molecular X-ray lasers
- Prof. Franz Kärtner (DESY, Center for Free-Electron Laser Science, Hamburg, Germany) on attosecond gated high-harmonic generation
- Prof. Jochen Küpper (University of Hamburg, Center for Free-Electron Laser Science, Hamburg Germany) on molecular X-ray lasing, molecular alignment
- Prof. Jan-Erik Rubensson, Prof. Raimund Feifel and Prof. Joseph Nordgren (Uppsala University, Uppsala, Sweden) on stimulated resonant X-ray Raman scattering in molecules
- Prof. Hans Jakob Wörner (Eidgenössisch Technische Hochschule, Zürich, Switzerland) on high harmonic generation of coherent electronic wave packets in NO
- Dr. Oriol Vendrell (DESY, Center for Free-Electron Laser Science, Hamburg, Germany) on dynamics of rotational motion in strong field X-ray processes

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

The department Biological Physics studies active dynamic phenomena in biology ranging from molecules to cells and tissues. From the point of view of physics, biological systems represent a highly organized and inherently dynamic form of condensed matter. This living matter is active and can exhibit spontaneous movements and flows, oscillations, the formation of complex patterns and structures as well as unusual material properties.

Spatio-temporal patterns emerge from the collective behaviors of many subunits on smaller scales. For example, intracellular dynamics result from the collective behaviours of many molecules, tissue dynamics reflects the collective behavior of cells. Biological dynamics typically combines active mechanical processes with chemical regulation. Such mechano-chemical dynamical systems represent a novel paradigm for pattern formation. The analysis of such systems opens original lines of biophysical research and can also lead to new physics.

In addition to the investigation of the physical principles which play a key role in the dynamics of cells and tissues, we study current problems of cell and developmental biology in close cooperation with biologists. These projects aim at a theoretical and quantitative description of biological processes (e.g. cell locomotion, cell division, pattern formation in cells and tissues). The goal is to develop theoretical methods and concepts to unravel the function and organization of living systems.

The department Biological Physics started its activities in 2002. The research of our department is characterized by many close interdisciplinary cooperations with experimental groups. Most important is a tight cooperation with the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG) in Dresden. This cooperation is built on a joint research program on the physics of biological systems. In 2012, this cooperation was extended and deepened by the creation of the Center for Systems Biology at Dresden as a joint operation of the two Max Planck Institutes. The center was started by three research groups. The group of Stephan Grill and the two newly hired groups of Michael Hiller and Ivo Sbalzarini. Furthermore, Gene Myers started as a new director at MPI-CBG to bring image informatics for the analysis of 3 and 4 dimensional microscopy image data to the center. In addition to the new center

for systems biology, a variety of collaborative projects exist between our department and the MPI-CBG. Our group is also linked to the International Max-Planck Research School for Cell, Developmental and Systems Biology, managed by the MPI-CBG. Finally, we also continue our collaborations with the Institut Curie in Paris and the AMOLF in Amsterdam.

Current research topics include:

Generic theories of active gels and of tissues The dynamics of the cell cytoskeleton is driven by active processes on the molecular scale such as the action of molecular motors. This leads on large scales to unconventional material properties and dynamic states that can be captured by generic hydrodynamic equations. These hydrodynamic equations for active gels take into account effects of active stresses that are internally generated. In the same spirit, tissue dynamics that results from active cellular behaviors can be studied in continuum limits and hydrodynamic descriptions. New developments are the study of fluctuations in such systems and the role of active chiral processes. Chirality results for example from the interaction of molecular motors with helical filaments. Such chiral effects in active systems can give rise to rich dynamics near surfaces with chiral asymmetries. Such chiral processes could be relevant for symmetry breaking in biological systems.

Physics of cells We are interested to study the spatial organization of cells and intracellular dynamics. Examples are endosome networks, cell division and the formation of intracellular structures. The sorting and processing of molecules in a cell occurs in distributed endosomal networks. We study how the large scale properties and dynamics of endosome networks emerges from stochastic processes on small scales such as endosome fusion, fission and conversion. Many intracellular structures exists that do not posess a membrane and are self-organized dynamic structures. Examples are the mitotic spindle, centrosomes or germ granules. We study the dynamics of such systems at different scales. In our mesoscopic approaches, for example, we take into account an interplay of liquid-liquid phase separation and chemical processes giving rise to the formation of well defined structures.

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

An important model system for the patterning of tissues during the development of organisms are epithelia, which are two dimensional tissues. An important example is our study of the development of the fly wing. This is an important model system for the patterning of two-dimensional tissues. A key result was the finding that interfaces between tissue compartments are organized with the help of increased mechanical tension and biased cell division axies. Such effects could account for the observed small interface roughness.

Physics of hearing Hair cells are highly sensitive mechanosensors which in our ears transduce sound vibrations to electrical signals. Our ear is able to operate over a vast dynamic range of 12 orders of magnitude and to detect extraordinarily weak stimuli. This is achieved by active processes which perform nonlinear frequency-selective amplification. This cochlear amplifier is based on the generic properties of dynamic oscillators. We are studying the interplay of active processes in the cochlea in the formation of cochlear waves. One key question is to understand the origin of spontaneous otoacoustic emissions which are a signature of active processes in the ear.

Perspectives The close collaboration between the mpi**pks** and the MPI-CBG aims to study the principles underlying spatiotemporal processes in cells and in tissues using a combination of theory and quantitative experiments. Modern microscopy techniques can provide a wealth of information in three dimensions on the time dependence of biological processes. In the new center for systems biology, additional groups with competences in image informatics have recently joined. This will provide us with powerful image analysis techniques to extract spatiotemporal information from microscopy images and to quantify experimental observations. The combination of theoretical physics and experimental biology with computer science will significantly strengthen our activities in quantitative biology and biophysics. This will allow us to move towards new challenges such as the theoretical study of the dynamics of cells and tissues in three dimensions.

Cooperations

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

Research Group: Physics of the Cytoskeleton
(Head: Dr. Guillaume Salbreux)

Living organisms have the ability to move, change shape, and organize themselves in space, through processes that require the production of forces. These forces are generated inside the cell by the cytoskeleton, a meshwork of polymers interacting with motor proteins using the energy provided by ATP hydrolysis. Our group studies how forces generated in the cytoskeleton affect cell shape and morphogenetic events, from the microscopic to the cellular and tissue level. We use a combination of coarse-grained descriptions of cytoskeletal structures and computer simulations to address these questions. Our group is working in close collaboration with experimentalists working on several biological model systems. Specifically, we are interested in:

Physics of cell division During cell division, most of the cellular actin and myosin is concentrated in the cortex, a thin layer of cytoskeleton connected to the cell membrane. The cortex plays a major role in setting cell shape and provide rigidity to the otherwise soft cell membrane. We investigate the role played by the cell cortex in mechanically dividing the cell into two equally sized daughter cells. We have shown that the dividing cell shape can be unstable to symmetry-breaking deformations, and that cell elasticity is necessary to stabilize the cell shape during division. We are analyzing cell shape oscillation resulting from symmetry-breaking instabilities to gain informations on the mechanical properties of dividing cells. We are also studying how the mechanical interplay of the actin cortex and cell membrane influences cell shape.

Physics of cell and nuclear migration Cell migration in a 3D confined environment is a new paradigm of cell motility, where cells appear to rely on actin cortex contraction and formation of membrane protrusions, called blebs, to generate motion. Using the simplified setup of migration in a channel, we are studying how cytoskeletal flows and shape deformation combine to give rise to cell motility. An interesting cellular process also relying on actomyosin contraction is interkinetic nuclear migration, a feature of neuroepithelial cell consisting of the motion of the cell nucleus towards the epithelia apical side, prior to cell division. We investigate forces involved in these processes with the help of physical models of cell mechanics. On a larger scale, we are also interested in trajectories exhibited by primordial germ cells in

the zebrafish embryo, which show distinct phases of directed motion and stalling, and the consequences of this motion on the efficiency of chemotaxis.

Actomyosin oscillation and patterns in cells and tissues It has been recently observed in a number of model systems that the actomyosin cortex can be highly dynamic, exhibiting density and shape oscillations, pulse propagation, and patterns of filament orientation. We investigate these processes using the framework of hydrodynamic equations for an active gel, where myosin molecular motors use the energy of ATP hydrolysis to induce active stresses. We particularly focus on spatiotemporal patterns appearing in an active gel with nematic order and whose material is undergoing turnover.

Morphogenesis of tissues How forces and mechanics play a role in morphogenetic processes in model systems such as *Drosophila* and zebrafish embryo is a key question in developmental biology. Forces generated inside the cell give rise to flow and deformations at the scale of the animal. With the help of coarse-grained description of tissues and cytoskeletal structures, we are studying the mechanics of epiboly in zebrafish gastrulation, a process during which embryonic tissues spread to engulf the yolk of the embryo. We are also more generally interested in the mechanics of epithelia, which are two-dimensional layers of connected cells. In collaboration with the experimental group of A. Classen in Munich we are studying the formation of cysts, out-of-plane bulges which form in *Drosophila* wing discs as a result of genetic mutations. To describe deformations of epithelia, we are developing a 3D vertex model where the cell surface is represented by triangulated polygons. Forces acting on the vertices are obtained by assuming that cells have a constrained volume and that cell-cell interfaces are submitted to a surface tension, thought to arise from cellular cytoskeletal networks. Within this framework, we are studying cell shape within an epithelium and 3D deformations of epithelia, using a combination of numerical simulations and analytical tools.

Cooperations

- Ewa Paluch, MPI-CBG Dresden, on the physics of the actin cortex in cell division and cell migration in confinement
- Stephan Grill, MPI-CBG and mpi**pks**, Dresden, on nematic ordering and pattern formation in the actomyosin cortex
- Caren Norden, MPI-CBG Dresden, on the mechanics of interkinetic nuclear migration in the zebrafish embryonic retina
- Jérome Solon, CRG Barcelona, on cell oscillations in dorsal closure
- Anne Classen, LMU Munich, on cyst formation in the Drosophila wing disc
- Carl-Philipp Heisenberg, IST Vienna and Stephan Grill, MPI-CBG, Dresden on the mechanics of zebrafish epiboly
- Suzanne Eaton, MPI-CBG and Frank Jülicher, mpi**pks**, on the mechanics of Drosophila wing disc development.

Research Group: Collective Dynamics of Cells
(Head: Dr. Vasily Zaburdaev)

The group "Collective Dynamics of Cells" started its work at the mpi**pks** in June 2012. In November 2012, the first postdoc Johannes Taktikos joined the group. Since December 2012 the group is a member of the IMPRS for Cell, Developmental and Systems Biology (IMPRS-CellDevoSys) and an affiliated group of the Center of Systems Biology in Dresden. We apply and develop methods of statistical physics to get a better understanding of multicellular dynamics and self-organization. In close collaboration with our experimental colleagues we try to tackle the following problems.

Clustering dynamics of N. gonorrhoeae bacteria In recent years a rapidly growing number of cases of gonorrhea infection was documented, with bacteria showing resistance to the standard set of antibiotics used to treat this disease. Motility of bacteria is essential for the progression of infection and therefore could become a potential target for the next generation of drugs. Our research aims to understand the microscopic mechanisms of *N. gonorrhoeae* motility. Many species of bacteria use long flexible filaments, called pili, to move on surfaces. Pili can extend from the cell membrane, attach to the surface and then retract, thus generating a pulling force. We have studied how an individual cell could employ multiple pili to propel itself. Pili allow several cells to merge in larger clusters, which are also motile. We develop a model of bacterial cluster formation based on the pili interaction of cells and show that a pili-mediated

mechanism is sufficient to explain the experimentally measured dynamics of clustering. As a future work we would like to understand how the mobility of larger clusters depends on their size. Such clusters possess nearly spherical shape with a diameter up to ten microns and comprising about a hundred of cells. The size of the clusters makes it possible to track their motion on a surface and also follow their rotational degrees of freedom. Our goal is to develop a model of a spherical cluster of cells which uses pili to move on a surface. This project is a challenging effort in all three facets of experiment, theory, and extensive numerical simulations.

Bacterial motility patterns and random walks Motility of individual cells is crucial for their ability to react on environmental changes and also allows the cells to aggregate and build microcolonies. In bacteria, motility is an essential condition for the formation of biofilms – complex multicellular communities of bacteria embedded into an extracellular matrix. This motivates us to study motility of bacteria and other microorganisms. We use the framework of generalized random walk models to describe the dispersal of cells. In addition we can analyze how different motility patterns effect the ability of cells to navigate to the source of nutrients by performing chemotaxis. With the help of extensive numerical simulations we would like to quantitatively explain experimentally observed chemotactic behavior of bacteria and use the modeling to make some predictions about the internal response of the cells to the chemical stimulus. As we employ random walk models and stochastic equations to describe the motion of cells it naturally leads to a deeper insight into theoretical aspects of those models. Therefore we are also actively involved in more fundamental analysis of theoretical aspects of various random walk systems, in particular those leading to anomalous transport behavior. An example of such work is presented in the research results section of this report.

The division Biological Physics at the **mpipks** has a long and fruitful history of collaboration with the MPI-CBG in Dresden. Our group continues to reinforce this connection by starting the following two projects.

Maternal to zygotic transition in zebra fish embryo Upon fertilization, the embryonic genome is inactive and transcription only starts during the maternal to zygotic transition (MZT). This feature is universal and occurs in animals and plants. Although recent studies involving mRNA deep sequencing provide a significant amount of new information about this process, it is still unclear how repression and activation of transcription in the early embryo are regulated. We would like to better understand the maternal to zygotic transition by using the zebra fish embryos as a model system. On the experimental side it is planed to observe genome activation on a single molecule and single cell level in real time, which is an extremely challenging but achievable goal. Our theoretical efforts would help to understand the emerging pattern of the genome activation on the scale of the whole embryo. In a parallel effort we would like to develop analytical models describing possible scenarios of the MZT and test their plausibility against the existing experimental data. In case of a potentially successful model, additional experiments could be designed to check its predictions. At the moment the most popular hypothesis of the MZT is the so-called excess repressor model. It is a phenomenological approach and the exact factor serving as a repressor remains elusive. In the case of zebra fish embryo, there are some indications that histones and their modifications could serve as such a repressor; it is our goal to explore this possibility. This project is a collaboration with the group of Nadine Vastenhouw at the MPI-CBG.

Physical role of meiotic nuclear oscillation for recombination of chromosomes Meiosis is a fundamental process in all eukaryotes leading to genetic diversity. Despite the accumulating knowledge on meiosis in various organisms, the details of this process and the mechanism of homologous chromosome recombination are still poorly understood. One of the central questions is how the chromosomes can align in a spatial and temporal manner for the proper recombination to occur. It has to happen with enormous precision since mistakes in the recombination and chromosome segregation can be fatal for the offspring. Fission yeast *Schizosaccharomyces pombe*, is an excellent model organism to study meiosis, because it has only three chromosomes (with approximately 14 million base pairs), and it is easily modified genetically. Additionally, meiosis can be induced in a simple manner. Meiotic division in the fission yeast *S. pombe* has a characteristic phase of nuclear oscillations that are necessary for a proper process of homologous chromosome pairing and recombination. The general biophysical mechanisms, responsible for the horsetail oscillations were recently described. However, their exact role in the chromosome recombination remains unclear. Our goal is to build a physical model of this process in order to reveal the biophysical mechanisms underlying chromosome pairing. To build an adequate model some essential information about the cell properties is required, but which is not available yet. For example there is no reliable data

concerning the compaction state of the chromatin during meiosis in yeast. To address this problem we proposed a series of experiments to be performed by using the soft X-ray spectro-microscopy together with the collaborating group of Thomas Pfohl in the University of Basel. Our principle collaborator on the whole project is the group of Iva Tolić-Nørrelykke at the MPI-CBG.

Cooperations

- *Clustering of N. gonorrhoeae bacteria*, Experiments: Group of Nicolas Biais, Columbia University/CUNY Brooklyn College, USA. Numerical simulations: Group of Michael Schmiedeberg, University of Düsseldorf
- *MZT*, Experiments: Group of Nadine Vastenhouw, MPI-CBG Dresden
- *Meiotic oscillations*, Experiments: Group of Iva Tolić-Nørrelykke, MPI-CBG Dresden (biology), and group of Thomas Pohl, University of Basel (soft X-ray microscopy). Theory, model, and simulations: Frank Jülicher, mpi**pks**, and Sergey Denisov, University of Augsburg
- *Bacterial trajectories and random walks*, Experiments: Group of Carsten Beta, University of Potsdam, Simulations and theory: Sergey Denisov and Peter Hänggi, University of Augsburg

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

This group was established in 1995 with a research programme in nonlinear dynamics and time series analysis. Over the years the focus has shifted and the scope was broadened. Our main guideline is the aim to understand, model, and predict fluctuations in open, i.e., driven systems. This comprises research in non-equilibrium statistical physics, low- and high-dimensional dynamical systems, nonlinear stochastic processes with Gaussian and non-Gaussian noises. A particular field of application is the Earth's atmosphere, which is evidently a very complex, driven dynamical system where predictions on short and long time spans are of utmost general interest.

Whereas mean values and average behaviour of systems are often easily assessable, fluctuations around such mean pose the real challenges. More precisely, in these settings we aim for an understanding of, e.g., magnitude distributions and temporal (and spatial, where applicable) correlations of fluctuations, and of the details of the mechanisms behind. Particular motivation arises from the study of extreme events, which often occur as natural disasters and then have large impact on human civilization. Extreme events in driven systems are very large but rare fluctuations, where first of all dynamical mechanisms (feedback loops) exist which drive the system so far off its normal state, but where secondly the frequency and magnitude of such excursions in phase space are constrained by physical conservation laws.

Non-equilibrium fluctuations and irreversibility For thermodynamic systems out of equilibrium, a number of strict relations for ratios of probabilities of fluctuations are known as *fluctuation theorems*. Opposed to open systems with a constant throughput of, e.g., energy, we focus on non-equilibrium processes which are strictly non-stationary since they are driven by the change of some control parameter. The well known Jarzynski integral fluctuation theorem and the detailed Crooks relation describe such processes. Thermodynamic fluctuations of such type are clearly relevant in nano-size systems only, since the amplitude of fluctuations drops to zero in the thermodynamic limit. We transfer this concept to fluctuations in a deterministic system, namely a turbulent two-dimensional velocity field which is subject to some global deformation. Not only do our numerical simulations show that Crooks relation holds in this case for arbitrarily large systems, but we are even able to prove its validity (PhD work of Julia Gundermann, see 2.19 for details). We are currently exploring, how far this will allow us to predict much better rare extreme events, since Crooks relation can be read as a way to compute the value of some very small probability, too small to be estimated from a finite data sample, from much larger probabilities. In other words, we want to use Crooks for the extrapolation of probability distributions towards their tails.

Another project in this range is concerned with the erasure of information from physical memory devices. Maxwell's demon and the Szillard motor are prominent examples for what is today known as conversion of information to work: Knowing the microstate of a system, one can, in principle, extract work from a single heat bath. One possible way how nonetheless the second law of thermodynamics can be established is to assume that the acquisition or the processing of information (about the microstate) leads to energy dissipation. This is exactly the result of our study (PhD work of Léo Granger) where we derived

a differential version of Landauer's principle: The amount of entropy production during erasure (or overwriting) of physically stored information is bound from below by the Shannon entropy which characterises the information content of the stored information, at every moment of some erasure process. In other words, since erasure by definition is an irreversible process, it must be an out-of-equilibrium process where inevitably some excess of entropy is generated.

Fluctuations in the Earth's atmosphere State-of-the-art models of the atmosphere are routinely used in weather forecasts. Formally, they are dynamical systems, and a forecast is the solution of an initial value problem for a finite time interval. By techniques called *data assimilation* one obtains the initial model state vector with about 10^8 components from a set of about 10^5 measurements of the current atmospheric state. This resembles the problem in dynamical systems theory called *shadowing*. Jochen Bröcker from our group (since October 2012 a lecturer at University of Reading) suggested novel variational approaches which are able to balance measurement errors on observations and model errors in model equations by an estimate of out-of-sample assimilation errors.

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

Atmospheric fluctuations and their modeling were in the focus of interest on the workshop "Exploring climate variability" at the ZiF Bielefeld in February/March 2013, which was organised jointly by us, Peter Imkeller (HU Berlin), and Ilya Pavlyukevich (Jena).

Stochastic processes with correlations and non-Gaussian noises Quite generally, long range temporal correlations are an interesting issue, since they might be easily misinterpreted as trends. Correlations can even be so strong that empirical time averages will never converge, which is called "weak ergodicity breaking". We study such phenomena in highly intermittent dynamical systems and in the model class of continuous time random walks (CTRW). Recently, together with Eli Barkai from Bar Ilan University and Markus Niemann from Oldenburg University (former PhD student of our group) we were able to precisely analyse properties of 1/f-noise generated by such type of intermittency (see 2.18). In 2011, together with Eli Barkai, Rainer Klages (London) and Roland Zweimüller (Vienna), we organized the workshop "Weak Chaos, Infinite Ergodic Theory, and Anomalous Dynamics" at the mpi**pks**.

Extreme events Yet another aspect of fluctuations is studied under the keyword extreme events. We continue our efforts in exploring and improving predictability. Besides the already mentioned approach through the Crooks relation, we continued detailed studies of weather extremes. A particular result for extreme temperature anomalies was our finding that data based statistical predictions, which are by orders of magnitude less expensive than so called numerical weather prediction, possess only slightly less predictive power than the latter on short lead times. In addition, we surprisingly found a very strong dependence of predictability on the performance measure by which it is measured, which shows how relevant it is first to decide on the performance measure and then to search for the best prediction scheme.

We also contribute with novel data analysis concepts to a joint research programme funded by the Volkswagenstiftung, where groups from Bonn, Oldenburg, Potsdam, and Dresden make a joint effort to explore harmful algae blooms and epileptic seizures as extremes in excitable media.

Cooperations

- Center for Dynamics at the TU Dresden: Holger Kantz is member of the board of directors of this Centre which will enhance the scientific interchange on dynamics in the Dresden area. We submitted a draft proposal for a DFG funded research group (Forschergruppe).
- Roland Ketzmerick, Physics Department, Technical University of Dresden (Chaos and intermittency in Hamiltonian systems).
- Ulrike Feudel (Oldenburg), Helmut Hillebrand (Oldenburg), Klaus Lehnertz (Bonn), Jürgen Kurths (PIK Potsdam) VW-project Extreme events in excitable media.

- Eli Barkai (Bar Ilan University) CTRW and $1/f$-noise.
- Martin Diestelhorst (University of Halle) experimental verification of Seifert's fluctuation theorem in a periodically driven electric resistor.
- Ilya Pavlyukevich, Peter Imkeller: ZiF Cooperation group "Exploring Climate Variablity"

1.9 Junior Research Groups

Research Group: Dynamical Systems and Social Dynamics
(Head: Dr. Eduardo G. Altmann)

The Otto Hahn group *Dynamical Systems and Social Dynamics* started in January 2011 and is guided by the belief that *complex* temporal behavior often emerges from *simple* evolution rules. Faithful to this principle, the aim of our research is to (i) characterize the complexity of observations and (ii) uncover the essential ingredients of dynamical models describing them. We focus on social systems for which detailed temporal data is available and on physical systems with chaotic transients. Common to all problems are the computational and mathematical methods (coming from dynamical systems theory, stochastic processes, and statistical physics) and the aim of understanding complex behavior using simple models. In the case of chaotic systems, models are well rooted in physical theories and are often chosen based on realistic configurations. In this case, models provide the starting point for investigations of generic phenomena, which are later generalized to larger classes of systems. In the case of social systems, undisputed quantitative theories are typically lacking, so that our starting point is data analysis. Here we benefit from the increasing availability of detailed datasets of human activities. Models are then judged according to their ability to describe the observations.

Problems which have been investigated in the last two years include:

Language dynamics The unprecedent amount of written texts available on the Internet enables us to track the frequency of usage of different words at different times and topics. We are interested not only in quantifying language change but also to trace the dynamics of ideas, opinions, and behavior expressed through the tracked words. We model these phenomena using stochastic growth models (e.g., vocabulary as a whole), evolutionary algorithms (e.g., spreading of new words), and models of population dynamics (e.g., words competing for the same meaning). In all cases the goal is to obtain models with predictive power which also provide a mechanistic understanding of the origin of the observations.

Predictions in fat-tailed distributions The attention of a community typically concentrates in a few out of many available objects. An example familiar to scientists are scientific publications and their corresponding fat-tailed distribution of citations. Similar fat-tailed distributions are widespread, in particular in the Internet (e.g., entries in discussion groups, views of videos). We combine stochastic models, time series analysis, and rigorous prediction methods from the natural sciences in order to develop strategies to predict the attention specific objects will receive. For the problem of magnitude prediction (e.g., number of views or citations), the quality of traditional predictors is greatly reduced due to the fat-tailed distributions, and the traditional quantification of the quality of predictors (e.g., the Brier score) may even diverge. Our goal is to design reliable and informative prediction schemes for this case. We are interested also in the problem of event prediction, which considers whether a specific object will belong to the group of most popular objects. Our assessment of the quality of the prediction provides also a rigorous quantification of the importance of different factors in the success or failure of specific objects.

Leaking chaotic systems The investigation of chaotic dynamical systems traditionally focused on two classes: closed systems, for which trajectories remain confined in a bounded region of the phase space; and open systems, for which trajectories diverge for long times. Leaking systems lie between these two extremes: there is a well-defined closed system on which a hole or leak is introduced. The interest in this problem comes from simulations and experiments (e.g., in optical microcavities) which show that observable quantities (e.g., emission patterns, the escape rate) depend sensitively and non-trivially on the properties of the leak (e.g., position, size). The aim of our research is to understand the origin of these dependencies in large classes of systems. For instance, we have obtained general expressions for the escape rate and the spectrum of fractal dimensions in systems with partial leaks (trajectories are partially absorbed/reflected). We also developed numerical methods to efficiently compute properties of

realistic systems, including methods to compute the spectrum of fractal dimensions of invariant sets and efficiently sample the phase space of high-dimensional systems.

Cooperations

- G. Cristadoro an M. Degli Esposti (Bologna, Italy) on long-range correlations in symbolic sequences.
- T. Tél (Budapest, Hungary) on transient chaos.
- J. M. V. P. Lopes (Porto, Portugal) on Monte Carlo sampling methods in complex systems.
- M. Sales and R. Guimerà (Tarragona, Spain) on stochastic growth processes.
- O. de Oliveira (São Carlos, Brazil) on computational natural language process and applications.
- D. Rybski (Potsdam, Germany) on scaling laws and statistical properties of languages.

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

The mesoscopic systems's group, funded by the DFG Emmy-Noether programme, finished its work at the mpi**pks** in March 2012 when the group leader, Martina Hentschel, became Professor in Theoretical Physics at the Technical University of Ilmenau, Germany. Most of the group members moved around the same time to promising positions in their home countries. The activities of the group continued to be in the field of many-body effects in mesoscopic systems including graphene (see the scientiffic report of the group below) as well as in the area of optical microcavities and microlasers with a total of 9 publications, inlcuding one Optics Letter and one Europhysics Letter. Georg Röder finished his PhD thesis on the X-ray edge problem in ballistic quantum dots in November 2011. Martina Hentschel was co-organizer of the WOMA conference 2011 in Pusan, Korea and co-organized the international conference "Wave chaos from the micro- to the macroscale" WCMM12 at the mpi**pks** Dresden in October 2012. She was invited to give plenary talks at the Spring Meeting of the German Physical Society in 2011 and at the Physikerinnentagung of the German Physical Society in November 2011. Martina Hentschel gave birth to a baby in 2012 and was awarded the Hertha Sponer Prize of the German Physical Society in 2011.

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

The Junior Research Group *Computational Nonlinear and Relativistic Optics* started to operate in fall 2007 at the mpi**pks**. In April 2009, the group leader Stefan Skupin became appointed as *Carl Zeiss* Junior Professor for *Computational Photonics* at the Friedrich Schiller University in Jena. Due to this second engagement, Stefan Skupin is only two days per week present at the mpi**pks**, and it became necessary to appoint a long-term Post-Doc as an assistant group leader. Until December 2012, Mickael Grech filled this position, however, he got permanently appointed as Chargé de recherche by the French CNRS at the Laboratoire d'Utilisation des Lasers Intenses (LULI) near Paris. Since 2013, Evangelos Siminos acts as new assistant group leader. In 2012, one of the two PhD. students, Christian Köhler, graduated and left the group to work with our long-term collaborator Dr. Luc Bergé at the French Commissariat à l'Énergie Atomique near Paris. The group's second student, Fabian Maucher, is expected to graduate in 2013. Thus, we are currently in the process of recruiting one or two new students. Last but not least, Jörg Götte joined the group in 2011 for a two-years Post-Doc, and the visitors program enabled several shorter visits of other senior scientists.

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

High intensity laser matter interaction With the development of the laser in the 60's the field of nonlinear optics was born. Light intensities achieved made it possible to observe effects induced by the light itself as it propagates through a medium. Nowadays, the rapid progress in laser technology almost continously opens new fields of research in laser matter interaction. In the past decade, the range of wavelengths which is accessible by exploiting frequency conversion from an optical pump has grown dramatically.

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

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

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

Another aspect of high intensity laser matter interaction we are currently looking at are turbulent dynamics in femtosecond multi-filamentation. Filament formation is ruled by two counteracting nonlinear optical mechanisms. One of these effects is self-focusing, which causes a beam collapse for sufficiently high powers. This effect is typically arrested by plasma formation, which defocuses optical radiation. This nonlinear optical system bears a modulation instability, which causes the break-up of a spatially homogeneous intensity profile into one or several highly localized filament strings above a critical power P_{crit}. Even though single-shot transverse beam profiles of multiple filaments have frequently been measured and simulated, little record is available on the detailed shot-to-shot dynamics inside their beam profiles. All the effects involved in filament formation are deterministic effects; therefore identical input beam profiles and gas-cell conditions are expected to yield identical filamentation patterns. Given that the system is highly nonlinear, one expects an effect of even the smallest fluctuations in the input profile, potentially giving rise to dramatic fluctuations of the resulting patterns from shot to shot. While most theoretical investigations indicate that noisy input pulses are enough to explain such fluctuations, the crucial role of thermal fluctuations and atmospheric turbulence along the beam path is currently debated. Moreover, once filaments are formed, they are known to interact, a degenerate variant of four-wave mixing, namely cross-phase modulation between individual filament strings automatically causes a phase front

tilt in the vicinity of each filament string, steering neighboring filaments into each other. Thus, multiple filamentation of femtosecond laser pulses is a promising system to observe so-called rogue waves, i.e., giant filaments with much higher energy than average, created in the rare event of merging of several ordinary filaments. Moreover, a more universal understanding of this phenomenon may prove useful for harnessing rogue wave events, their avoidance, or their controlled generation. Such control holds fascinating possibilities, where the limiting effect of filamentation in optical materials could be converted from nuisance into a useful effect, allowing the transport of much higher energies in a self-confined geometry than currently perceived possible.

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

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

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

Recently, we proposed a scheme for the creation of three-dimensional bright solitons in a BEC. The approach is based on optical dressing of a groundstate atom BEC to highly excited Rydberg states. We were able to identify an appropriate range of Rydberg states that provides sign-definite attractive nonlinearities, and thus prevents condensate collapse as occurring in dipolar gases. In fact, the stability of higher order localized structures is intimately linked to the efficient suppression of wave-collapse, and we could proof absence of collapse for a certain class of nonlinearity rigorously.

Currently, we are working on the impact of random perturbations both in propagational as well as transverse directions on solitons in nonlocal media. Both numerical simulations and analytical estimates show that the stability of fundamental bright solitons in the presence of random perturbations increases dramatically with the nonlocality-induced finite correlation length of the noise in the transverse plane. In fact, solitons are practically insensitive to noise when the correlation length of the noise becomes comparable to the extent of the wave packet. In near future, we want to investigate the interplay between wave collapse and random perturbations.

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

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

Our research at the mpi**pks** is devoted to laser-based ion acceleration and its applications. Multi-MeV ion beams generated during the interaction of an intense laser pulse with a plasma can indeed initiate

a thermonuclear reaction in the so-called fast-ignitor scenario for inertial confinement fusion. Due to their good laminarity, collimation and short duration, they are also used for time-resolved radiography in plasma experiments. Last but not least, high-quality ion beams may also be used for medical applications such as isotope creation and hadron-therapy.

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

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

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

Besides, we recently revisited the effective increase of the critical density associated with the interaction of relativistically intense laser pulses with overcritical plasmas, known as relativistic self-induced transparency (RSIT), for the case of circular polarization. Our comparison of particle-in-cell simulations to the predictions of a relativistic cold-fluid model for the transparency threshold demonstrated that kinetic effects, such as electron heating, can lead to a substantial increase of the effective critical density compared to cold-fluid theory. We showed that perturbations due to pulse profile dependent electron heating exceeding a certain finite threshold can force electrons to escape into the vacuum, leading to laser pulse propagation. We think that our results will trigger further investigations in this domain, as the reported dependency of the RSIT threshold on the pulse profile could provide a versatile tool for high-contrast CP laser pulse characterization

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

Joint research program *mpipks* and MPI-CBG

In 2004 the Max Planck Institute for the Physics of Complex Systems and the Max Planck Institute of Molecular Cell Biology and Genetics started the joint research program 'Physics of Biological Systems' to strengthen the collaborations between the two institutes. The objective of the program is to develop physical techniques - both experimental and theoretical - for analyzing biological systems. Until mid-2012, the program comprised three Junior Research Groups. The group of Dr. Michael Hiller is located at the mpi**pks** and works on Computational Biology and Evolutionary Genomics. The group of Dr. Iva Tolić-Nørrelykke (Interior Design of the Cell) is located at the MPI-CBG and studies how the cell organizes its interior over its lifetime. The group of Dr. Stephan Grill (Motor Systems) is located at both institutes and addresses cell-scale emergent physical properties and the collective function of molecular machines. In summer 2012, the joint research program 'Physics of Biological Systems' was merged in the newly founded 'Center for Systems Biology Dresden'. Jointly run by tne mpi**pks** and the MPI-CBG

the center provides a unique research environment bringing together experimental biology, theoretical physics, bioinformatics and image analysis to shed light on the physical principles that underlie living systems.

Junior Research Group: Motor Systems
(Head: Dr. Stephan W. Grill)

Our group is interested in how molecular machines, the workhorses of the cell, function collectively to give rise to the complex dynamical processes observed in living organisms. The whole is greater than the sum of the parts - in this spirit we pursue an understanding of how molecular mechanisms give rise to specific behaviors that emerge at length and time scales relevant for processes at the cell biological level, using a combined experimental and theoretical approach. Our main focus concerns the question how biochemical networks interact with mechanical ones to enact morphogenetic change. Answering this question requires (I) a physical description of the underlying mechanical processes, (II) an understanding of the regulatory components and their behaviors, and (III) an identification of the possible means of interaction. Working on all three points in the past several years, we have revealed how the *C. elegans* zygote polarizes and how the zebrafish embryo undergoes epiboly during gastrulation. In a second set of projects we investigate transcription by RNA polymerase in relation to molecular events that occur in the machinery that is involved. This is done by combining single-molecule optical tweezer experiments on RNA polymerase I and II with a theoretical treatment in the framework of statistical mechanics.

Morphogenetic Mechanochemical Pattern Formation

Summary A central focus of our work has been to reveal generic forms of coupling between mechanics and biochemistry. The establishment of cellular and developmental form rests on this interplay. Biochemical regulatory pathways directly active deformation and reshaping of cells and tissues. Components of these regulatory pathways are transported by flow and deformation arising from active mechanical processes inside cells. In some instances one can successfully decouple the biochemistry from the mechanics. This is the approach that was taken sixty years ago by Alan Turing when he started the field of reaction-diffusion. However, we are learning more and more that generally this is not possible. My group has been studying the process of establishment of cell polarity in the *C. elegans* zygote, a classical example of coupling of mechanical and biochemical pathways for enacting morphogenetic change. Here, flows in the actomyosin cell cortex trigger the formation of an intracellular pattern in the distribution of PAR proteins. Generally, the actomyosin cortex is responsible for much of the reshaping and mechanical restructuring that proceeds at both the cellular and the tissue scale. To understand the mechanisms by which patterning, structure and form arises in development, we must first find an appropriate mechanical description of the actomyosin cell cortex, and then integrate with biochemical regulation. It is essential that we find these mechanical descriptions. They represent fundamental laws of morphogenesis that describe how cells or tissues deform and restructure themselves. They define the rules of the game of morphogenetic processes, they characterize the playing field on which regulatory molecular pathways are acting. We need ways of identifying them, and we need systematic approaches that link molecular scale physical mechanisms to those on cell and tissue scales. Morphogenesis is one of the great remaining mysteries, and tackling it requires an interdisciplinary approach that links cell/developmental biology with biophysics experiments and with theory. This has been our approach for investigating the mechanochemistry of polarity establishment. At the cellular scale, we have shed light on how cortical flow, through advection, triggers the formation of a pattern in the PAR polarity system to polarize the cell. We found that PAR proteins undergo exchange between well mixed cytoplasmic populations, and laterally diffusing membrane-associated states. We discovered that cortical flow, by inducing transient PAR segregation, serves as a mechanical trigger for the formation of a PAR pattern in a multistable PAR reaction-diffusion system. At the multicellular scale and in work that was done in collaboration with the Group of Guillaume Salbreux at the mpi**pks**, we have identified a crucial role for flow of actomyosin into an actomyosin ring for driving epiboly during zebrafish gastrulation. Taken together, our work has uncovered that many aspects of polarity establishment in *C. elegans* and epiboly in zebrafish are governed by simple mesoscale biophysical laws, and can be understood as processes of morphogenetic mechanochemical pattern formation.

Future plans Future plans concern (I) the development of a generic theory of pattern formation in coupled active mechanical and biochemical systems, and (II) the utilization of this theory to investigate

morphogenetic events at the cellular and the developmental scale. At the cellular scale we plan to continue our investigations of cortical flow and polarization of the *C. elegans* zygote, to understand the feedback from the PAR system to cortical force generation. At the developmental scale we plan to investigate the physical basis of *C. elegans* epithelial morphogenesis, to reveal how actomyosin-based force generation determines tissue reshaping. We are also extending our work in zebrafish gastrulation, where we investigate which mechanisms ensure the stationary structure of the actomyosin ring. In all these projects, the actomyosin cytoskeleton will continue to be a specific focus of our research. Actomyosin is pivotal in many types of developmental rearrangements, and we plan to find mechanical descriptions that accurately characterize the essential aspects of its coarse-grained and mesoscale active mechanical behavior. These include the local ordering of actin filaments, the clustering and pulsatory behavior of myosin in situations of high contractility, and large-scale rotatory and chiral actomyosin flow. We will combine high-resolution optical microscopy with advanced image analysis techniques for an experimental analysis of filament alignment, clustering and chiral flow. We will extend our physical description to short times to incorporate elastic effects, and we will include nematic order and active torques to provide a theoretical analysis of filament alignment, clustering and chiral flow. Finally, we will integrate these descriptions with proper formulations of biochemical feedback and control, to reveal the principles by which mechanochemical patterning, structure and form arises in development.

Single Molecule Transcription

Summary 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 amino acid sequence that forms the protein product, which is encoded by the sequence of DNA that was originally read out. Since the production of 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. Understanding the micromechanical events that underly RNA polymerase transcription on both naked DNA and on chromatin templates remains one of the great challenges in Biology. In the past 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. In theoretical work, we focused on rate-limiting off-pathway events during transcription. We examined the dynamics of backtracking, a state thought to be crucial for detecting and removing copy errors. Pause lifetimes follow a power law behavior, indicating that the polymerase performs a one-dimensional random walk while backtracked and engaged in error correction. We revealed that a further consequence of random-walk backtracking is that it generates two asymptotic subsets of pauses distinct both in duration and trajectory. Both classes of pauses have been observed in experiments, and we now suggest that both are a consequence of a single process, random-walk backtracking. Furthermore, the ability of the machine to move backwards along the copy template allows for retrospective proofreading of past copy errors. In recent work we investigated the transcriptional fidelity achieved by diffusive proofreading within the general framework of kinetic proofreading schemes. We showed that diffusive proofreading increases transcriptional fidelity to a degree that accounts for the difference between what is physiologically observed and what is expected from base pairing energies alone. Furthermore, by considering transcriptional performance at the level of the gene, we revealed that frequent backtracking leads to an enormous increase in the rate at which extended transcripts of high fidelity can be produced.

Future plans Future plans concern (I) backtracking and pausing during RNA Polymerase I transcription, and (II) mechanisms of chromatin transcription by RNA Polymerase II. We are currently pursuing both sets of experiments on our high-resolution dual-trap optical tweezer apparatus. On the theoretical side, we are extending our statistical mechanics treatment of RNA polymerase backtracking to include sequence-dependent effects.

Cooperations

- C.-P. Heisenberg, IST, Klosterneuburg, Austria: Zebrafish Gastrulation
- J. M. R. Parrondo, Universidad Complutense de Madrid, Spain: Irregular dynamics for transcriptional proofreading
- P. Cramer, Gene Center and Department of Biochemistry, Ludwig-Maximilians-Universität München: Transcription by RNA Polymerase I
- C. Müller, European Molecular Biology Laboratory, Heidelberg Germany: Transcription by RNA Polymerase III
- J .Ahringer, The Gurdon Institute, University of Cambridge, U.K.: PAR Suppressors

- F. Schnorrer, MPI für Biochemie, Martinsried: Muscle Tension
- A. A. Hyman, Max Planck Institute of Molecular Biology and Genetics: Cortical Polarization
- F. Jülicher, Max Planck Institute for the Physics of Complex Systems, Dresden: Active Polar Gels
- G. Salbreux, Max Planck Institute for the Physics of Complex Systems, Dresden: Active Nematic Gels

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

The group on Dynamics of Biological Networks (BioND) was hosted for four years at the Max-Planck-Institute for Physics of Complex Systems. Presently, the group is in the transition of moving to the University of Bristol, while the last Dresden-based members are finishing their work. Over the years the members of the group have published 47 publications including two papers in Science, two in Physical Review Letters as well as two books.

The central aim of the group is to gain a heightened understanding of complex systems through the development of new approaches combining insights from statistical physics, nonlinear dynamics and network science. The defining feature of complex systems is their ability to exhibit emergent properties, which do not arise from the constituents of the system, but from their interactions. When describing a system as a network one simplifies the constituents, but retains the complexity of the pattern of their interactions. Therefore, network models can often provide a simplified picture of a real-world complex system without simplifying the complexity away. The hope is then that the simplification enables a deeper understanding of the process of emergence in the system. To achieve this goal, analytical approaches are needed that are capable of describing both structural and dynamical properties of the systems. The BioND group aims at developing such approaches and applying them to important actual problems in applications.

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.

During the initial two years of work we focused on the consolidation of the generalized modelling approach, by supporting generalized modelling by a rigorous mathematical theory. This has greatly increased the capabilities of generalized models and also facilitated the adoption of the generalized modeling approach by other labs. In the past two years we were able to capitalize on this success and use generalized models to resolve questions from a wide range of fields. For instance generalized models played a major rule in the development of a procedure for the design of dynamical motifs in networks. These motifs are sets of a small number of network nodes that can be embedded in larger networks and have distinct consequences for the system-level dynamics regardless of the embedding structure. Furthermore, generalized models were used to formulate new approaches for the identification of important species in ecosystems and for the detection of early warning signs for critical transitions.

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

In the past two years a major focus in this area was to develop methodologies for the analysis of adaptive networks with discrete states in the network nodes. We supplemented our previous work on moment expansions for these networks by the development of a new method, which yields excellent analytical results specifically in the cases where moment expansions fail. Together these two approaches form a powerful tool-kit for the study of simple adaptive network models. We subsequently shifted our focus to more difficult classes of systems such as weighted, continuous, and strongly heterogeneous adaptive networks. Here we have made significant methodological progress with the development of new

approaches (signature-stability analysis, triple-jump method for heterogeneous systems), which we used in recent publications to gain insights into synchronization of large oscillator networks, the evolution of cooperation in biological populations, and social opinion formation.

Junior Research Group: Computational Biology and Evolutionary Genomics
(Head: Dr. Michael Hiller)

The Junior Research Group *Computational Biology and Evolutionary Genomics* started in Oct 2011 jointly at the **mpipks** and MPI-CBG, as part of the new center for systems biology. With an overarching interest to convert biological data into knowledge, the group focuses on the development and application of computational biology approaches to link the observable characteristics of species (phenotypes) to the underlying locus in the DNA (genotype).

Evolution has led to an amazing diversity of phenotypes in all major species clades. Since DNA as the blueprint of life encodes the phenotypes of an organism, phenotypic differences between species must be due to differences in their DNA. Advances in sequencing technology make it possible to read the entire DNA sequence (the genome) of many species. Nevertheless, we know very little about which genomic differences underlie phenotypic differences that make up the diversity observed in nature. The main reason is that any pair of species, even when as closely related as human and chimpanzee, exhibits millions of genomic changes as well as countless phenotypic changes. While this N:N relationship makes it hard to study how phenotypic differences are encoded in the genome using a pair of species, the availability of scores of other genomes allows us now to use multi-species comparative approaches to address this question using the power of comparative and evolutionary genomics.

The goal of the group is to develop computational algorithms and methods to associate phenotypic differences between several species to differences in genomic elements in order to explore the underlying mechanisms and to infer general evolutionary principles. This will give insights into questions like: How did nature's incredible phenotypic diversity evolve? How does a biological system change and adapt to loss of some of its components? How do complex molecular systems change in evolution as the result of species' phenotypic changes?

Our work focuses on two strategies that can be described as "forward" and "reverse genomics". Forward genomics starts with a given independently-evolved phenotypic difference and systematically searches whole genomes for differences that correlate and match to the phenotypic pattern. Reverse genomics starts with the systematic detection of genomic differences that likely have functional consequences and uses exploration-driven approaches that integrate available functional annotations as well as statistical enrichment tests to predict phenotypic changes for individual or entire sets of genomic differences. The lab is jointly affiliated with the MPI-CBG, which allows us to experimentally test if and how the genomic differences pinpointed by the computational approaches are involved in changing molecular and morphological phenotypes in a variety of model organisms.

Research Group: Microtubules and Motor Proteins in Cell Division
(Head: Dr. Iva Tolić-Nørrelykke)

A cell is not a bag full of randomly dispersed molecules, molecular assemblies, and organelles. The cell interior is instead neatly organized in a dynamic yet controlled manner. Dynamic organization of the cell interior requires constant exploration of the intracellular space to adjust the position of cell components in a response to changes such as cell growth, progression through the cell cycle, and signals from the environment. To this aim the cell uses microtubules and actin filaments, motor proteins, and other cytoskeleton-associated proteins. We are interested in how motor proteins and microtubules self-organize to generate large-scale structures and movements in the cell. The main projects in the lab are focused on the mechanism of nuclear oscillations that help chromosome pairing in meiosis, the mechanisms of kinetochore capture and spindle assembly, as well as on segregation of damaged proteins in dividing cells. Our approach is live cell imaging of microtubules and motors at the single-molecule level in fission yeast and mammalian cells, in combination with genetic and biophysical manipulations, e.g., laser ablation. We aim at quantitative descriptions and development of simple theoretical models that help us understand the self-organization processes in the cell.

How Microtubules Find Chromosomes For a mother cell to divide its genetic material equally between the two daughter cells, the chromosomes have to attach to microtubules, which will pull them apart. The linkers between chromosomes and microtubules are kinetochores, protein complexes on the chromosome. The central question, how microtubules find kinetochores, is still under debate. We observed in fission yeast that kinetochores are captured by microtubules pivoting around the spindle pole body, instead of growing towards the kinetochores. By introducing a theoretical model, we show that the observed angular movement of microtubules is sufficient to explain the process of kinetochore capture. Our theory predicts that the speed of the capture process depends mainly on how fast microtubules pivot. We confirmed this prediction experimentally by speeding up and slowing down microtubule pivoting. Thus, microtubules explore space by pivoting, as they search for intracellular targets such as kinetochores (Kalinina *et al.*, *Nat Cell Biol* 2012).

Nuclear Oscillations To exert forces, motor proteins bind with one end to cytoskeletal fibers, such as microtubules and actin filaments, and with the other end to the cell cortex, a vesicle, or another motor. A general question is how motors self-organize to generate large-scale movements in the cell. As an example of a system where a motor binds to a microtubule and to the cell cortex, we study dynein, which, during meiotic prophase in fission yeast, drives oscillations of the spindle pole body (SPB) and of the nucleus. These oscillations are crucial for proper chromosome pairing and recombination. By combining quantitative live cell imaging and laser ablation with a theoretical description, we have shown that the mechanism of these oscillations relies on the asymmetric distribution of dyneins, with more dyneins bound to the leading than to the trailing microtubule (Vogel, Pavin *et al.*, *PLoS Biol* 2009). The observed asymmetry is a consequence of preferred unbinding of dynein from the trailing microtubule. Our work provided 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.

Targeting of Dynein: Single-molecule Observations of Dynein in vivo We next investigated the mechanism by which dyneins target sites where they can exert force. We set up the experiments to observe the movement of single dyneins in vivo. We were able to follow single dyneins moving on the microtubule and diffusing in the cytoplasm. Surprisingly, we were also able to directly visualize binding of dynein from the cytoplasm to the microtubule and to quantify this process. These measurements were possible because we pushed our Total Internal Reflection Fluorescence (TIRF) microscope to the limit by using a high laser power and the highest possible speed of imaging, 200 frames/s. Direct single-molecule observations enabled us to identify the main steps of the dynein binding process: (i) from the cytoplasm to the microtubule, and (ii) from the microtubule to the cortical anchors. We uncovered that dyneins on the microtubule move, surprisingly, either in a diffusive or a directed manner, with the switch from diffusion to directed movement occurring upon binding of dynein to the cortical anchor. By using genetics, we have shown that this binding is sufficient to activate dynein. The dual behavior of dynein on the microtubule, together with the two steps of binding, constitute the mechanism by which dyneins find cortical anchors in order to generate large-scale movements in the cell. This work is currently under revision (Ananthanarayanan *et al.*: Dynein diffuses along the microtubule and becomes activated upon binding to cortical anchors in vivo).

The Role of Kinesin-8 in Nuclear Centering In fission yeast, microtubules push against the cell edge, thereby positioning the nucleus in the cell center, which in turn positions the cell division plane. Microtubule dynamic properties, including catastrophe, are regulated by proteins such as kinesin-8 motors. The effect of kinesin-8 on microtubule dynamics has been studied experimentally and theoretically, however, the role of kinesin-8 motors in nuclear positioning is not known. We have shown that the nucleus is centered better in wild-type cells than in those lacking kinesin-8 motors. We developed a physical model describing how kinesin-8 motors accumulate at the plus end of dynamic microtubules in a length-dependent manner, to regulate their catastrophe rate and consequently the time the microtubule spends in contact with the cell end pushing the nucleus. Our model reproduces the improved centering in the presence of motors. The model predicts a characteristic time for the re-centering of a displaced nucleus, which we confirmed experimentally by displacing the nucleus using optical tweezers. We observed a decrease in the velocity of the spindle pole body as it stretched the nucleus, which we interpret as a decrease in the microtubule growth velocity with increasing compressive force of the microtubule. In summary, we propose a positioning mechanism in which kinesin-8 motors improve nuclear centering by regulating microtubule catastrophe. This work is currently under review (Maghelli *et al.*: Kinesin-8 motors improve nuclear centering in fission yeast).

Segregation of Protein Aggregates at Cell Division Asymmetric segregation of damaged proteins at cell division generates a cell that retains damage and a clean cell that ensures the survival of the population. Yet, the mechanisms underlying damage segregation have remained largely elusive. We have shown that misfolded protein aggregates in fission yeast segregate symmetrically or asymmetrically, where the transition between these two modes is facilitated by fusion of aggregates. Using the GFP-labeled chaperone Hsp104 to monitor protein aggregates in vivo, we found that aggregate dynamics is consistent with a stochastic aggregation model. Upon stress aggregate nucleation increases, and extensive fusion forms large aggregates, which segregate asymmetrically at division. The cells that inherit large aggregates typically die. Our results show a new mode of damage segregation, where the transition from symmetric to asymmetric segregation promotes survival in stressful environments. This work is currently under revision (Coelho *et al.*: Protein aggregate fusion facilitates a transition between symmetric and asymmetric damage segregation).

Cooperations

- Theoreticians:
  - Nenad Pavin, mpi**pks** and University of Zagreb, Croatia: Modeling of nuclear oscillations, dynein dynamics, nuclear centering, kinetochore capture
  - Frank Jülicher, mpi**pks**: Modeling of nuclear oscillations, dynein dynamics, kinetochore capture
  - Vasily Zaburdaev, mpi**pks**: Modeling of chromosome pairing
  - Thilo Gross, mpi**pks** and University of Bristol: Modeling of protein aggregate dynamics
  - Benjamin Lindner, mpi**pks** and Bernstein Center Berlin: Modeling of kinetochore capture

- Experimentalists:
  - Simon Alberti, MPI-CBG, Dresden: Protein aggregates
  - Stefan Diez, MPI-CBG and TU Dresden: *In vitro* reconstitution of nuclear oscillations
  - Juraj Gregan, University of Vienna: Forces acting on kinetochores in yeast
  - Daniela Cimini, Virginia Tech: Forces acting on kinetochores in mammalian cells

Joint research program *mpipks* and MPI-CPfS

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

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

The Joint Junior Research Group *Collective Phenomena in Solid State and Materials Science* is co-sponsored by the mpi**pks**, the MPI-CPfS and the *Innovationsfond* of the President of Max Planck Society. As the group is a joint research group of two institutes, special efforts are made to integrate the group into both institutes. A particular attraction of the nature of the group's set-up is that it is located at two institutes involved in cutting-edge research on both the theoretical and the experimental aspects of modern condensed matter physics and materials science. Research interests of the group center around the understanding of correlations in and out of thermal equilibrium in strongly correlated electron systems, in particular on quantum criticality in rare earth intermetallic compounds. Intermetallic rare earth and actinide compounds are extended lattice systems where the competition between localized and itinerant

degrees of freedom gives rise to a complex behavior and a plethora of competing ground states where the relevant energy scales emerge out of the bare couplings that determine the high-temperature behavior. As a consequence, theoretical models like the so-called Kondo lattice model are effective models designed to describe the universal aspects of the problem. Thermodynamic and (bulk) transport measurements, i.e. the traditional bulk measures that are available at low temperatures, are more and more augmented by local probes that have become available, e.g. neutron scattering techniques or most recently scanning tunneling microscopy for heavy fermions. These novel experimental tools give access to the microscopic coupling constants that enter theoretical models but in turn require effective theories that go beyond the universal aspects of the problem. The Max Planck Institute for Chemical Physics of Solids is at the forefront of experimental research in 4f- and 5f electron systems and has been playing a key role in establishing the existence of unconventional quantum criticality in such systems. Quantum criticalities promise to offer a novel organization principle or paradigm to address universal features of the general phase diagram of correlated matter. Such quantum criticalities occur as matter is tuned through a continuous zero-temperature phase transitions and are found to affect the properties of matter in a wide temperature and parameter range fanning out from the singular zero-temperature critical points. So far, the existence of quantum critical points has been established beyond reasonable doubt only in heavy fermion systems although growing evidence exists that quantum criticality also governs the phase diagram of other strongly correlated materials, like e.g. the high-temperature cuprate superconductors. In the traditional approach to quantum criticality, the critical regime is described in terms of a Ginzburg-Landau-Wilson functional of the order parameter and its fluctuations where the order parameter is a physical quantity characterizing the ordered side of the critical point. Quantum mechanics enters in this approach only in increasing the effective spatial dimensions in which the Ginzburg-Landau-Wilson functional is defined. As a result, this classical theory in elevated dimensions predicts mean field behavior for many systems. In the context of magnetic quantum criticality, the classical Ginzburg-Landau-Wilson approach is known as the spin-density wave theory. Experimental and theoretical work for heavy fermion systems has established the existence of at least one other class of quantum critical points. This additional class of quantum critical points defies a description in terms of a Ginzburg-Landau-Wilson functional. Characteristic to all quantum critical points is the diverging correlation length as criticality is approached. This divergence is at the heart of the scale-invariant energy spectrum and the origin of 'universality' i.e. the phenomenon that the power law divergence of physical quantities is largely independent of physical details of the system. At present, neither a field theoretic formulation for the new class of quantum critical points is known nor a general classification of quantum critical points into universality classes is available.

With these developments in the broad area of instabilities in strongly correlated electron systems is mind, the group focuses on

- developing phenomenological theories as a framework to understand and describe experiments performed on quantum critical systems. This also involves to relate theoretical results to the in general more complicated experimental setting.
- Studying the properties of paradigmatic models of strongly correlated electron systems on a lattice in and out of equilibrium. This is done both by using analytical approaches were possible together with state-of-the art numerical algorithms.
- Relating experimental probes, *e.g.* scanning tunneling spectroscopy or photo-emission to the basic building blocks of many body theory. In particular for local probes like the scanning tunneling microscope this is not trivial but may be key to a better understanding of correlated matter.

Cooperations

In addition to the projects between the **mpi**pks and MPI-CPfS, we initiated a number of projects with external collaborators. Joint projects currently exist with

- Dr. Theo Costi from the *Institute for Advanced Simulation* at the Research Centre Jülich on applications and extensions of the numerical renormalization group technique.
- Prof. Dr. Enrique Munoz Tavera from the Pontificia Universidad Católica in Santiago de Chile on the development of a renormalized dual fermion perturbation theory on the Keldysh contour to describe steady-state transport.
- Dr. Gavin Scott from Alcatel-Lucent and Prof. Dr. Douglas Natelson from Rice University on transport characterization of nano-scale devices.

- Prof. Dr. Qimiao Si from Rice University, Houston and Prof. Dr. Kevin Ingersent, University of Florida at Gainesville. The long-term goal of the collaboration with Qimiao Si and Kevin Ingersent and the members of their groups is the construction of the critical field theory of the particular unconventional quantum critical point that recently were observed in a number of intermetallic rare earth compounds. We try tackle this problem by a two-pronged approach. On the one hand, we obtain a microscopic understanding of the physics near zero-temperature instabilities in certain models. This has so far been accomplished for the spin-isotropic Bose-Fermi Kondo model and the so-called pseudogap Bose-Fermi Anderson model. On the other hand, symmetry considerations can be used to pose important constraints on the underlying critical field theory.
- Dr. Gang Li and Prof. Dr. Werner Hanke from Universität Würzburg. We are working on a ladder dual fermion resummation around the dynamical mean field result (DMFT) of the Hubbard model on the triangular lattice to address the interplay of electron correlation and frustration. This research is motivated by several classes of materials, where this interplay is underlies the emergence of unconventional phases. For example, the κ-(BEDT-TTF)$_2$X family and the layered cobaltate $Na_xCoO_2{\cdot}yH_2$ are triangular systems that develop superconductivity at sufficiently low temperatures.
- Prof. Dr. Emanuel Gull from University of Michigan on a dual fermion description for the charge order transition in the Falicov-Kimball model.
- Prof. Dr. Dirk Morr from the University of Illinois at Chicago. Together with D. Morr and his group we pursue the question of how site disorder influences the quantum critical properties of the Kondo lattice. In addition, we intend to develop a theoretical framework for 'quasiparticle interference imaging' based on a SU(N) approach that is likely to be relevant to upcoming Scanning tunneling microscopy measurements on doped $YbRh_2Si_2$. Quasiparticle interferences have recently been utilized in the hidden order compound URu_2Si_2 by the Davis group to trace the evolution of the band structure across the hidden order transition (A. Schmidt et al., *Nature* **465**, 570 (2010)).
- Prof. Dr. Hans Kroha from Universität Bonn. While a number of numerical tools exist to treat the short-time evolution of strongly correlated systems, the long-time limit of non-stationary problems has not received much attention. The Floquet technique is one of the few means to treat the long-time limit of periodically driven systems. In this project, we apply this technique to time-dependent strongly interacting problems.

1.10 Max Planck Fellow Group

Max Planck Fellow Group: Quantum Chaos and Quantum Dynamics
(Head: Prof. Dr. Roland Ketzmerick)

The group was founded in September 2010 on the basis of the Max Planck fellowship of Prof. Roland Ketzmerick (Technische Universität Dresden) for the purpose of strengthening the collaboration between TU Dresden and the mpi**pks**. The group is co-headed by Dr. André Eckardt. Further group members currently are one Diploma student (Marcus Bugner), three PhD students (Clemens Löbner, Christoph Sträter, Daniel Vorberg), two associated guest scientists (Jeremy Le Deunff, Soo-Young Lee), as well as two external members (PD Arnd Bäcker from TU Dresden, Prof. Holger Schanz from Hochschule Magdeburg-Stendal).

The interests of the group range from quantum signatures of regular and chaotic dynamics with the current focus on a semiclassical theory for tunneling and four-dimensional maps, over statistical physics of open many-body Floquet systems, to ultracold atomic quantum gases with a special interest on optical lattices, time-periodically driven systems, geometric frustration, and artificial gauge fields.

Quantum Signatures of Regular and Chaotic Dynamics We are interested in the properties of quantum systems where the underlying classical dynamics is non-integrable, in particular when regular and chaotic dynamics coexist. One of the main topics is the development of a semiclassical theory for tunneling between regular and chaotic phase-space regions. In contrast to the well-understood 1D tunneling through an energetic barrier, the use of complex paths for tunneling in the presence of chaos is a major challenge. We also investigate the universal quantum properties of classical partial barriers which are ubiquitous in the chaotic component of phase space. For open quantum systems these partial barriers affect the fractal properties of the chaotic saddle, the localization of eigenstates on this fractal, and lead for the counting

function of the number of resonances to a modified fractal Weyl law. We study wave-packet dynamics in open quantum billards generalizing the concepts of the Goos-Hänchen shift and Fresnel filtering from optical microcavities. In higher dimensional systems, which play an important role in many areas of physics, regular tori do not separate regions in phase space. Thus one typically has regular motion which is surrounded on arbitrary fine scales by chaotic motion, leading for example to Arnol'd diffusion. We investigate methods for the visualization of the underlying structures in phase space for four-dimensional maps. This is used in searching for the mechanism of power-law trapping in these systems and allows for studying the quantum-classical correspondence by displaying Husimi functions together with the classical phase space.

Research in this area is strongly linked with the activities of the 2011 Advanced Study Group *Towards a Semiclassical Theory of Dynamical Tunneling*, the Center for Dynamics Dresden, and the German Science Foundation Research Unit FOR 760 *Scattering Systems with Complex Dynamics* headed by R. Ketzmerick.

Statistical Physics of Open Many-Body Floquet Systems We are studying the standard questions of Statistical Physics for many-body Floquet systems, i.e. systems governed by a time-periodic Hamiltonian instead of a time-independent one. Specifically we concentrate on a driven system with weak coupling to a thermal bath. The driven system will assume an asymptotic state that neither obeys detailed balance in the Floquet-Fock space nor posseses mean occupations given by Boltzmann factors. We are investigating the ideal Floquet quantum gas, in particular the consequences of bosonic or fermionic quantum statistics in the quantum degenerate regime. We are addressing questions like: whether (and if yes when) Bose condensation can be expected; whether non-trivial correlations can be engineered from the coupling to the bath; whether (and if yes how) the semiclassical chaotic or regular character of the Floquet states matters. For that purpose we employ Floquet-Markov theory in combination with both numerical and analytical methods (wave-function Monte-Carlo simulations, mean-field theory). Future plans also concern the design and properties of quantum thermal machines and the role of interactions.

Ultracold Atomic Quantum Gases Ultracold atomic quantum gases are realized by tapping and cooling neutral atoms. Their great appeal lies in the combination of quantum optical precision and controllability with many-body physics. These systems are extremely clean, highly tunable (also in a time-dependent fashion during the experiment) and well isolated from coupling to the environment. Optically created lattice potentials allow to realize paradigmatic Hubbard-type lattice models and to reach the interesting regime of strong coupling. Moreover, densities and few-particle correlation functions can be measured both *in situ* with single-site resolution and, after time of flight, with respect to momentum. This makes atomic quantum gases a unique platform for engineering quantum many-body physics.

We are interested in the properties of optical lattice systems under the influence of strong time-periodic forcing. Here one aim is to engineer the properties of the many-body Floquet states of these *dressed lattice systems*, in order to realize exotic quantum phases. In close collaboration with the experimenal group of Klaus Sengstock in Hamburg, we are working on the realization and characterization of lattice systems with frustrated kinetics and artificial gauge fields (both abelian and non-abelian). We are also investigating methods to access orbital degrees of freedom associated with excited Bloch bands in optical lattices. Current work is, moreover, concerned with kinetic frustration as it results from Pauli exclusion in non-bipartite lattice geometries, with the question whether inhomogeneity can be a useful tool for adiabatically growing ordered quantum phases, and with large-spin ($> 1/2$) spinor dynamics in fermionic quantum gases.

Cooperations

- We have fruitful collaborations within the mpi**pks**
  - Prof. Holger Kantz on stochastic perturbations of symplectic maps.
  - Dr. Eduardo Altmann on classical and quantum aspects of open dynamical systems.

- as well as externally with the experimental groups of
  - Prof. Hans-Jürgen Stöckmann (University of Marburg, FOR760) on microwave billiards showing resonance-assisted tunneling.
  - Prof. Markus Oberthaler (University of Heidelberg, FOR760) on regular and chaotic dynamics in Fock space using condensates.

  - Prof. Klaus Sengstock (University of Hamburg) on the realization of artificial gauge fields in optical lattice systems and on fermionic spinor dynamics.

- and with the theory groups of
  - Prof. Steven Tomsovic (Washington State University, USA) on quantum signatures of partial barriers.
  - Prof. Akira Shudo (Tokyo Metropolitan University, Japan) on complex paths for regular-to-chaotic tunneling.
  - Prof. Peter Schlagheck (University of Liège, Belgium) on semiclassics of resonance-assisted tunneling.
  - Prof. Maciej Lewenstein (ICFO-The Institute of Photonic Sciences, Spain) on frustrated lattice systems and the creation of artificial gauge fields.

1.11 Advanced Study Groups

Advanced Study Group 2011/2013: Statistical Physics of Collective Motion
(Convenor: Prof. Dr. Hugues Chaté)

Scientific context

The recent years have witnessed the explosive growth, within the statistical physics community, of works dealing with "active matter", loosely understood as the situations where energy is spent locally to produce some kind of directed (non-random) displacement. In this context, particular interest has been paid to the phenomenon of collective motion. The growing interest of physicists has been accompanied by the emergence of novel experimental/ observational data and findings in fields as diverse a animal behavior, (multi- and sub-)cellular biology, crowd management, ad-hoc networks, and distributed robotics. Here as elsewhere, modern technology allows for the collection of larger and larger datasets, and physicists are increasingly involved. There is a definite sense of a burgeoning cross-disciplinary community. As of now, this growth has also triggered some level of confusion between the various communities involved, which is quite natural since the viewpoints/interests of the people involved are sometimes very different. But confusion is also present within physics. For instance, but significantly, the nature of the ordered, collective motion phases in the most studied model, the Vicsek model, is still considered by some as an open problem. Many other microscopic "agent-based" models have been proposed and studied, leading to a wealth of papers with sometimes contradicting conclusions. Nevertheless, there is a growing recognition that some degree of universality exists, which needs to be clarified. Another line of research is that of continuous descriptions of collective motion phenomena, in terms of density and order parameter fields. As usual, it is expected that, at some coarse-grained level, such equations will make the above-mentioned universality explicit. We are currently witnessing some of this, but here again, the situation is complicated by competing results obtained following different paths.

Structure, calendar, summary of activities

The Advanced Study Group (ASG) on the "Statistical physics of collective motion" was created in the above context in order to bring together some of the major players on the theoretical side of this emerging subfield of physics with two major aims:

- bringing some order and reducing the misunderstandings among theoreticians
- defining/proposing, in close collaboration with experimentalists, novel experiments susceptible of unlocking key pending theoretical issues

The ASG was installed in September 2011 and will conclude its activities at the end of June 2013, having met during three two-month sessions. Its convenor is *Hugues Chaté* (CEA-Saclay, France) and its members are *Igor Aronson* (Argonne National Lab, USA), *Eric Bertin* (ENS-Lyon, france), *Cristián Huepe* (unaffiliated researcher, USA), *Sriram Ramaswamy* (TIFR Center for Interdisciplinary Research, Hyderabad, India), and *John Toner* (U. Oregon, USA).

During September 2011, the ASG activities were alongside the one-month program "Dynact11" co-organized by H. Chaté, K. Kruse, and M. Bär at the mpi**pks**. Under the full title "Collective Dynamics and

Pattern Formation in Active Matter Systems", this combination of conference, workshop, lectures and seminars marked the start of the ASG (see http://www.pks.mpg.de/~dynact11). The group members benefited then from the presence in Dresden of most of the prominent researchers in the field.

In June 2013, the ASG will organize a focus workshop on "Connecting theory and experiments in active matter" at the mpi**pks** (see http://www.mpipks-dresden.mpg.de/~cteam13). This short and deliberately small event will bring around the same table researchers performing in vitro experiments using purified biological components (filaments, motor proteins, etc.) and theoreticians working in the modeling/understanding of active matter including of course ASG members. The emphasis will be put on discussing which experiments could be done to test theoretical ideas, as well as the theoretical problems posed by already existing experimental results.

The ASG has also benefited from the visits of other scientists which typically resulted in new collaborations and/or the strengthening/extension of existing ones: B. Delamotte (UPMC, Paris), A.E. Turgut and E. Ferrante (IRIDIA, Brussels), C. Weber (LMU, Munich), F. Ginelli (U. Aberdeen, Scotland), Leiming Chen (Xuzhou, China), G. Theraulaz (CRCA, Toulouse), G. Grégoire (UPD, Paris), Xiaqing Shi (Suzhou, China), K. Nagai (U. Tokyo, Japan), Y. Sumino (Aichi, Japan), R. Montagne (UFRPE, Brazil), J. Tailleur (UPD, Paris).

Numerous interactions and some new collaborations also occurred with researchers in Dresden, both at the mpi**pks** and MPI-CBG.

Cooperations

Several collaborations between ASG members and/or ASG invitees and/or the mpi**pks** researchers have started at the occasion of the ASG activity periods. Several of them have already led to publications. Below is a list of some of the most notable results achieved so far.

- *Revisiting the Toner-Tu theory of flocking*: Following brainstorming sessions among ASG members together with Dynact11 participants J.-F. Joanny and M.C. Marchetti, Toner realized that the foundations of his seminal and very influential papers of 1995 and 1998 are not as firm as believed initially. This is now clearly explained in [1]. The consequences are that extra assumptions, not justifiable a priori, are needed for the theoretical results derived in 1995 to be valid. As a result, a posteriori confirmations from numerical/experimental data are crucial.
- *"Boltzmann-Ginzburg-Landau" approach to collective motion*: Aronson, Chaté, Bertin, and Ginelli developed a kinetic theory framework to derive hydrodynamic equations from simple, Vicsek-style, microscopic models. Combining classic kinetic theory with weakly nonlinear Ginzburg-Landau-like ideas allows to control all terms in a systematic expansion yielding well-behaved nonlinear field equations. Several cases are studied, some of which have already been published [1, 2].
- *Langevin equations for active nematics*: Ramaswamy, Bertin, Chaté, and Ginelli recently applied the "Boltzmann-Ginzburg-Landau" to the case of active nematics and used Ito calculus to complement these deterministic field equations with noise terms derived properly from the original microscopic model [4]. This in effect constitutes the first instance where Langevin equations/field theories are derived entirely from a microscopic model in active matter studies.
- *Active smectics* Ramaswamy, Toner and Chen made the first theoretical predictions about active matter systems which develop smectic order in addition to orientational order [5, 6]. In a second step, Chaté and Romanczuk (from the mpi**pks**) developed the first microscopic model giving rise to active smectic phases. Being a simple extension of the Vicsek model, this model is both simple and elegant, and its study already revealed the evidence for novel collective phenomena.
- *Elasticity-driven collective motion in active solids and active crystals*: Huepe, Ferrante, and Turgut showed that collective motion can arise in active solids and crystals just as the result of their elasticity properties [7]. Their model, derived from an earlier robotic system, was discussed at length during ASG meetings.
- *Origin of non-thermal noise in active mesoscopic systems*: Aronson and Weber, using motility assays as paradigmatic systems for the study of active matter, showed that coupling local active force exertion to local energy dissipation leads to a drastic increase in the likelihood of anomalous, extreme events in the curvature distributions of filaments driven by molecular motors.
- *In silico approach to vibrated polar disks*: Chaté and Weber, together with Dauchot and Frey, constructed an "*in silico*" version of the vibrated polar disks experiments performed by Deseigne, Dauchot, and Chaté. This detailed, quantitatively faithful model, allowed to explore systems sizes

and boundary conditions out of reach of the experimental system. Among the obtained results are the possibility of true long-range polar order in this system, and an intriguing phase diagram calling for further studies of the dense ordered phases of active matter systems. [8]

In addition to the above achievements, the ASG has been an excellent opportunity for respectively completing and constructing the following two review articles to appear in *Reviews of Modern Physics*:

- "Soft active matter", by M.C Marchetti *et al.*, to appear. [9]
- "Interacting self-propelled particles: minimal models and universality classes", by H. Chaté *et al.*, in preparation. [10]

Publications and unpublished documents

[1] J. Toner, Phys. Rev. E **86** (2012) 031918.
[2] A. Peshkov, *et al.*, Phys. Rev. Lett. **109** (2012) 098101.
[3] A. Peshkov, *et al.*, Phys. Rev. Lett. **109** (2012) 268701.
[4] F. Ginelli, *et al.*, submitted to N. J. Phys. (2013).
[5] T.C. Adhyapak, S.R. Ramaswamy, J. Toner, submitted to Phys. Rev. Lett. (2013).
[6] L. Chen, J. Toner, submitted to Phys. Rev. Lett. (2013).
[7] E. Ferrante, A.E. Turgut, M. Dorigo, C. Huepe, submitted to Phys. Rev. Lett. (2013).
[8] C.A. Weber, *et al.*, submitted to Phys. Rev. Lett. (2013).
[9] M.C. Marchetti, *et al.*, to appear in Rev. Mod. Phys. (2013).
[10] H. Chaté, *et al.*, to be submitted to Rev. Mod. Phys. (2014).

Advanced Study Group 2011: Towards a Semiclassical Theory of Dynamical Tunneling
(Convenor: Prof. Dr. Steven Tomsovic)

Long term members: Arnd Bäcker (TU Dresden & mpi**pks**), Srihari Keshavamurthy a (IIT Kanpur, India), Roland Ketzmerick (TU Dresden & mpi**pks**), Peter Schlagheck (UL, Liege, Belgium), Akira Shudo (TMU Tokyo); plus 19 more focus event participants and a number of Ph.D. students.

The Advanced Study Group (ASG) *Towards a Semiclassical Theory of Dynamical Tunneling* took place over four and a half months beginning April, 2011. The main goals and activities were applied to two central topics:

1. *Combination and unification of different semiclassical approaches to tunneling* To a very rough extent, the existing semiclassical approaches to describe quantum tunneling processes can be classified into WKB-type methods, employed to describe direct and resonance-assisted tunneling, which are essentially based on the complexification of classical invariant manifolds, and path-integral-type methods which are based on the representation of the quantum propagator in terms of complex classical trajectories. Both types of methods have their strong points and limitations, and a central task of the ASG was to establish a common unifying framework for both of them. This task has been achieved to a limited extent. Indeed, a genuinely semiclassical theory of direct tunneling could be obtained through the inclusion of complex trajectories (Mertig *et al.*, Ref. [1]) The role of nonlinear resonances in complex trajectory-based semiclassical approaches, on the other hand, still represents an open issue under debate (Shudo and Ikeda, Ref. [2]).

2. *Exploration of dynamical tunneling in systems with more than two degrees of freedom* Tunneling processes in molecular systems, to mention a relevant example, most generally involve more than two degrees of freedom, and a semiclassical determination of the corresponding time scales characterizing tunneling-induced decay or transfer processes is therefore concerned with a high-dimensional phase space. A central aim of the ASG was therefore to extend the existing semiclassical descriptions of tunneling to systems with more than two degrees of freedom. As far as resonance-assisted tunneling is concerned, the theoretical foundations of this task were laid by an internal working note written by P. Schlagheck (Ref. [7]) and distributed among the members of the ASG. Two main questions are identified in this context:

   (a) How does direct and resonance-assisted tunneling proceed in systems with more than two degrees of freedom, and how can the associated coupling rates be evaluated in practice?

(b) How does the possibility of classical diffusion within the Arnol'd web manifest in the eigenstates or transport observables of the quantum system?

These questions are at present addressed in a joint effort focusing on the nearintegrable (S. Keshavamurthy/J. Madronero/P. Schlagheck/S. Tomsovic) and mixed regular-chaotic regime (A. Bäcker/R. Ketzmerick/P. Schlagheck).

In order update each other on the progress that we have made on these two main topics since the end of the ASG, we organized an informal one-week post ASG meeting at the **mpipks** from 15th to 19th October 2012. The invited key participants of this meeting were Srihari Keshavamurthy (Kanpur), Akira Shudo (Tokyo), Amaury Mouchet (Tours), and Javier Madronero (Duisburg), in addition to Peter Schlagheck (Liège), Arnd Bäcker and Roland Ketzmerick (Dresden) who were the main co-organizers.

Seminars

We organized weekly Thursday seminars every week except for during the focus event. They were intended to be very informal, with introductory material presented, and questions asked by the listeners. This was very successful and rarely did a talk last less than 2 hours due to all the extensive questions being asked. The talks are listed below. In addition, every Friday we held a meeting to discuss open physics research questions of interest to the ASG, except one or two Fridays dedicated to administrative organization of the focus event. Usually, one person was responsible for initiating a discussion in which they had some particular interest. These discussions also mostly lasted a couple of hours.

Thursday talks:

Jérémy Le Deunff: Resonant tunneling and normal forms
Akira Shudo: *Dynamical tunneling in the anti-integrable limit*
Akira Shudo: *Dynamical tunneling in the anti-integrable limit II*
Steven Tomsovic: *What is being measured in the scanning gate microscopy of a quantum point contact?*
Stephen Creagh: *Looking for tunnelling in boundary integral methods*
Steven Tomsovic: *Extreme value statistics for random waves*
Alfredo Miguel Ozorio de Almeida: *Initial value representations for the Loschmidt echo*
Peter Schlagheck and Martin Richter: *Secular perturbation theory in systems with two and three degrees of freedom*
Srihari Keshavamurthy: *Classical and Quantum transport on the Arnold Web: an introduction*
Clemens Löbner: *Integrable Approximation for Regular Islands in Billiards*
Arseni Goussev: *A Huygens-Fresnel-type approximation for quantum propagators: Wave packet diffraction and interference*
Andreas Buchleitner: *Nonlinear resonances - from atoms to ultracold atoms*
Srihari Keshavamurthy: *Transport on the Arnold web: Chirikov's calculation*
Javier Madronero: *Complexity in the 3-body Coulomb problem: fluctuations in the spectrum of highly doubly excited states*
Italo Guarneri: *Projection approach to resonance assisted tunneling*
Normann Mertig: *Power-law level statistics due to dynamical tunneling*
Steven Tomsovic: *Random matrix theory for long-range ocean acoustics*

Focus event:

We held a four day focus event organized to facilitate discussions with a larger group of people. There were 25 participants, but only twelve seminars during the event, three per morning. Each afternoon, discussion sessions were organized to explore further the morning talks in greater detail. There were half a dozen posters up the entire event.

Stephen Creagh: *Resonant tunneling from cavities*
Shmuel Fishman: *Quantum chaos of a mixed, open system of kicked cold atoms*
Kensuke Ikeda: *Complex semiclassical description of chaotic tunneling in quasi-stationary regime*
Srihari Keshavamurthy: *Dynamical Tunneling in three degrees of freedom and beyond: The final frontier?*
Steffen Lück: *Regular-to-chaotic tunneling rates using the fictitious integrable system approach*
Amaury Mouchet: *The role of resonances in tunneling*
Evgenii Narimanov: *Quantum Chaos in Hyperbolic Metamaterials*

Louis Pecora: *Changes in Distributions of Tunneling Rates Through a Barrier between Regular and Chaotic Symmetric Well Systems*
Susumu Shinohara: *Chaos-assisted emission from microcavity lasers*
Peter Schlagheck: *Resonance-assisted tunneling in mixed regular-chaotic systems*
Akira Shudo: *What does theory of complex dynamics tell us?*
Kin'ya Takahashi: *Stable-unstable manifold guided tunneling for continuous time systems*

Publications and unpublished documents

[1] N. Mertig, S. Lück, A. Bäcker, R. Ketzmerick, and A. Shudo *Complex paths for regular-to-chaotic tunneling rates*, arXiv:1207.0985 (2012).

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Chapter 2

Selection of Research Results

2.1 Fractional Chern Insulator Hierarchy

EMIL J. BERGHOLTZ, ANDREAS M. LÄUCHLI, RODERICH MOESSNER

Introduction The discovery of fractional quantum Hall (FQH) states kick-started the field of topological condensed matter physics. Fractional Chern insulators (FCIs) are their lattice analogs which have recently been predicted to appear due to interactions within nearly dispersionless bands with non-zero Chern number, C [1–3]. Contrary to their continuum analogs, these intriguing states do not require an external magnetic field and might in principle be realized at room temperature, making them very promising for futuristic applications such as topological quantum computation [4].

Given the initial numerical discovery of a FCI state at filling $\nu = 1/3$ in a flat $C = 1$ Chern band [3, 5, 6], a number of questions immediately arise. Firstly, which FCIs can actually be realized and under what conditions? Secondly, are there lattice specific states which compete with the FCI states? Thirdly, what are the key differences between FCI physics in Chern bands compared to the familiar setting of Landau levels in the continuum appropriate for describing FQH states in conventional semiconductor heterojunctions?

In our recent work [7] we contribute to all of these questions. In particular we provide a heuristic prediction of which filling fractions we can expect to find stable FCIs as well as their their relative stability by relating the lattice interactions to Haldane's pseudopotentials in the continuum [8]. By use of large-scale exact diagonalization studies we are able to confirm that these predictions can indeed account for the chief part of the phase diagram as a function of the electronic filling fraction in topological flat (Chern) bands: we find compelling evidence of a large number of FCI states akin to the emergent hierarchy of incompressible liquid states familiar from conventional QH physics. At high filling fractions, however, we observe clear deviations from this simple picture, which we are able to account for by a new interaction-driven instability towards compressible states that is absent in continuum systems, and which is responsible for the absence of some FCIs in the lattice case.

Setup To illustrate our generic findings regarding interactions in flat Chern bands we use the two-band checkerboard model introduced in [2, 3] as our workhorse (Fig. 1(a)). Here $t_1 e^{\pm i\phi}$ is a nearest-neighbor hopping with an orientation dependent complex phase, and t_2 denotes the next-nearest-neighbor hopping amplitude. After Fourier transformation, the single-electron (kinetic) Hamiltonian reads

$$H_0 = \sum_{\mathbf{k}\in \mathrm{BZ}} (c^\dagger_{\mathbf{k}A}, c^\dagger_{\mathbf{k}B}) h(\mathbf{k}) (c_{\mathbf{k}A}, c_{\mathbf{k}B})^T, \qquad (1)$$

where $h(\mathbf{k})$ is $h(\mathbf{k}) = \sum_i d_i(\mathbf{k})\sigma_i$, with $d_x(\mathbf{k}) = 4t_1 \cos(\phi)\cos(k_x/2)\cos(k_y/2)$, $d_y(\mathbf{k}) = 4t_1 \sin(\phi)\sin(k_x/2)\sin(k_y/2)$, and $d_z(\mathbf{k}) = 2t_2[\cos(k_x) - \cos(k_y)]$, and σ_i are the Pauli matrices. For $t_2 \neq 0, \infty$ one obtains two separated bands characterized by Chern number $C = \pm 1$ which means that the bands support one chiral edge state each (in opposite directions).

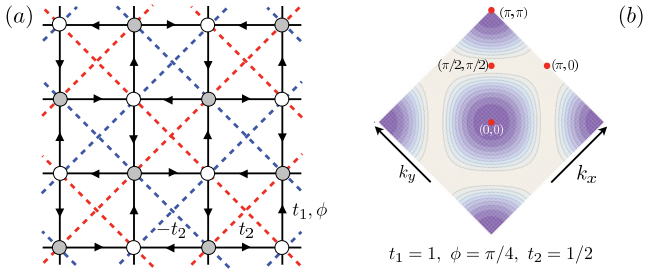

Figure 1: (a) Illustration of the checkerboard lattice model with the relevant hopping amplitudes. (b) Berry curvature in the first Brillouin zone for the indicated set of parameters. Dark (light) coloring denotes small (large) Berry curvature.

While the topologically quantized Chern number, $C = \frac{1}{2\pi}\int_{BZ} F_{12}(\mathbf{k}) d^2k$, can in general only assume integer values, its microscopic source given by the the Berry curvature, $F_{12}(\mathbf{k})$, necessarily varies in the Brillouin zone and depends on the microscopic parameters (Fig. 1(b)). The varying Berry curvature is indeed a striking and generic effect of the underlying lattice which is absent in the continuum setting.

In the following we consider nearest neighbor repulsion, $H_{\mathrm{int}} = V \sum_{\langle i,j\rangle} n_i n_j$, projected into the partially filled band, leading to a projected Hamiltonian of the form

$$H = \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} V_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} c^\dagger_{\mathbf{k}_1} c^\dagger_{\mathbf{k}_2} c_{\mathbf{k}_3} c_{\mathbf{k}_4}, \qquad (2)$$

where the residual dispersion is ignored as we wish to highlight the new phenomena arising e.g. due to the non-constant Berry curvature, as opposed to remnant energy dispersion. These approximations make sense in the limit where the energy gap between the bands is large compared to the interaction strength, which in turn is much larger than the band dispersion.

Pseudopotential analogy and hierarchy states To establish a connection to Haldane's pseudopotentials defined in the continuum [8] with the lattice setting, we consider the problem of two particles interacting within the flat Chern band: In Fig. 2(a) we display the non-zero eigenvalues along a path in the Brillouin zone. The spectrum depends on the total momentum,

$\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2$, underscoring the lack of translation invariance. We observe two dominant eigenvalues of mean value $\approx 0.4V$ while there is also second pair of eigenvalues about 10 times smaller. Careful counting of these energy levels and comparing with the continuum spectra reveals a pseudopotential analogy in which we label the two non-zero pairs of eigenvalues of the projected two-particle Chern band problem as $\mathcal{V}_1$ (the larger pair) and $\mathcal{V}_3$ (the smaller pair) as indicated in Fig. 2(a).

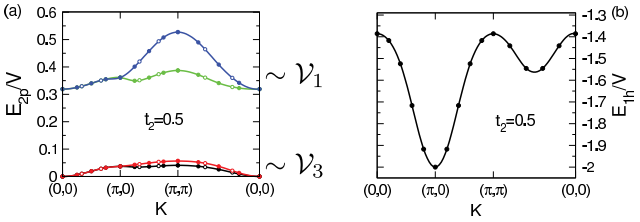

Figure 2: (a) Non-zero energy eigenvalues of the two-particle problem. (b) Energy of a single hole in the lower band along a cut through. the Brillouin zone.

Summarizing the evidence given in [7], we find hierarchy multiplets of incompressible states at fillings $\nu = 1/3, 2/5, 3/7, 4/9, 5/9, 4/7, 3/5$ which are associated with the relatively large energy scale $\mathcal{V}_1$ as well as weaker states at $\nu = 1/5, 2/7$ going along with the smaller energy scale $\mathcal{V}_3$.

Competing compressible states The lack of particle hole-symmetry in the above list of observed FCIs naturally leads us to the qualitative distinctions from conventional QH physics.

Performing a particle-hole transformation, $c_{\mathbf{k}} \rightarrow c^\dagger_{\mathbf{k}}$ within one of the bands, the projected Hamiltonian transforms to

$$H \rightarrow H^* + \sum_{\mathbf{k}} E_h(\mathbf{k}) c^\dagger_{\mathbf{k}} c_{\mathbf{k}}, \qquad (3)$$

which crucially includes an effective single-hole energy $E_h(\mathbf{k})$. This term amounts to a trivial overall energy shift in a Landau level. By contrast, it introduces an effective hole dispersion, even for an entirely flat Chern band, due to the lack of translation invariance in reciprocal space. We display an example of $E_h(\mathbf{k})$ in Fig. 2(b). Indeed this particle-hole asymmetry generally leads to a deformation of $n(\mathbf{k})$ and in fact dominates the physics near $\nu = 1$ where no FCIs are realized, as highlighted in Fig. 3.

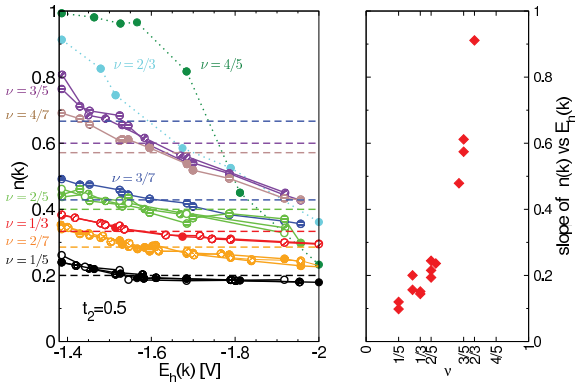

Figure 3: Left: Momentum space orbital occupation $n(\mathbf{k}) = \langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \rangle$ plotted as a function of the single-hole energy $E_h(\mathbf{k})$. Solid lines correspond to FCI phases while dashed lines denote fractions which are most likely not FCI states, as indicated by the Fermi surface-like feature in $n(\mathbf{k})$. Right: A measure of the slope of $n(E_h(\mathbf{k}))$, the divergence of which signals the boundary of FCI states.

Summary and outlook We have established a powerful analogy between strongly correlated lattice states, the FCIs, and the continuum FQH by introducing a characterization of the band projected lattice interaction similar to Haldane's pseudopotantial description. We have furthermore numerically established a number of new FCI states in accordance with this classification and provided insights into the nature of the generic lattice effects that lead to the breakdown of the lattice-continuum analogy in the form of an interaction driven instability towards compressible states.

Our results also suggests that, given a specific topological flat band model, the easily tractable two-body and single-hole problems already provide an efficient diagnostic of the phase diagram of the model.

A similar approach might also shed light on the phase diagram of the less understood flat band models with $C > 1$, which have recently been shown to host new intriguing correlated phases [9].

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2.2 Order by disorder in the classical kagome Heisenberg antiferromagnet

GIA-WEI CHERN AND R. MOESSNER

The first experiments on the 'kagome bilayer' material SCGO [1, 2] triggered a wave of interest in kagome antiferromagnets in particular, and frustrated systems in general which persists to this day. A cluster of early seminal theoretical papers [3–7] established kagome magnets as model systems for novel ordering phenomena discussing, in particular, spin liquidity, partial order, disorder-free glassiness and order by disorder. The kagome magnet is unusual as it exhibits, at low temperature (T), coplanar (nematic) ordering driven exclusively by thermal fluctuations.

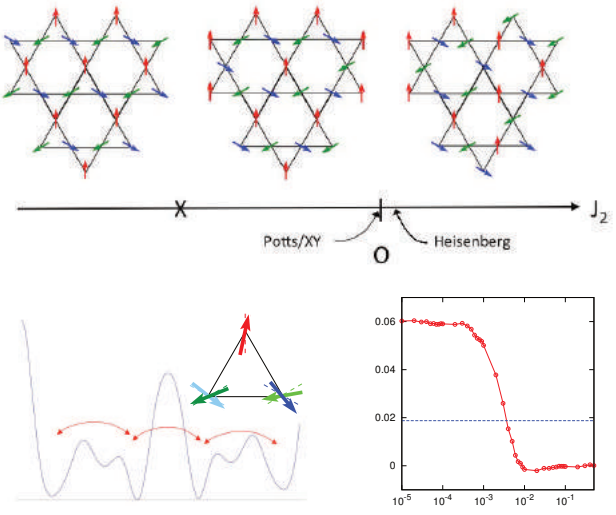

Figure 1: Top: candidate phases of the kagome antiferromagnet (from left to right: $q = 0$; Kosterlitz-Thouless phase; $q = \sqrt{3} \times \sqrt{3}$) in the phase diagram of an extended Potts model. $J_2 = 0$ corresponds to the pure Potts model on the kagome lattice, the unweighted ensemble of coplanar Heisenberg ground states. Bottom left: cartoon of the effective entropy landscape for ground states–soft fluctuations yield minima at co-planar states. Our algorithm surmounts the entropic free energy barriers. The resulting ensemble average encodes a small but nonzero spin order. Inset: transitions between harmonically equivalent configurations–spins on loops of alternating color are rotated such that the angle a spin makes with its local Potts axis is not changed, as the dark green/blue spins are exchanged for the light ones. Bottom right: temperature-dependence of spin correlations half way across a finite-size system. For $T < 10^{-3}$, correlations are approximately T-idependent.

Remarkably, for the *classical* kagome Heisenberg magnet, the nature of low-temperature phase has not been established, despite the deceptive simplicity of its Hamiltonian, encoding only antiferromagnetic nearest-neighbour interactions between classical unit-length spins $\mathbf{S}_i$: $H = \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$. The reason is that classical Monte Carlo has not been able to sample the different local free energy minima separated by entropic barriers [8]. In particular, the question whether there is, or is not, (dipolar) ordering of the spins in addition to nematic ordering has tantalisingly remained open for two decades.

We have developed a Monte Carlo algorithm which equilibrates down to hitherto unreachable a low-temperatures $T \ll 10^{-3}$, below which correlations no longer change. The algorithm implements a mapping of configurations into each other which are equivalent as far as the linearised equations of motion are concerned [9] – whether or not to accept a move thus depends only on the *anharmonic* terms responsible for the low-temperature state selection. As we explain below, we use the results to determine the best parameters in effective low-energy models, for our problem, including a stiffness in a height model, an effective field theory; as well as a further-neighbour coupling in an extended Potts model. In particular the latter can then be simulated for $> 10^6$ spins, which enables us to verify the critical behavior encapsulated by the height model. This allows us to conclude that – modulo Mermin-Wagner physics – the system exhibits spin ordering with a – for a classically magnet – remarkably small ordered moment, which we estimate to be about an order of magnitude below the saturated moment.

As the ground state is continuously degenerate, the energy landscape has many zero-energy directions (flat valleys). However, at non-zero temperature, in the free energy landscape – which incorporates entropic effects – the flat valleys are replaced by robust local minima at each coplanar state. The coplanar states are discrete. These can be mapped onto the ground states of the antiferromagnetic Potts model on the kagome lattice (which is, in turn, equivalent to the three-colouring model of the honeycomb lattice): each spin points in one of three directions at mutual angles of 120° with one another. Labelling these with the colours red, green and blue, the coplanar states are those where each triangle hosts a spin of each colour (Fig. 1). Below, we use the fact that these discrete models are exactly soluble [11], e.g. it is known that there are exponentially many coplanar states, $N_c \sim 1.13^N$, where N is the total number of spins.

Correlations at low temperature Our first central result is the discovery of a limiting low-temperature regime where the correlations cease to change as T is lowered further below $T \sim 10^{-3}$ (Fig. 1). This implies that the effective weights differentiating between different coplanar states become temperature independent, which can perturbatively be understood as follows. The fluctuations selecting an ordered state are subdominant compared to those which select the

nematic order: the modes which cost no energy are dressed by the finite-energy ones when anharmonic effects are taken into account. Perturbatively, cubic (quartic) terms appear to second (first) order. The corresponding contributions turn out to be suppressed by a factor of T compared to the leading ones [10]. Temperature therefore drops out of the resulting effective weights for $T \to 0$. Our numerics establishes that this holds for the full problem, and not just to leading order in a (potentially divergent) perturbation theory.

Enhanced correlations at low T: In Fig. 2, we present the correlators necessary for the demonstration of order in the low temperature regime. We focus on the order parameter corresponding to a tripling of the unit cell, $m_{\sqrt{3}}$, as in the right state depicted in the phase diagram, Fig. 1. For comparison we show the correlations of the (unweighted) average over the coplanar Potts states, which do not take into account anharmonic fluctuations. $m_{\sqrt{3}}$ deviates *upwards* from the decay of the Potts correlations, while the decay of m_0, corresponding to the left state in Fig. 1, is even faster than at higher temperatures (not shown). Next, we analyse this data in detail with the aid of effective field theories and an effective Hamiltonian.

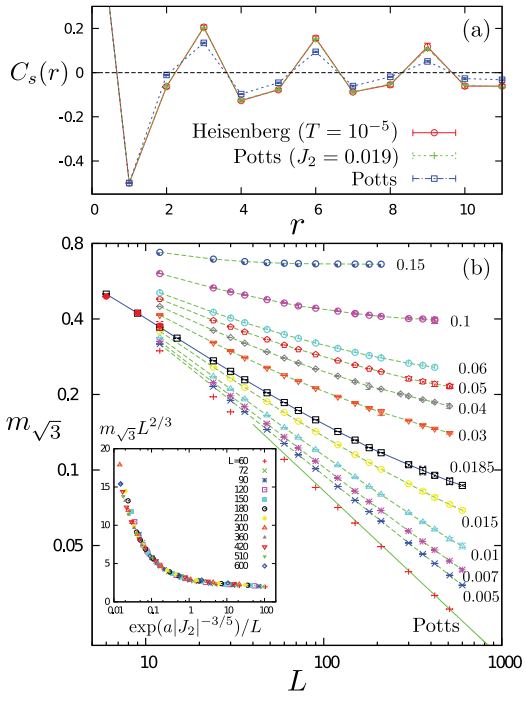

Figure 2: (a) Spin correlations of the Heisenberg model at $T = 10^{-5}$ and the extended Potts model with $J_2 = 0.019$ on a lattice with 396 spins. (b) Order parameter $m_{\sqrt{3}}$ for the extended Potts model as function of linear system size L for different values of J_2. The solid red points for small systems are from the Heisenberg simulations. Inset: scaling collapse of data for $L \geq 60$.

Based on Baxter's observation that the average over coplanar states without entropic weighting, is *at a critical point* in the limit of $T \to 0$ [11], to settle the question whether the kagome magnet is in turn ordered, one needs to establish whether the appropriate tuning parameter – the stiffness of a so-called height field [12] – increases rather than decreasing or remaining the same: for decreasing stiffness, the system would move away from the critical point into the KT phase whereas, for an increase, ordering ensues. Fig. 3 shows that the ratio of stiffnesses, $\lim_{q\to 0} \Theta(q^2) > 1$, which implies that the magnet is driven into an ordered phase. To confirm this full scenario, we have extracted a parameter for an extended Potts model including further-neighbour interactions to account for the entropic weights (Fig. 2, top). This model can be simulated for $> 10^6$ sites!

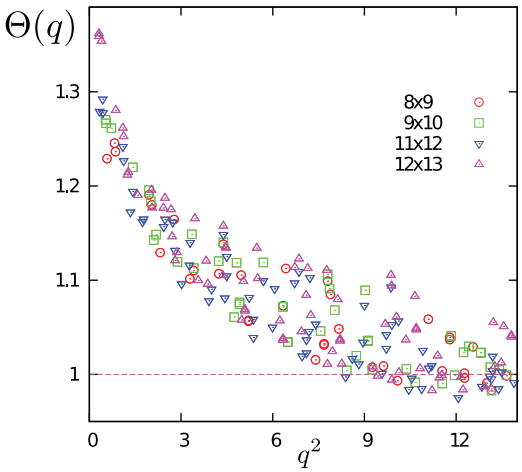

Figure 3: A ratio $\Theta(q) > 1$ for $q^2 \to 0$ reflects the increased stiffness of the Heisenberg model compared to the Potts model, and the resultant ordering at low temperature.

The effective Potts model does indeed exhibit a KT phase transition exactly as predicted by the effective field theory, evidenced by a scaling form, $\mathcal{F}$ of the order parameter (Fig. 2 inset)

$$m_{\sqrt{3}} L^{2/3} = \mathcal{F}\big(\xi(J_2)/L\big),$$

with $\xi = \exp(a|J_2|^{-3/5})$ is the correlation length and $a \approx 0.385$ is the only fitting parameter. In the thermodynamic limit, $m_{\sqrt{3}} \sim \mathcal{A}\,\xi^{-2/3}$. Estimating the constant $\mathcal{A}$ from large $|J_2|$, where $m_{\sqrt{3}}$ can be directly read off, a small but non-zero ordered moment about an order of magnitude below the full moment is obtained.

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2.3 Superconductivity and the pseudogap in the two-dimensional Hubbard model

EMANUEL GULL[1,2] AND ANDREW J. MILLIS[3]

Lamellar perovskite-based copper oxide compounds display three remarkable properties: d-wave superconductivity, with unprecedentedly high transition temperatures, a nontrivial ("Mott") insulating state and a "pseudogap" regime of suppressed density of states. P. W. Anderson [1] argued that these have a common origin as strong-correlation phenomena that could be understood in terms of the two-dimensional Hubbard model, but the interplay between the pseudogap and the superconductivity has remained controversial, with some authors suggesting the pseudogap is a signature of unusual superconducting fluctuations and others suggesting it is a competing phase or regime.

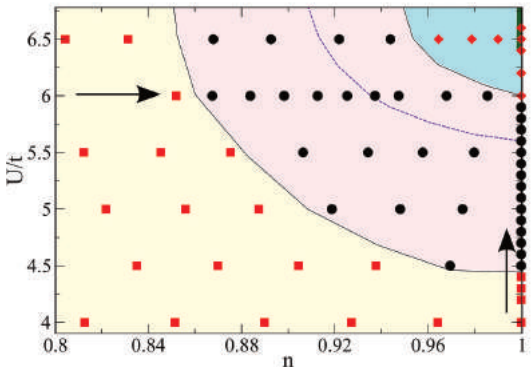

Figure 1: Phase diagram of two dimensional square lattice Hubbard model in plane of density n and interaction strength U at inverse temperature $\beta = 60$ as obtained in 8-site cluster dynamical mean field theory. Mott insulator at half filling for $U/t > 6.4$ indicated by heavy green bar; superconducting region indicated by black circles, pseudogapped but non-superconducting region with red diamonds and Fermi liquid non-superconducting state by red squares. Boundary of normal state pseudogap is indicated as a purple dashed line.

We used new numerical techniques [2] to solve the Hubbard model in the dynamical cluster approximation, which becomes exact as cluster size tends to infinity. Our methods enable the study of interactions strong enough and temperatures low enough so that the properties of the superconducting state and its relation to the Mott insulator and the pseudogap can be determined for clusters large enough to be representative of the thermodynamic limit and show that in the Hubbard model the two phenomena, while both linked to proximity to the Mott insulating state, are competing phenomena [3, 4].

Superconductivity is found to occur in a dome separated from the Mott insulating state by the pseudogap. The emergence of superconductivity from the pseudogap regime leads to a decrease in the gap (i.e. the creation of new states within the pseudogap), in agreement with recent angle-resolved photoemission data.

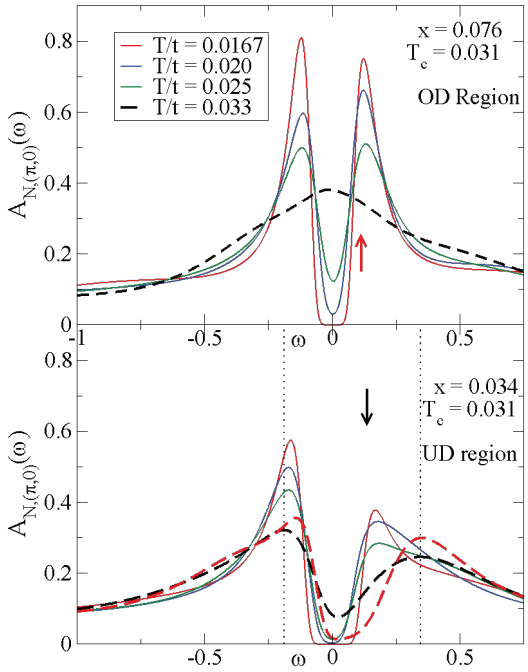

Figure 2: Analytically continued spectral function computed at $U = 6$ for antinodal sector showing temperature evolution of gap structure for a typical optimally doped/overdoped state ($x = 0.076$, upper panel) and underdoped pseudogap state ($x = 0.034$, lower panel). Solid lines: superconducting spectral function. Heavy dashed lines: normal state spectral function, obtained for $T = t/30$. Light dashed line (lower panel): normal state density of states at $T = t/60$ obtained by suppressing superconductivity. Arrows mark spectral function maxima used to determine superconducting gap size Delta. Dotted lines: pseudogap energy at $T = t/30$ obtained from maximum in spectral function.

Fig. 1 presents the phase diagram determined from a comprehensive survey of parameter space for $N_c = 8$, which previous work shows adequately represents the normal state physics of the model [5]. Studies of selected U and doping values in the computationally much more expensive $N_c = 16$ site cluster confirm that the physics found for $N_c = 8$ is generic. The phase diagram in the absence of superconductivity has been determined previously. One key feature is the presence of a fully gapped ("Mott") insulating phase for density

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$n = 1$ and $U > U_c \approx 6t$ indicated by the vertical heavy green line.

The Mott phase is separated from the normal Fermi-liquid phase by a pseudogap regime characterized by a suppression of density of states near the $(0, \pi), (\pi, 0)$ regions of the Brillouin zone, with states near the zone diagonal remaining unaffected. The onset of the normal state pseudogap is indicated by the dashed purple line in Fig. 1.

Fig. 2 presents the frequency and temperature dependence of the density of states. The upper panel shows spectra representative of dopings higher than, or interactions weaker than, the values which maximize T_c, so that superconductivity emerges from a relatively conventional normal state. The spectra are consistent with expectations from standard theory [6]: the onset of superconductivity is associated with a suppression of density of states at low frequency and with the formation of density of states ("coherence") peaks at slightly higher energies. The behavior of the superconducting gap (defined as half of the peak to peak distance) is conventional in the sense that the area in the coherence peaks comes mainly from the states removed at $|\omega| < \Delta$. The gap amplitude develops very rapidly with temperature: only at the temperature closest to T_c is the peak to peak splitting appreciably different from its value at the lowest T.

The situation is quite different when superconductivity emerges from the pseudogap regime. Representative spectra are shown in the lower panel of Fig. 2. The normal state pseudogap is visible at $T > T_c$ as a suppression of the density of states at low frequencies with a broad gap structure at higher frequencies. The normal state pseudogap maxima are marked by dashed lines. The development of superconductivity is characterized by the formation of coherence peaks at energies below the pseudogap, i.e. by a decrease in gap magnitude as the superconducting state is entered. Furthermore, most (typically more than 50%) of the spectral weight in the coherence peak is drawn from frequencies greater than than the superconducting gap energies. This behavior is consistent with recent experimental reports [7] that in underdoped cuprates the emergence of superconductivity out of the pseudogap regime is associated with the formation of new states at energies lower than the pseudogap energy and that the superconducting gap is tied to the pseudogap.

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2.4 Entanglement Spectrum of the two-dimensional Bose Hubbard Model

VINCENZO ALBA, MASUDUL HAQUE, ANDREAS M. LÄUCHLI

Introduction In recent years the cross fertilization between quantum information and condensed matter has led to new insights into the physics of quantum many body systems [1]. In particular the concept of *entanglement spectrum* [2] has established itself as an informative and intriguing theme. Considering a bipartion of a system into parts A and B, the entanglement spectrum (ES), $\{\xi_i\}$, is defined in terms of the Schmidt decomposition

$$|\psi\rangle = \sum_i e^{-\xi_i/2} |\psi_i^A\rangle \otimes |\psi_i^B\rangle. \quad (1)$$

Here $|\psi\rangle$ is the ground state, and the states $|\psi_i^A\rangle$ ($|\psi_i^B\rangle$) form an orthonormal basis for subsystem A (B). The ES $\{\xi_i = -\log\lambda_i\}$ can also be thought of as the spectrum of the so called entanglement hamiltonian $\mathcal{H}_E \equiv -\log\rho_A$ where the reduced density matrix ρ_A is obtained after tracing out the B part of the system density matrix $|\psi\rangle\langle\psi|$.

Many results are now available for the ES and entanglement entropies of one-dimensional (1D) systems. In contrast, higher dimensions are far less explored. Much of the ES literature on 2D systems focuses on topological phases. A detailed understanding of generic ES features for more common 2D systems is not currently available.

The Bose-Hubbard model We consider the two dimensional Bose-Hubbard model on a cylinder of length L (with open boundary conditions) and circumference W (with periodic boundary conditions). The Hamiltonian is $\mathcal{H} = -\sum_{\langle ij\rangle}(b_i^\dagger b_j + h.c.) + \frac{U}{2}\sum_i n_i(n_i-1)$ where b_i are bosonic operators, $n_i = b_i^\dagger b_i$, and U is the on-site repulsion. We restrict to the case of unit filling. To calculate the ES we divide the cylinder in two parts A and B of size V_A and V_B respectively, with W the boundary length (Fig. 1 top right). The number of bosons $N_A(N_B)$ in $A(B)$ is a good quantum number for the ES and can be used to label the ES levels. We introduce $\delta N_A \equiv N_A - V_A$ measuring the excess of bosons in A compared to unit filling.

The ES in the Mott insulator In the $U\to\infty$ limit, the ground state is a product state with one boson per site. The ES has only one level, $\xi_0 = 0$. As in Ref. [3], the ES at large U can be constructed through boundary-linked perturbation theory, treating the hopping term $\mathcal{H}_p \equiv -\sum_{\langle ij\rangle}(b_i^\dagger b_j + h.c.)$ as perturbation.

Fig. 1 (left) plots the ES $\{\xi\}$ for a system at $U = 100$. We denote with α the perturbative order giving the leading contribution to the ES levels. As in gapped 1D systems [3], the separation ($\sim \log U$) between consecutive α reflects the perturbative nature of the ES. In the center bottom we show the configurations giving dominant contribution to selected groups of ES levels. At each δN_A and $\alpha > 0$ there is more than one level. The multiplicities are determined by the boundary length W, and can be understood in terms of hopping processes across the boundary. On the ES envelope (dotted line in Fig. 1 left), the group of levels at δN_A is obtained by transferring δN_A bosons from subsystem B to A. This process appears at order δN_A (with amplitude $U^{-\delta N_A}$). The multiplicity $m(\delta N_A)$ is obtained as the number of ways of moving δN_A bosons across the boundary to give distinct configurations, i.e. $m(\delta N_A) = C(W, \delta N_A)$ with C the binomial coefficient (see (**a**)(**b**) in Fig. 1 right).

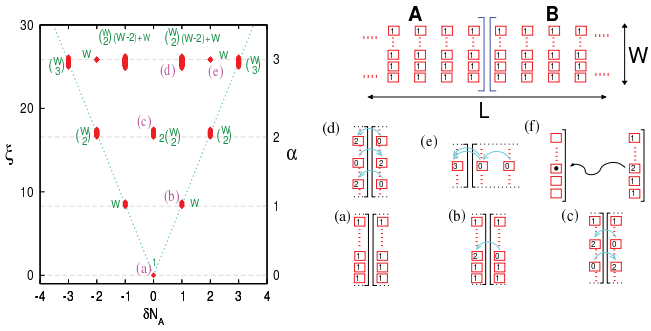

Figure 1: ES in the Mott phase. **Left**: perturbative structure, DMRG data for equally bipartitioned cylinder, $W = 8, L = 32, U = 100$. **Right**: bosonic configurations corresponding to leading order configurations for some $\delta N_A \geq 0$ levels. Only occupancies on sites nearer the boundary are shown (omitted sites are singly occupied).

Similar boundary perturbative processes help explain ES levels above the envelope; c.f., (**c**)(**d**)(**e**) in Fig. 1 left and center. At $\alpha < 3$ the leading order of all ES levels (not only the envelope) is given by pure boundary processes. At higher orders ($\alpha \geq 3$) processes further away from the boundary start contributing to the leading order of some ES levels, e.g., (**e**) in Fig. 1. The corresponding configurations involve hoppings perpendicular to the boundary, and thus are similar to the physics of ES configurations in 1D chains [3]. This is reflected in the linear multiplicity ($\sim W$) in (**e**). Generically, the multiplicities grow exponentially with α ($\sim W^\alpha$). This growth of multiplicity is related to the area law of entanglement entropy which limits the performance of DMRG in 2D systems even in gapped phases.

The ES in the superfluid phase In the superfluid phase ($U \lesssim 16.739$) the ES looks dramatically different (Fig. 2). There is a clearer separation between a low-lying "envelope" and the rest of the ES, but the envelope now has quadratic dependence on δN_A, and there is only a single envelope level at each δN_A. These

features are due to the fact that the underlying superfluid state has spontaneous breaking of $U(1)$ symmetry in the thermodynamic limit. We can explain some of these features through a correspondence with the tower of states spectrum [4], which is the physical low-energy spectrum obtained when a system with spontaneously broken continuous symmetry is placed in a finite volume. Since the finite-size ES is plotted against quantum numbers whose conservation is spontaneously broken only in the thermodynamic limit, it is naturally related to the TOS spectrum. For the lower part of the ES, $\mathcal{H}_E \sim \mathcal{H}_T/T_E$, where $\mathcal{H}_T$ is the TOS Hamiltonian, T_E is an effective temperature given by $T_E = v_s/\mathcal{L}$ with v_s the velocity of the gapless excitations (for the Bose Hubbard this is the sound velocity), and $\mathcal{L} \approx W$ is the linear size of the system [5]. The form of T_E reflects the finite size behavior of the sound-wave gap. For the Bose-Hubbard the TOS Hamiltonian is $\mathcal{H}_T \sim (\delta\hat{N})^2/(\chi V)$ where $\hat{N}$ is the total particle number operator and $\chi \equiv dn/d\mu$ is the compressiblity. This suggests that $\mathcal{H}_E \sim \frac{W}{v_s \chi V_A}(\delta N_A)^2 \sim (\delta N_A)^2/(v_s \chi W)$.

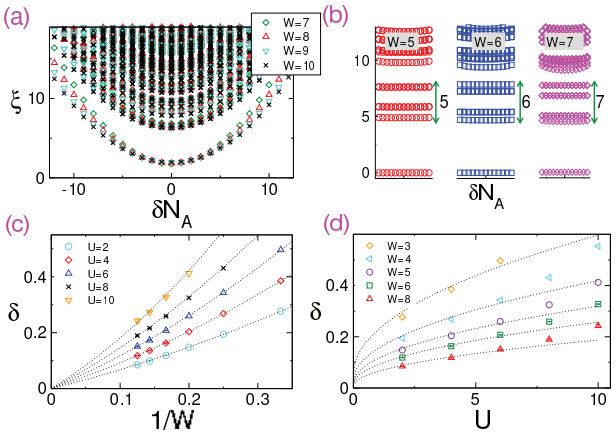

Figure 2: (**a**) ES in the superfluid phase (DMRG data at $U = 2$ for size $L/4 = W$). (**b**) The same ES as in (**a**) but after subtracting the contribution of the envelope. (**c**) Spacing δ (defined in text and Fig. 3) plotted versus $1/W$; various U. Dotted lines are fits to $A/W + B/W^2$. (**d**) δ as function of U. Dotted lines are fits to $\delta \sim \sqrt{U}$ (expected for $U \to 0$).

We characterize this scenario through the quantities Δ ("TOS gap") and δ ("envelope curvature"), defined pictorially in Fig. 3. In the thermodynamic limit $\mathcal{H}_E \sim \mathcal{O}(1/W)$, then $\delta \sim \mathcal{O}(1/W)$. Furthermore, in the limit $U \to 0$ at fixed W, using $\chi^{-1} \sim U$ and $v_s \sim \sqrt{U}$ one obtains $\delta \sim \sqrt{U}$. Finally, assuming that the lowest excitations above the ES envelope are sound-wave like one can write $\mathcal{H}_E \sim [\mathcal{H}_T + \mathcal{H}_{sw}]/T_E$ where $\mathcal{H}_{sw}$ describes the sound wave excitations. Since $T_E \sim 1/W$ this suggests that the gap Δ remains finite in the thermodynamic limit, although logarithmic decay cannot be ruled out [5].

Numerical data in Figs. 2 and 3 shows a finite gap Δ for all W and a quadratic behavior of the ES envelope, supporting the tower of states picture. Figs. 2 (**c**) and 2 (**d**) show good agreement with the predictions $\delta \sim 1/W$ and $\delta \sim \sqrt{U}$.

The Mott-superfluid transition Across the phase transition ($U_c \approx 16.739$), Δ and δ show "dual" behaviors (Fig. 3 bottom). In the Mott insulating phase, $\Delta \sim 1/W^2$, while in the superfluid Δ converges to a possibly nonzero value or vanishes only logarithmically with W [5]. In contrast, the W-dependence of δ is: $\delta \sim \text{const.}$ in the Mott insulator, $\delta \to 0$ in the superfluid.

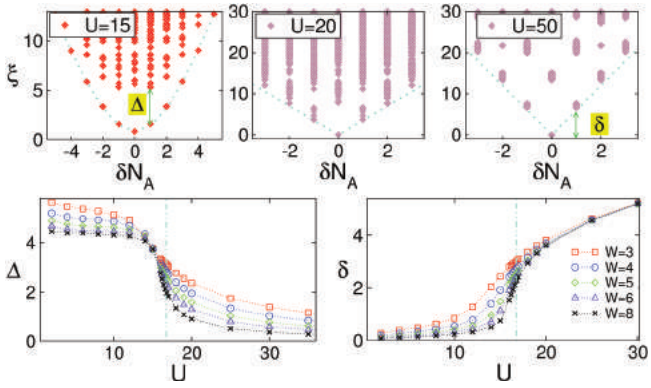

Figure 3: **(top)** Restructuring of ES across the Mott-superfluid transition (DMRG data for $W = 8 = L/4$, equal bipartitions). The arrows explain the definitions of the quantities Δ and δ. **(bottom)** Δ and δ plotted versus U for several values of the boundary length W. The vertical line denotes the critical value U_c.

Discussion Our results open up a number of research directions. First, identifying the TOS in the ground state ES implies that one can use ground state analysis to explore exotic symmetry breaking scenarios (e.g. [4, 6]), avoiding the expensive requirement of calculating many eigenstates. On the other hand our analysis points to an advantage of DMRG calculations with explicitly broken symmetry, leading to a collapse of the redundant tower of states. Third, it would be interesting to explicitly see the TOS structure appear for gapless phases where the symmetry breaking is more complex than the $U(1)$ symmetry broken in our case.

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2.5 Topological phases in one-dimensional spin systems

JONAS KJÄLL, FRANK POLLMANN

Different phases of matter are usually identified by measuring local order parameters. These order parameters are associated with spontaneous symmetry breaking [1]. For example, in the Z_2 symmetric Ising model, we find an ordered and a disordered phase which can be distinguished by an order parameter measuring the magnetization. Over the last decades, it has been discovered that distinct quantum phases (separated by quantum phase transitions) can occur even when there is no spontaneous breaking of a global symmetry and thus no local order parameter. These phases are usually referred to as "non-trivial topological phases" [2]. One of the simplest examples of a topological phase is the Haldane phase in quantum spin chains [3]. By tuning various parameters, such as anisotropy terms, this state can be driven through a critical point. Yet, on both sides of the critical point, there is no spontaneous symmetry breaking. A mystery then is how to characterize the phases and to find some *non-local* order parameter or another property that changes at the critical point.

We showed in Refs. [6, 7] that the topological phases in quantum-spin chains are characterized by the projective representations of the symmetries present. The projective representations are derived from an effective boundary theory of the model. These so-called "symmetry protected topological phases" (SPTP) can be protected by any of the following symmetries: spatial inversion symmetry, time reversal symmetry or the $Z_2 \times Z_2$ symmetry (rotations by π about a pair of orthogonal axes). This approach was furthermore shown to give a complete classification of phases in one dimension [8]. In Ref. [9] we proposed a method which allows us to directly extract the projective representation from density matrix renormaization group (DMRG) simulations. From the projective representation we then find the complete factor set, which is known to define the topological phases. We also derived non-local order parameters which can be evaluated in numerical simulations or potentially be measured in cold-atom experiments using *high-resolution imaging* [10]. With these works, we have a complete mathematical framework for the classification and detection of SPTP at hand.

Physically, the different SPTP in spin chains are characterized by their boundary spin. That is, the spin fractionalizes into two localized *half-integer* edge spins in the case of the odd integer Heisenberg spin chain (one on each edge), and into two *integer* edge spins in the case of even integer spins. There is a crucial difference between these two cases. In the odd integer case, the Haldane phase is a SPTP as the half-integer edge spin cannot be removed unless the system undergoes a phase transition or all the relevant symmetries are explicitly broken. In contrast, in the even case, the integer spins at the edge are not protected and thus the ground state can be adiabatically turned into a trivial (product) state, without breaking any symmetries. This motivates a notation of two distinct phases, an odd-Haldane (OH) and an even-Haldane (EH) phase. As proposed by Oshikawa [11], all the Haldane phases corresponding to lower integer spin can in principle be realized in the presence of on-site anisotropies.

In Ref. [12], we studied a concrete quantum spin-2 model and showed that it exhibits both the OH and the EH phase. While the spin-1 phase diagram is well established, various studies have obtained different results for the spin-2 phase diagram, see for example Refs. [13, 14]. In particular, no easy route had been found to stabilize the OH phase. For our study, we developed an efficient variant of the infinite system DMRG algorithms in terms of matrix-product-states (MPS).

The model Hamiltonian we investigated is of the form

$$H = H_{\mathrm{XXZ}} + H_D. \tag{1}$$

The first term describes the XXZ quantum-spin chain

$$H_{\mathrm{XXZ}} = J \sum_n \left(S^x_n S^x_{n+1} + S^y_n S^y_{n+1} + \Delta S^z_n S^z_{n+1} \right), \tag{2}$$

where S^α_n, with $\alpha = x, y, z$, is the α-component of the spin-S operator at site n and Δ is the XXZ anisotropic interaction parameter. The term H_D represents an on-site anisotropy, which for spin S has the general form

$$H_{\mathrm{D}} = \sum_n \sum_p^{2S} D_p (S^z_n)^p. \tag{3}$$

Depending on the values of the D_p's, this on-site anisotropy can favor different eigenstates $|m_\alpha\rangle$ of a noninteracting spin $\vec{S}$, and allows for realization of more phases than the XXZ model alone. A large positive D_2 (or a large D_4) favors a product state of the form $|\psi_D\rangle = \bigotimes_n |0\rangle_n$, where $|0\rangle_n$ is the eigenstate of S^z_n with eigenvalue $m_z = 0$. This is because the higher m_z eigenstates have been energetically projected out, and there remains only an effective spin-0 degree of freedom. In the limit $D_4 \to \infty$ with $D_2 = -D_4$, only the states with $m_z = \pm 2$ are projected out, and an effective spin-1 degree of freedom remains. Adding the previously unconsidered D_4, it is thus expected to make it easier to realize the spin-1 phases, such as the OH phase, in the spin-2 chain.

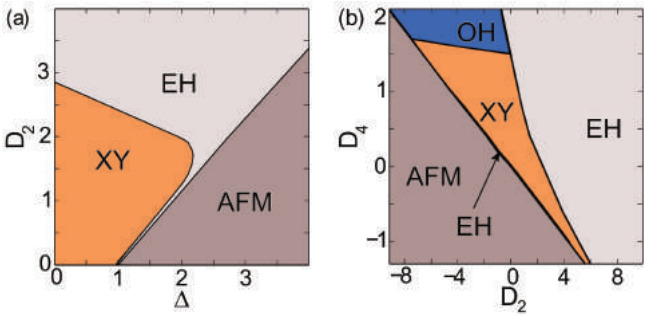

Figure 1: Spin-2 phase diagrams: Panel (a) shows the phase diagram for $D_4 = 0$ and panel (b) for $\Delta = 1.0$. Examples of data used to obtain the phase boundaries are presented in Fig. 2.

The spin-2 phase diagram for the upper right corner $\Delta \geq 0, D_2 \geq 0$ at $D_4 = 0$ is shown in Fig. 1(a). Most noticeable, there is no direct transition from the XY phase into the AFM phase. Instead, these phases are separated everywhere by the EH phase which is continuously present to large D_2. This answers one of our main questions; the Heisenberg point and the large-D region are continuously connected. This is in accordance with the theoretical finding that the edge spins are integer and thus not protected.

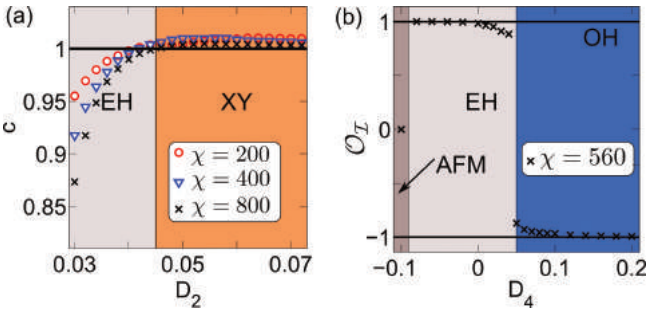

Figure 2: Examples of data used to detect phase transitions for different bond dimensions χ used in the MPS representation. (a): The transition into the critical XY phase is best localized by calculating the central charge c using finite entanglement scaling. (b): The transition from a trivial (EH) to a topological (OH) phase is identified using a non-local order parameter $\mathcal{O}_\mathcal{I}$ that is based on the inversion symmetry.

In order to map out the phase boundaries of the critical XY phase, it turned out to be very useful to apply the *finite entanglement scaling* method [15]. The phase transition between the critical XY phase and the EH phase is of Berezinskii-Kosterlitz-Thouless (BKT) type and thus notoriously hard to pinpoint numerically. We consider the scaling of entanglement entropy S_E as a function of the bond dimension χ of the matrices used in the MPS representation of the ground state. The entanglement entropy S_E is the von-Neumann entropy of the reduced density matrix for the bipartition of the system into two half-chains. In critical systems, which are described by a conformal field theory, the scaling properties of S_E allow us then to calculate the central charge c using

$$S_E = \frac{c}{6} \log(\xi) + s_0, \tag{4}$$

with s_0 being a non-universal constant. The data we used to locate the transition is shown in Fig. 2(a). The XY phase is characterized by a central charge $c = 1$. As the phase boundary to the gapped EH phase is crossed, the estimated central charge decreases with increasing bond dimension χ (and scales to zero as $\chi \to \infty$).

We furthermore showed that the topological OH phase, which is not present in Fig. 1(a), can be easily reached with the addition of the D_4-term. The experimentally most interesting region is the one with small on-site anisotropy. As an example, the D_2, D_4 plane at $\Delta = 1$ is shown in Fig. 1(b). Increasing Δ, the XY phase disappears. Since the EH and OH phase cannot be distinguished by any local order parameter, we use a non-local order parameter $\mathcal{O}_\mathcal{I}$ [9] based on the inversion symmetry of the system. The quantity $\mathcal{O}_\mathcal{I}$ can be directly extracted from the MPS representation and tells us which class the ground state belongs to. The results in Fig. 2(b) clearly show a transition between the two phases which do not break any symmetry. We use $\mathcal{O}_\mathcal{I}$ instead of the usual string-order parameter to detect the OH phase because it provides a clearer distinction between the phases. We observe a transition from the EH phase with $O_\mathcal{I} = 1$ to an OH with $O_\mathcal{I} = -1$ which extends almost to the $D_4 = 0$ plane here.

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2.6 Exotic Ising dynamics in a Bose-Hubbard model

LUIS SEABRA AND FRANK POLLMANN

The search for phases which support exotic excitations in condensed matter has benefited greatly in the last few years from the tremendous advances in cold atomic gases [1]. Here, we explore the dynamical properties of a one-dimensional pairing Bose-Hubbard model, describing two different bosonic atomic species confined to a 1D optical lattice and interacting via Feshbach resonance. We show that the dynamical features represent a faithful simulation of the low-energy effective Ising model in transverse and longitudinal fields, paving the way to the observation of exotic Ising dynamics [2], such as the emergence of E_8 symmetry [3], in a cold-atoms setting.

We consider the following Hamiltonian, see e.g., Ref. [4],

$$\mathcal{H} = \sum_{i\alpha} \epsilon_\alpha n_{i\alpha} - \sum_{i\alpha} t_\alpha (b^\dagger_{i\alpha} b_{i+1\alpha} + \text{H.c.}) + \sum_{i\alpha\alpha'} \frac{U_{\alpha\alpha'}}{2} n_{i\alpha}(n_{i\alpha'} - \delta_{\alpha\alpha'}) + g \sum_i (b^\dagger_{im} b_{ia} b_{ia} + \text{H.c.}), \tag{1}$$

describing two species of bosons $b_{i\alpha}$ hopping on a 1D lattice. Atoms are labeled by $\alpha = a$ while molecules are labeled by $\alpha = m$ and $n_{i\alpha} = b^\dagger_{i\alpha} b_{i\alpha}$. Here ϵ_α are on-site potentials, t_α are hopping parameters between nearest neighbours sites, and $U_{\alpha\alpha'}$ are on-site interactions. Two atoms form a molecule via s-wave pairing, driven by a Feshbach resonance g.

The low-energy behavior of the model Eq. (1) in the Mott regime with a filling factor of $\rho_T = 2$ can be described via an effective Ising model [4]

$$\mathcal{H}_I = -J \sum_i S^z_i S^z_{i+1} + h \sum_i S^z_i + \Gamma \sum_i S^x_i. \tag{2}$$

The effective spin degrees of freedom are $|\Uparrow\rangle \equiv |1;0\rangle$ and $|\Downarrow\rangle \equiv |0;2\rangle$ in the basis of occupation numbers $|n_a; n_m\rangle$, see Fig. 1(a). The spin operators have a direct physical interpretation: $S^z_i = (n_{im} - n_{ia}/2)/2 \equiv \Delta n_i/2$ measures the *relative* density of bosons at site i, while $S^x_i = 1/(2\sqrt{2})[m^\dagger_i a_i a_i + m_i a^\dagger_i a^\dagger_i]$ and $S^y_i = 1/(2\sqrt{2}i)[m^\dagger_i a_i a_i - m_i a^\dagger_i a^\dagger_i]$ account for fluctuations between the two species.

We find the ground state of the bosonic model Eq. (1) using the infinite density matrix renormalization group method (iDMRG) method, which yields a matrix-product state representation (MPS) of the ground-state wave-function directly in the thermodynamic limit. We then use the infinite time evolving block decimation (iTEBD) method to compute the transverse dynamical factor structure $S^y(k,\omega)$ of the effective spin representation of the bosonic model.

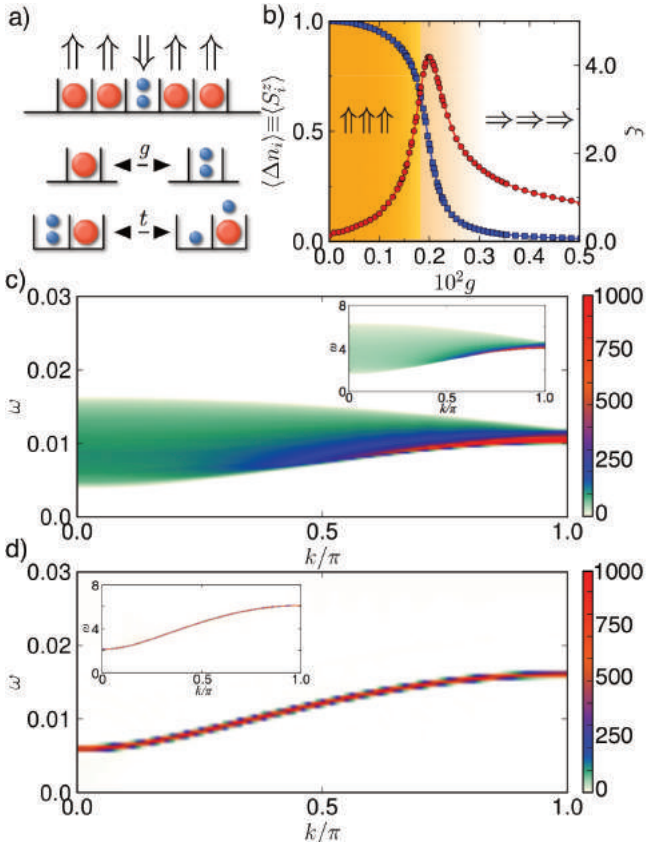

Figure 1: (a) Mapping between the pairing Bose-Hubbard model, Eq. (1), in the second Mott lobe and the Ising chain, Eq. (2). Two atoms (one molecule) per site map(s) to effective spin-down (spin-up). A local excitation converts one molecule into two atoms, which then propagates via boson hopping and Feshbach resonance, (Ising interaction J and transverse field Γ, respectively). (b) Phase diagram of the bosonic model for $t_a = 0.0504$ ($J = 0.01$) and constraints detailed in the text, measured by relative boson density. A crossover between a phase with roughly one molecule per site (small g) and disordered phase at large g is detected by the peak in the correlation length. (c) Dynamical structure factor for $g = 0.00106$ (Γ=0.3J) and $\Delta\epsilon_m$=-1.5×10^{-4}. The continuum of excitations reproduces that of the transverse-field Ising chain (inset). (d) Dynamical structure factor for $g = 0.003535$ ($\Gamma = J$), showing the quadratic single quasi-particle line, as also found in the Ising chain (inset).

We tune the system to an effective *ferromagnetic* Ising chain by choosing $t_a = 0.0504$, resulting in $J = 0.01$, and imposing the following constraints on the bosonic parameters : $t_a = 2t_m$, $\epsilon_a = 0$, $U_{aa} = 2$ and $U_{am} = 2U_{aa}$. We start by setting the effective longitudinal field h to zero, by tuning ϵ_m. The above choice of parameters leaves the Feshbach resonance g, i.e., the transverse field $\Gamma = 2g\sqrt{2}$, as the only free parameter.

While, previously, emphasis was placed on the phase-diagram where the effective model is the *antiferromagnetic* Ising chain, here we focus on parameters which yield an effective *ferromagnetic* model. The ground-state phase diagram, cf. Fig. 1(b), consists of two distinct phases connected by a crossover, close to a true critical point. At low values of g, an ordered phase is found, the "molecular state". This state is a descendent of a simple product state with one molecule localized per site. In the spin language, this state is a ferromagnetic state with a finite magnetization. By increasing the value of g, the system is tuned to a disordered phase where there is no preference between the molecular and atomic states, i.e., $\sum_i \Delta n_i \to 0$.

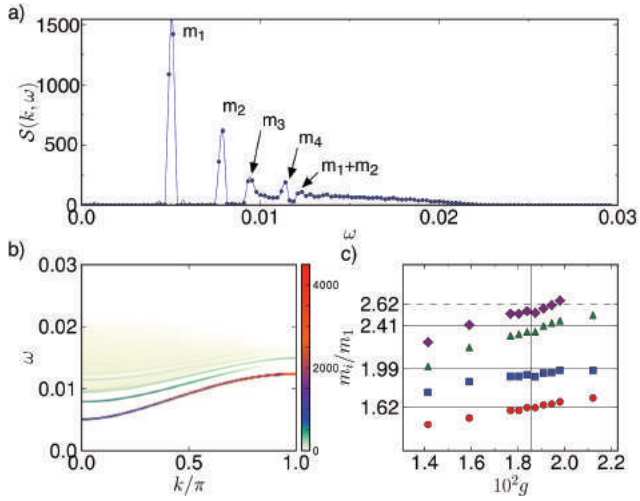

Figure 2: Signatures of the emerging E_8 symmetry in a Bose-Hubbard model. (a) Cut at $k = 0$ of the dynamical structure factor function for $g = 1.80 \times 10^{-3}$ ($\Gamma = J/2$) and $\Delta\epsilon_m = -5 \times 10^{-4}$, showing several massive excitations. (b) Dynamical structure factor resolved in momentum space. (c) Lowest mass ratios as a function of transverse effective field Γ, for fixed $\Delta\epsilon_m = 10^{-3}$. Horizontal lines are analytical values for the E_8 masses predicted by Ref. [3].

The non-equilibrium dynamics and low-energy excitation spectrum of the bosonic model in the region shown in Fig. 1(c) are also well captured by the Ising chain description. In the low-g molecular ordered state the dynamical structure factor function $S^y(k,\omega)$ displays a broad continuum of excitations around the minimum at $k = 0$ and sharpening near the Brillouin zone edge at $k = \pi$ is approached. This perfectly reproduces the behavior of the same quantity in the transverse-field Ising chain, see e.g., Ref. [5], as shown in the inset. The continuum of excitations arises from the unconfined movement of a pair of domain walls in opposite directions. In the large-g disordered state a well-defined quasi-particle excitation appears, Fig. 1(d), in excellent correspondence with the single spin-flip quasi-particle of the Ising chain, cf. inset.

The addition of a longitudinal field to the Ising chain in the ordered phase destroys the continuum of excitations by confining the motion of the pair of domain-walls. In the bosonic model under study, an effective longitudinal field has the same effect, breaking up the continuum that is present without a field (not shown).

Near the quantum critical point ($\Gamma = J/2, |h| \ll |\Gamma|$), the E_8 symmetry of the perturbed Ising chain manifests itself in eight massive particles [3]. Five different excitations are clearly identified in the cut at $k = 0$ of the dynamical structure factor function of the Bose-Hubbard model Eq. (1), cf. Fig. 2(a). These correspond to four massive particles and one bound state $m_1 + m_2$ of the E_8 theory. The successive ratios of their masses agree rather well with the analytically predicted mass ratios from Ref. [3], represented by horizontal lines in Fig. 2(c). The observation of this highly non-trivial sequence in the energy spectrum is a clear evidence for the emergent E_8 symmetry at the perturbed critical point [5].

Systems of hundreds of cold atoms confined to quasi 1D optical lattices have been extensively explored in the last decade. Recent experimental developments have made it possible to trap heteronuclear bosonic mixtures in 1D geometries [6], which naturally lead to Bose-Hubbard models similar to Eq. (1). The relevant perturbations in the bosonic model are the biasing potentials ϵ_α and the Feshbach detuning g, whose effects in tuning effective longitudinal field and fluctuations are well accounted for in Fig. 2(c). By fixing all other parameters and sweeping the Feshbach detuning term, it should be possible to observe the ratios of resonances predicted by the E_8 theory. Recent developments in manipulating heteronuclear bosonic mixtures in 1D arrays, and in techniques directly accessing the low-energy excitation spectrum, open up the fascinating possibility of observing the fingerprints of E_8 symmetry in a cold atoms experiment.

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2.7 Dominant Interaction Hamiltonians

CARLOS ZAGOYA, MARTIN GERLACH, FRANK GROSSMANN AND JAN M ROST

We introduce the concept of Dominant Interaction Hamiltonians (DIH), where the full problem is described by several approximate, but simpler – ideally integrable hamiltonians. Each hamiltonian has a phase space region for which it is dominant. At the boundaries the hamiltonians are switched. The final goal is to develop a fast yet fairly accurate numerical approach, which at the same time, provides insight into the physical mechanisms of the many particle dynamics described through the switching sequences. Two examples are discussed, high harmonic generation, where we can derive an analytical wave function within the DIH concept, and planar electron-ion scattering with two active electrons.

Presently, the concept is classical (in the example of planar electron-ion scattering), and has been extended to a semiclassical treatment (in the example of high harmonic generation) since it relies on the underlying local classical dynamics. However, it has the advantage over well known partition concepts in quantum mechanics, e.g., the R-matrix approach which is based on a spatial separation of regions, that it takes into account explicitly the momentum of particles through the separation of regions in phase space, sketched in Fig. 1.

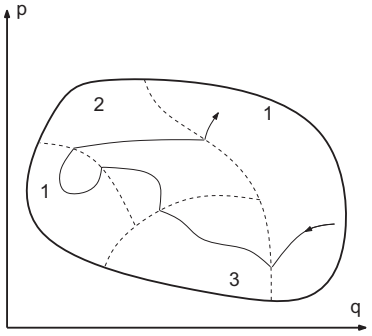

Figure 1: Sketch of phase space partition through DIH with a hypothetical trajectory passing different DIHs in the sequence 132121.

Switching conditions for the two-electron problem In our first example we construct DIH for electron-ion scattering with two active electrons, initially a projectile and a bound target electron. Clearly, if the two electrons are far apart, the electron-electron interaction is weak and the hamiltonian may be approximated by two independent electrons where the one closer to the ion (let us assume with label $i = 1$) sees the full nuclear charge Z with potential ZV_1 and the outer one feels a screened charge, $(Z-1)V_2$, which constitutes with the electron-nuclear attractions $V_i = -1/r_i$ an integrable approximation investigated a long time ago [1]. The switch of the roles of the two electrons happens at $r_1 = r_2$, where r_i are the electron-nucleus distances.

event	'1'	'2'
condition	$F = 1$	$r_1 = r_2$
action	$\vec{p}_2' - \vec{p}_1' = K_{\rm NF}(\vec{p}_2 - \vec{p}_1)$	$r_1 \leftrightarrow r_2$
effect	$\Delta l_i \neq 0, \Delta E_i \neq 0$	$\Delta E_i \neq 0$

Table 1: Switching conditions of DIH for the two-electron problem with primed (unprimed) quantities indicating variables after (before) the switch; the function F is defined in Eq. (1). Note that total energy $E = E_1 + E_2$ and total angular momentum $L = l_1 + l_2$ are conserved.

We label such a switch with '2', see table 1. There is a second dominant interaction to be considered which was never done before, and this is, when both electrons are close to each other. In this case the hamiltonian for the relative motion of the two electrons with the interaction $V_{12} = |\vec{r}_1 - \vec{r}_2|^{-1}$ rules the dynamics while the electronic center of mass moves freely and the entire hamiltonian in this approximation is again integrable. However, rather than acting over a finite time interval, this hamiltonian, once dominant works directly against its dominance since V_{12} is repulsive. Hence, the dominant electron-electron interaction V_{12} exerts a 'kick' to the system, labeled as '1' in table 1. It is applied if V_{12} and the average ZV_i are with $F = 1$ equal, where

$$F \equiv \left| \frac{2V_{12}}{ZV_1 + ZV_2} \right| , \qquad (1)$$

while the propagation is always executed with the independent electron hamiltonians discussed before.

Characterization of the dynamics through switching sequences As it is well known [2], the inherently classical approximation allows only a semiquantitative agreement with the full quantum calculation for the present two-electron planar scattering problem [4]. Surprisingly, the DIH results compare as well as the full classical calculation to the quantum results. Moreover, they provide insight into the dynamics through the classification of the switching sequences along the trajectories. Elastic scattering is dominated by trajectories with a switching sequence '12' while the inelastic peak is characterized well by '22'. This can be seen from the DIH dynamics, but also by applying the rules for the classification of dominant interaction regions only for labeling the trajectories propagated fully classically (see Fig. 2). We conclude that DIH in this case facilitates the classical description without significant loss of accuracy and the additional benefit of a classification for the trajectories through the switching sequence which has a physical meaning.

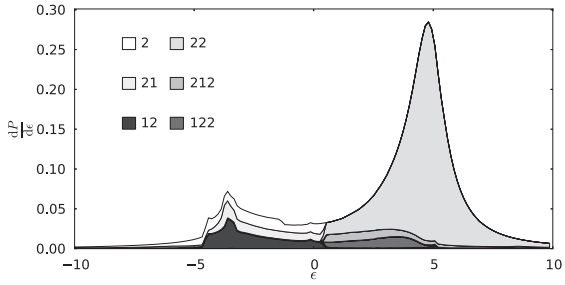

Figure 2: Electronic energy spectrum from full classical dynamics with contributions shaded according to their DIH event sequences (see table 1).

Semiclassical DIH approach for high harmonics Our goal is to eventually formulate with DIH a quantum approach. As an intermediate step we have investigated strong field dynamics of an electron in the field of a nuclear charge Z using DIH. It is well known that the high harmonic (HH) yield and in particular the cutoff with the preceding plateau (see Fig. 4) depends sensitively on an accurate description of interferences [3]. Hence, HH generated from laser assisted electron-ion scattering is a good problem to test the DIH approach semi-classically for which a one-dimensional formulation with a soft-core Coulomb potential in the direction of the linear polarization of the laser is sufficient. In the length gauge the switching is physically intuitive.

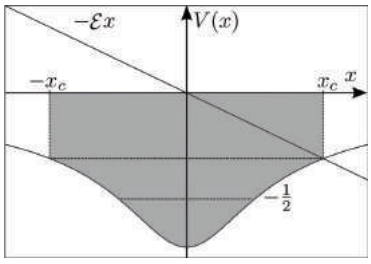

Figure 3: Soft-core Coulomb and laser potential ($-x\mathcal{E}$). Shaded areas represent the switching regions, after [6].

For large distances the electron moves only under the influence of the laser field while for short distances it is exclusively exposed to the attractive ionic potential $V(x)$, the position x_c of equal strength $x_c\mathcal{E}(t) = V(x_c)$ defines the spatial switching, see Fig 3. For the complete switching also the condition in momentum space must be defined: $p_c = 0$ ensures that the electron spends relatively long time close to this point in phase space facilitating the switching. For bound orbits under the ionic potential this constitutes their turning point defining automatically the energy with $E = V(x_c)$. It is conserved until the electron gets driven by the laser field again after the next switch. Eventually, a small fraction of trajectories corresponding to electrons driven by the laser field are trapped in the ionic potential and collect a phase in time (through their classical action) quite different from the freely floating ones. This difference leads to substantial interference which appears as a plateau of high harmonics in the energy domain in good agreement with the quantum solution (Fig. 4). In the DIH formulation together with the semiclassical initial value representation of Gaussian wave packets, it is even possible to construct a fully analytical wave function which produces the spectrum in Fig. 4 [5].

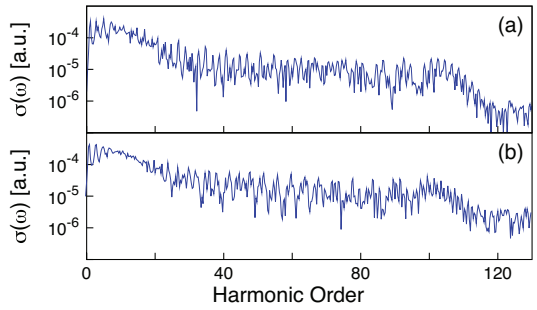

Figure 4: HH spectrum, (a) full quantum result, (b) DIH result. The cutoff for scattering from an ion under a laser field, $E_{\rm cut} = 2U_p + I_p$, determines the highest harmonic order, $N_{\rm max} = E_{\rm cut}/\omega = 105$, where $U_p = \mathcal{E}_0^2/(4\omega^2)$ is the ponderomotive potential.

The potential of DIH lies not only in the chance to find approximations which can be treated numerically very efficiently (e.g., for HHG we need a factor 100 fewer trajectories for the HHG spectrum based on DIH compared to the full semiclassical one), but leads also to interesting conceptual questions: while the continuous classical dynamics may be chaotic, the approximate DIH dynamics can be integrable. The chaotic character is in this case transferred to the discrete switching sequences which constitute formally a map to be investigated in the future.

We thank Sebastian Wüster for support with the numerical wave packet calculations in [4] and Christian Goletz for contributing the quantum calculations in [5,6].

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2.8 Non-adiabatic dynamics in molecular- and Rydberg-aggregates

SEBASTIAN WÜSTER, ALEXANDER EISFELD, JAN M ROST

Coupling of excitonic and nuclear degrees of freedom plays an important role in many chemical and biological processes. For example the efficient exciation energy transfer in photosynthesis strongly depends on the coupling of electronic transition of the (bacterio)chlorophyll molecules to internal vibrations and that of the surrounding protein [3, 4]. The resonant dipole-dipole interaction that is responsible for the transfer of energy has a strong distant and orientation dependence. The resulting center of mass or orientational motion is not well understood. It had been speculated that the relaxation in certain types of molecular aggregates proceeds via a conical intersection (CI) which is reached by torsional motion of the molecules w.r.t. each other [5]. We have investigate this relaxation dynamics [6] and demonstrated that the torsional relaxation can be distinguished from other possible relaxation mechanisms using fs pump-probe spectroscopy.

While in molecular systems the analysis of torsional or center-of-mass motion is complicated by internal vibration and the coupling to the (usually) aqueous environment, we have shown in previous publications that ultra-cold atoms are well suited to study the intriguing interplay of excitonic and nuclear dynamics in a controlled way [7], in particular regarding non-adiabatic transitions. In the following discussion we will focus on how CIs emerge due to the resonant dipole-dipole interaction between Rydberg atoms.

General description Consider N atoms of mass M whose positions $\mathbf{r}_n$ are grouped into the $3N$ component vector $\mathbf{R} = \{\mathbf{r}_n\}$. We assume that each particle can be either in some electronic ground state $|g\rangle$ or some excited state $|h\rangle$. The single excitation Hilbert space for the electronic degree of freedom is then spanned by $|\pi_n\rangle \equiv |g \cdots h \cdots g\rangle$, with the n'th particle excited. We incorporate particle motion and electronic excitation transfer by dipole-dipole interactions into the Hamiltonian

$$\hat{H} = -\sum_n^N \frac{\nabla^2_{\mathbf{r}_n}}{2M} + \hat{H}_{el}(\mathbf{R}), \tag{1}$$

with

$$\hat{H}_{\rm el}(\mathbf{R}) = \sum_{n,m}^N V_{nm}(\mathbf{r}_n, \mathbf{r}_m)|\pi_n\rangle\langle\pi_m|, \tag{2}$$

where V_{nm} is the dipole-dipole interaction between the particles. When ignoring the angular dependence of the interaction we have $V_{nm} \propto -\mu^2/|R_{nm}|^3$ with $R_{nm} = |\mathbf{r}_n - \mathbf{r}_m|$. Atomic units are implied unless otherwise indicated.

The total quantum state is $|\Psi(\mathbf{R})\rangle = \sum_{n=1}^N \phi_n(\mathbf{R})|\pi_n\rangle$, where $\phi_n(\mathbf{R})$ is the wave function of particle motion in the electronic state $|\pi_n\rangle$. From the time dependent Schrödinger equation one obtains the set of coupled equations $i\frac{\partial}{\partial t}\phi_n(\mathbf{R}) = \sum_{m=1}^N \left[-\frac{\nabla^2_{R_m}}{2M}\phi_n(\mathbf{R}) + V_{nm}\phi_m(\mathbf{R})\right]$.

To analyze the resulting dynamics it is often convenient to consider a Born-Oppenheimer separation. The eigenstates of the electronic Hamiltonian fulfill $H^{\rm el}(\mathbf{R})|\varphi_j(\mathbf{R})\rangle = U_j(\mathbf{R})|\varphi_j(\mathbf{R})\rangle$. The energies $U_j(\mathbf{R})$ then define N adiabatic potential energy surfaces for particle motion. A particle stays on a definite surface, if non-adiabatic couplings between the surfaces can be ignored. These non-adiabatic couplings become large at a conical intersection.

A setup to study the dynamics at a CI in a controlled manner We consider three particles confined one-dimensionally on a ring, with coordinates as in Fig. 1. On the ring the position of atom n is specified by its 2D polar angle θ_n. The centre-of-mass type angle $\theta_{CM} = \sum_n \theta_n/3$ decouples, and the dynamics of interest is fully described by the two relative angles $\theta_{12} = \theta_2 - \theta_1$ and $\theta_{23} = \theta_3 - \theta_2$.

In Fig. 1 we show the three potential energy surfaces obtained by diagonalizing $\hat{H}_{\rm el}$.

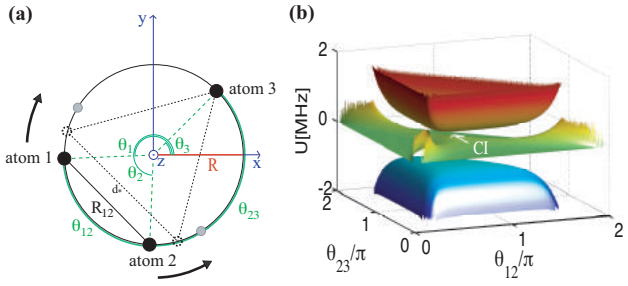

Figure 1: Ring trimer. (a) Three atoms confined to a ring with radius R in the x-y plane. (b) Born-Oppenheimer surfaces for the electronic Hamiltonian (1). From top to bottom $U_{\rm rep}$, $U_{\rm mid}$ $U_{\rm att}$. For better visibility we shifted the repulsive (attractive) surface up (down) by $\Delta U = 0.37$ MHz, and magnified the middle surface by a factor $f_m = 5$. At the marked CI location, $U_{\rm rep}$ and $U_{\rm mid}$ would touch without the shifts.

The top (red) and bottom (blue) surfaces are globally repulsive or attractive, respectively. Each of them is associated with a different delocalized excitation. Energetically between these, we find a middle surface that touches the repulsive one in a conical intersection at $\theta_{12} = \theta_{23} = 2\pi/3$. In the following we show how this intersection affects adiabatic excitation transport.

We also introduce the adiabatic form of the wavefunction $|\Psi\rangle = \sum_{j=1}^{3} \tilde{\phi}_j(\theta_{12},\theta_{23})|\varphi_j(\theta_{12},\theta_{23})\rangle$. Finally, let us define the population of the n'th diabatic (adiabatic) state as $p_n = \int d\mathbf{R}|\phi_n|^2$ ($\tilde{p}_j = \int d\mathbf{R}|\tilde{\phi}_j|^2$). For adiabatic states and surfaces, we will use subscripts rep $= 1$, mid $= 2$, att $= 3$ as in Fig. 1. The setup described above allows one to observe how CIs affect many-body dynamics. Here we will discuss electronic de-coherence. The possibility to directly observe Berry's phase is described in Ref. [1].

Electronic de-coherence Consider the case where initially the system is on the repulsive adiabatic surface and the particles form an isosceles triangle as sketched in Fig. 1a. The initial distance between particles 1 and 2 is chosen smaller than the separation $d^* = \sqrt{3}R$ at the conical intersection. Each atom has initially a narrow Gaussian angular distribution. The detailed construction of the initial state is described in [7]. From this initial state, the repulsion drives the configuration over the CI. We use $R = 9.8\mu$m for the radius of the ring. The atomic parameters $\mu = 180$ a.u. and $M = 11000$ correspond to laser dressed Lithium, as will be explained later.

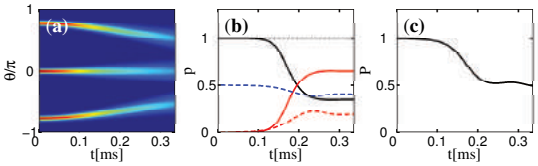

Figure 2: (a) Total atomic density, given by $n(\theta) = \sum_{m=1}^{N} n_{\{m\}}(\theta_m)|_{\theta_m\to\theta}$ with $n_{\{m\}}(\theta_m) = \sum_{n=1}^{N}\int d^{N-1}\theta_{\{m\}}|\phi_n(\theta)|^2$, where $\int d^{N-1}\theta_{\{m\}}$ denotes integration over all but the m'th particle coordinate. Note that the θ-axis is periodic, hence the highest and lowest particle are near neighbors and initially repel. The configuration passes the CI location when all three inter-particle distances are equal, around $t = 0.17$ ms. (b) Adiabatic populations p_{rep} (solid, black), p_{mid} (solid, red), electronic populations $p_1 = p_3$ (dashed, blue), p_2 (dashed, red) and total population (dotted, black). (c) Purity $P = \text{Tr}[\hat{\sigma}^2]$ of the reduced electronic density matrix, described in the text.

The close proximity pair of particles initially accelerates adiabatically, as evident from the constant surface populations in Fig. 2b. However, as the many-body wave function passes the conical intersection, more than 60% of the total population is transferred from the repulsive to the middle surface. Fig. 2c shows an accompanying drop in purity of the reduced electronic density matrix $\hat{\sigma} = \sum_{n,m}\sigma_{nm}|\pi_n\rangle\langle\pi_m|$, with $\sigma_{nm} = \int d^N\mathbf{R}\,\phi_n^*(\mathbf{R})\phi_m(\mathbf{R})$. The operator $\hat{\sigma}$ describes the electronic state, disregarding knowledge of particle positions. The observed decoherence of the electronic state is a consequence of the spatially disjunct splitting of the wave-packet on two surfaces and ensuing entanglement between the particle position and aggregate electronic state. It will occur generically for all dynamics close to the CI.

Experimental realization: Rydberg dressing We have shown that Rydberg dressing can be used to facilitate the experimental realization, since it allows us to control the various parameters in a controled way [2]. For this we require two non-interacting ground (or meta-stable) states $|g\rangle$, $|h\rangle$, each of which is off-resonantly coupled to a Rydberg level $|g\rangle \leftrightarrow |s\rangle$, $|h\rangle \leftrightarrow |p\rangle$ by two separate transitions, both with Rabi-frequency Ω and detuning Δ. The detuning parameter $\alpha = \Omega/2\Delta$ controls the population transferred to the Rydberg levels $|s\rangle$, $|p\rangle$, of order $\sim \alpha^2$, and the interaction-strength for the ground state atoms ($\sim \alpha^4$).

The simulations presented above correspond to ^{7}Li atoms, acquiring long-range interactions through laser dressing with $\alpha = 0.15$ via the Rydberg level $\nu = 100$.

Conclusions We have demonstrated that Rydberg atoms can be used to study fundamental properties of coupled electronic and nuclear dynamics [1, 2, 8], as demonstrated previously for adiabatic entanglement transfer and here for non-adiabatic transitions at a CI. Laser dressings gives us a great freedom to design potential energy surfaces. By choosing different potentials for the states $|g\rangle$ and $|h\rangle$ it becomes possible to consider each atom as a prototypical molecule with different Born-Oppenheimer surfaces in the ground and excited state. The (dressed) dipole-dipole coupling between the atoms then leads to the basic model to describe molecular aggregates where exciton vibrational coupling is important and cannot be described within an adiabatic approximation [9]. In particular we are now in the situation to consider beside internal vibrations also the center-of-mass motion of the atoms/molecules to study energy relaxation and exciton self-trapping. Such investigations would be quite demanding using numerical simulations.

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2.9 Strongly Coupled Plasmas via Rydberg-Blockade of Cold Atoms

G. BANNASCH, T. C. KILLIAN AND T. POHL

We propose and analyze a new scheme to produce ultracold neutral plasmas deep in the strongly coupled regime. Our method exploits the interaction blockade between cold atoms excited to high-lying Rydberg states. We observe universal behavior of the resulting plasma coupling strength, providing a direct connection between the physics of strongly correlated Rydberg gases and ultracold plasmas. The approach is shown to reduce currently accessible temperatures by more than an order of magnitude, which opens up a new regime for ultracold plasma research and cold ion-beam applications with readily available experimental techniques.

Strongly coupled Coulomb systems occupy an exotic regime of plasma physics [1] where correlated dynamics due to strong interactions dominates random thermal motion of the charges. While plasmas generally constitute the most abundant state of matter, strongly coupled systems are rather scarce and typically require extremely high densities that occur in such exotic settings as the interior of stars and giant gas planets or inertial-confinement fusion experiments. On the other hand, ultracold neutral plasmas (UNPs), produced by direct photoionization of laser-cooled atoms [2,3], represent a promising alternative for creating and studying strongly coupled plasmas, which provides unique opportunities to probe dynamical phenomena [3]. Their low temperatures yield strong coupling conditions at such small densities that typical evolution timescales are slowed down tremendously. Amongst other, this has enabled recent experiments to investigate relaxation processes [4] at ultralow plasma temperatures, allowing for the first time to measure relaxation rates in the strongly coupled domain (see Fig. 1). Such conditions also hold great promise for applications in nanotechnology, where UNPs are utilized to create high-brightness ion beams [6] for fabricating and characterizing nanoscale objects.

Plasmas can be classified into weakly and strongly coupled systems by means of their Coulomb coupling parameter $\Gamma = \frac{e^2}{a\,k_{\rm B}T}$, where e is the electron charge, $k_{\rm B}$ is the Boltzmann constant, and $a = (\frac{4}{3}\pi\rho)^{-\frac{1}{3}}$ is the Wigner-Seitz radius for a plasma of density ρ. A plasma is termed strongly coupled, when the average potential energy $\sim e^2/a$ of the charges exceeds their thermal energy $\sim k_{\rm B}T$, i.e. when $\Gamma > 1$. Yet, the intriguing possibilities to achieve high Γ in UNPs are currently limited by intrinsic ion heating [3] that takes place right after plasma creation and pushes the plasma-ions just to the edge of the strong-coupling regime.

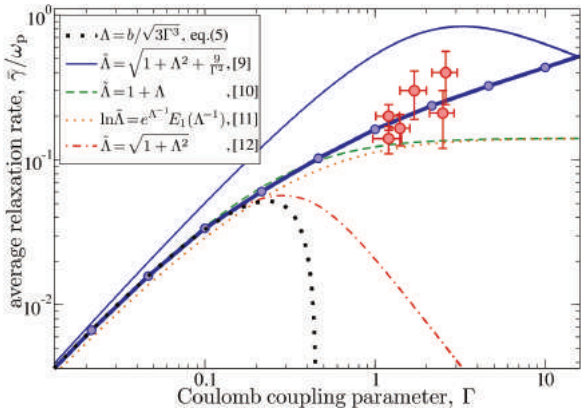

Figure 1: Average relaxation rate as a function of coupling strength Γ [4]. Circles represent experimental results, obtained from fluorescence measurements of selected ions, marked by velocity selective optical pumping. The thick solid line shows MD simulations for a wider range of parameters. For weak coupling it approaches the Landau-Spitzer prediction [5] which, however, breaks down in the strongly coupled regime.

Here we describe a new UNP-production scheme that considerably suppresses this heating with currently available and well established experimental techniques. The approach is based on the strong correlations between Rydberg atoms that emerge when a cold gas of atoms is laser-excited to a high-lying electronic state.

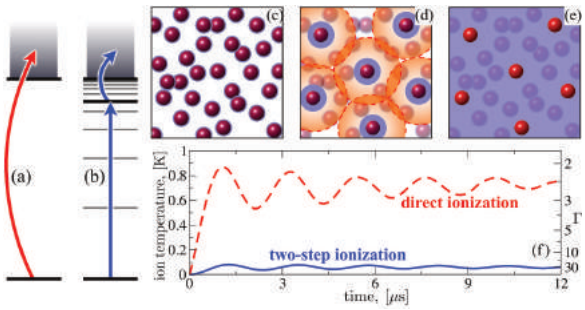

Figure 2: Schematics of the (a) conventional direct-ionization scheme for UNP production and (b) the two-step production proposed in this work. The new scheme proceeds over configurations in (c)-(e) (see text) and leads to a considerably reduced ion heating (f).

Figure 2 illustrates the basic idea in comparison to the conventional approach for UNP creation. In the latter case, direct photoionization of cold atoms [Fig.2(a)] produces a disordered configuration of ions. Subsequent rearrangement establishes inter-particle correlations, and leads to a rapid rise of the temperature to $T_{\rm i} \sim 1$ K, corresponding to $\Gamma \approx 2$ irrespective of the initial ion density and atom temperature [3], as shown in Fig.2(f).

This strong heating can be reduced with a two-step ionization scheme [see Fig.2(b)], where the ground state atoms are first excited to high-lying Rydberg states

and subsequently ionized. In the first excitation step we take advantage of the so called Rydberg blockade [7], which prevents simultaneous excitation of nearby atoms due to the enormous van der Waals interaction between Rydberg atoms. The corresponding length scale on which atoms are blocked, the blockade radius r_b, can be estimated from the respective interaction energy of the Rydberg excitation [9], which increases with the principal quantum number n of the excited state, and is close to the typical correlation length of a strongly coupled plasma, $r_\mathrm{b} \approx 1.2\,a$. A Single Rydberg atom can thereby inhibit the excitation of up to a few 10^3 atoms. As illustrated in Fig.2(d), this gives rise to strong Rydberg-Rydberg atom correlations. Their subsequent ionization thus produces a pre-correlated plasma [Fig.2(e)] that evolves to an equilibrium state with a much higher Coulomb coupling parameter [Fig.2(f)].

The many-body excitation dynamics can be described in terms of transition rates [8], leading to a set rate equations that can be solved efficiently via classical Monte Carlo simulations. The conversion of the atomic correlations into ionic ones, requires efficient ionization of the Rydberg states while leaving the ground state atoms undisturbed. Short microwave pulses are well suited for this task, as we could show by classical trajectory Monte-Carlo simulations [9].

Finally, we performed molecular dynamics simulations to investigate the subsequent relaxation of the pre-correlated ions, whose initial positions correspond to those of the Rydberg atoms obtained from the Monte-Carlo simulations of the excitation step. Such simulations yield the temperature dynamics shown in Fig.2(f), which demonstrates a more than tenfold enhancement of the Coulomb coupling parameter. This places the produced plasma deep into the strongly coupled regime with strong liquid like correlations.

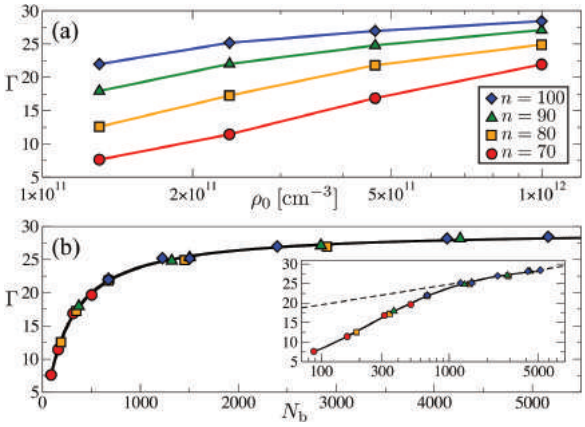

Figure 3: (a) Final Coulomb coupling parameter Γ as a function of the ground state atom density ρ_0 and different Rydberg levels n. (b) Same data, but as a function of the number N_b [eq.(1)] of blocked atoms.

As shown in Fig. 3 the Coulomb coupling parameter Γ increases with both the atomic density ρ_0 and the principal quantum number n of the Rydberg state. This behavior can be qualitatively understood from the increasing degree of correlations in cold Rydberg gases with ρ_0 and the strength of the van der Waals interactions. We can quantify this relation by defining the number of blockaded atoms

$$N_\mathrm{b} = \frac{4}{3}\pi r_\mathrm{b}^3\,\rho_0\ , \qquad (1)$$

which corresponds to the total number of atoms within one blockade sphere of radius r_b. Indeed all data points collapse on a single universal curve as a function of N_b [see Fig.3(b)].

The proposed scheme, therefore, represents a viable way to tremendously boost currently achievable coupling strength, which would otherwise be constrained to $\Gamma \approx 2$. The demonstrated tenfold cooling directly translates into an enhanced brightness of UNP-based ion beams, which enhances the spatial beam resolution for nanotechnology applications.

Several extensions of the proposed scheme appear worth pursuing. First, the conversion from a Rydberg gas to an UNP can also be realized by other approaches than microwave ionization. For example, by ionizing a fraction of the remaining ground state atoms using a second laser pulse right after the Rydberg excitation, one produces energetic electrons that will lead to rapid electron impact ionization of the highly excited Rydberg atoms. Second, a correlated plasma with $T \lesssim 100$ mK seems well suited for subsequent laser-cooling, which thus far was hampered by the strong heating out of the Doppler range. Third, long-range dipolar Rydberg interactions, induced by resonant pair-state couplings or external electric fields, may give rise to atomic correlations that are closer to those of long-range interacting Coulomb systems and, therefore, may further enhance the coupling strengths of the resulting plasma. Finally, Rydberg excitation by standing-wave light fields is expected to increase atomic correlations substantially. If the lattice constant matches the blockade radius, we expect strong excitation ordering that could push Γ to values not far below the crystalline-plasma regime ($\Gamma \approx 174$ [1]).

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2.10 Spin squeezing in a Strontium lattice clock

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Squeezed states of quantum spin ensembles are special kind of entangled many-body states that display reduced quantum fluctuations in some observable compared to coherent many-body states of uncorrelated particles. This makes them a valuable resource for high precision frequency metrology and could tremendously boost the performance of atomic lattice clocks. Here, we theoretically demonstrate a viable approach to spin squeezing in Strontium lattice clocks via optical dressing to a highly excited Rydberg state. We present a simple protocol for preparing entangled states in such a Strontium-Rydberg clock in current lattice clock experiments with the addition of a single excitation laser and without affecting the subsequent measurement.

The precise measurement of frequency in atomic systems has important applications both in fundamental science, such as searches for physics beyond the standard model, and in technologies such as satellite navigation. Clocks based on optical transitions have begun to surpass the performance of microwave standards, currently used to define the second. In fact, comparisons between optical clocks based on single ions [1] or ensembles of neutral atoms [2] are now the most precise measurements ever made. The ensemble approach is spearheaded by the strontium lattice clock, where a fractional instability of 10^{-17} [2] was recently obtained with clocks operating close to the limit imposed by the quantum projection noise associated with measurements on N independent atoms.

Squeezing, or quantum correlations between the atoms, can be used to beat this limit and improve the signal-to-noise ratio. The usage of squeezing to improve frequency measurements was first proposed [3] and demonstrated in the context of ion traps. Recent state-of-the-art experiments have broken the projection noise limit on microwave clock transitions. However, as the state-of-the-art moves towards optical standards, an outstanding challenge is to find an effective method for generating squeezed sates in lattice clocks. Here, we describe an approach based on switchable spin interactions, induced by far off-resonant optical dressing to highly excited atomic states [4] and exploiting to availability of two valence electrons in alkaline earth atoms such as Strontium. While one valence electron is employed to create strong interactions, the remaining one serves for optical trapping of the atoms independently of their internal state.

Setup We consider N Strontium atoms confined in an optical lattice with a single atom per site and lattice spacing a. The Sr clock operates on the transition between the $5s^2$ singlet ground state $|g\rangle$ and the long-lived metastable $5s5p$ triplet state $|e\rangle$, which is coherently driven by a laser with Rabi frequency Ω, as illustrated in Fig. 1a. In addition, a second laser with Rabi frequency Ω_D couples the intermediate state $|e\rangle$ to a Rydberg $5sns$ triplet state $|r\rangle$ with a large detuning Δ. Choosing $\Delta \gg \Omega_D$, only a very small fraction $\epsilon = (\Omega_D/2\Delta)^2$ of the Rydberg state is admixed to the intermediate state, such that the three-level system effectively reduces to a two-level system with a long lifetime of 10ms to 10^3ms. The effective interaction [5] between two such Rydberg dressed intermediate states of atoms at positions $\mathbf{r}_i$ and $\mathbf{r}_j$ yields a soft core van der Waals potential of the form (Fig. 1 b)

$$V_{ij} = V_0 \frac{R_c^6}{r_{ij}^6 + R_c^6}. \tag{1}$$

Here, $R_c = \left(\frac{C_6}{2\hbar|\Delta|}\right)^{1/6}$ denotes the Rydberg blockade [6] radius that depends on the van der Waals C_6 coefficient and the potential height is given by $V_0 = \left(\frac{\Omega_D}{2\Delta}\right)^3 \hbar\Omega_D$. Both parameters are widely tunable via the laser parameters Δ and Ω_D.

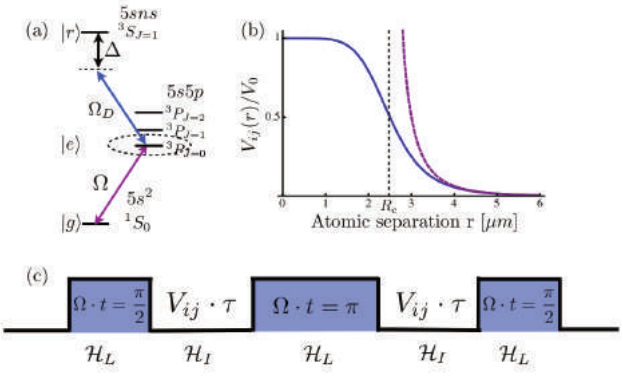

Figure 1: (a) Schematics of the considered three-level atom. One laser field drives the clock transition between the singlet ground state ($|g\rangle$) and the long-lived triplet state ($|e\rangle$) with a Rabi frequency Ω. A second laser couples the clock state $|e\rangle$ to a triplet Rydberg state $|r\rangle$ with Ω_D and detuning $\Delta \gg \Omega_D$, thereby inducing an effective interaction potential shown in (b). The dashed purple line represents the van der Waals type tail of the potential. (c) Squeezing protocol, based on a spin echo-type sequence of driving and interaction phases controlled by the intents of the two laser fields. The duration t of the $\Omega(t)$ pulse is chosen such that it leads to a $\pi/2$ or π spin rotation, while the interaction time τ determines the amount of produced squeezing.

Hamiltonian The switchable interaction V_{ij} which can be turned on and off by the dressing laser allows

one to decompose the Hamiltonian into two independent building blocks $\mathcal{H} = \mathcal{H}_L + \mathcal{H}_I$ where

$$\mathcal{H}_L = \frac{\hbar\Omega}{2}\sum_{i=1}^{N}(\hat{\sigma}^i_{eg} + \hat{\sigma}^i_{ge}), \quad \mathcal{H}_I = \sum_{i<j}^{N} V_{ij}\hat{\sigma}^i_{ee}\hat{\sigma}^j_{ee}, \qquad (2)$$

with the two-level transition and projection operators $\hat{\sigma}_{\alpha\beta}$ ($\alpha, \beta = g, e$). The laser coupling term $\mathcal{H}_L$ drives coherent transitions between the ground and clock state, $|g\rangle$ and $|e\rangle$, respectively, while $\mathcal{H}_I$ induces squeezing due to state dependent spin rotations. Consequently, this type of scheme is referred to as "one-axis twisting" [7,8] and leads to squeezing.

Squeezing protocol The amount of squeezing can be quantified by introducing the squeezing parameter ξ^2 [3], which is the squared signal-to-noise improvement of the resulting squeezed state with respect to an uncorrelated coherent state. For a squeezed state $\xi^2 < 1$, where the lower bound is set by the fundamental quantum mechanical Heisenberg limit $1/N$. A lower squeezing parameter, indicates a stronger suppression of quantum fluctuations, and therefore a higher measurement accuracy. Here we consider a spin squeezing protocol in which the two blocks of the Hamiltonian in Eq. 2 are applied sequentially (see Fig. 1 c) within an spin echo-type sequence. Initially we start with all atoms in the ground state. Then a $\pi/2$ pulse brings each atom into an superposition state of $|g\rangle$ and $|e\rangle$. Now the interaction is switched on for a time τ, leading to atomic correlations. To compensate for undesired global spin rotations a π pulse followed by a subsequent interaction phase of duration τ is applied. Finally the state is brought back into the ground state by another $\pi/2$ pulse.

Results The consecutive application of only one building block at a time allows us to solve the entire quantum dynamics analytically, which yields simple expressions that can be evaluated efficiently for large of several 10^3 atoms. As expected squeezing improves with larger interaction range R_c and is very strong for realistic values of up to ten lattice sites (Fig. 2 b). Importantly, the interaction time τ during which the Rydberg states are coupled to the clock state can be brought into the sub-millisecond regime (Fig. 2 c). This is much shorter than the lifetime of the dressed Rydberg state $|e\rangle$ so that decay can be neglected. With higher dimensionality of the optical lattice, squeezing is strongly enhanced and quickly approaches the Heisenberg limit (Fig. 2 a,b).

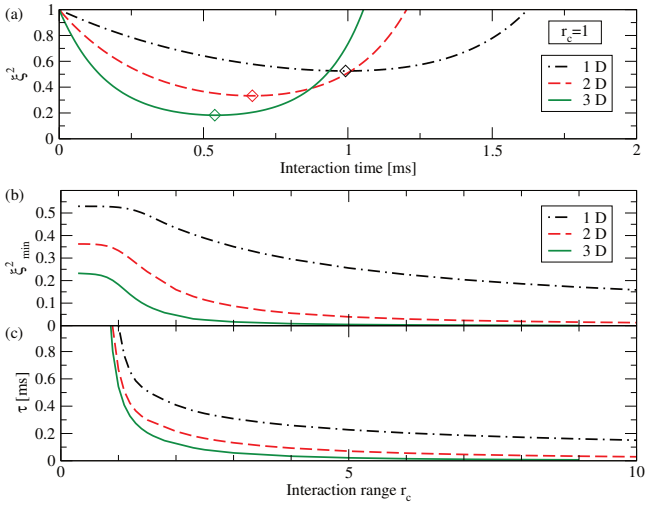

Figure 2: (a) Dynamical evolution of the squeezing parameter ξ^2 shown for different dimensions of the optical lattice for the exemplary value of an interaction range per lattice spacing $r_c = R_c/a = 1$. The diamonds indicate the minimum ξ^2_{min} of the squeezing parameter. Panel (b) shows ξ^2_{min} as a function of the interaction range and Panel (c) the corresponding interaction time τ to obtain this optimal squeezing.

Conclusion We have shown that by introducing one additional laser into a common Strontium lattice clock, one can produce strong and well controllable interactions between the effective spins. Within an optimized squeezing protocol, these interactions produce strongly squeezed states within a few milliseconds. An important distinguishing feature of the present scheme is that the additional interactions are completely switched off after the squeezing has been produced. It therefore does not affect the subsequent measurement process and there presents a promising approach towards a significant improvement current clock accuracies.

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2.11 Stimulated Electronic X-Ray Raman Scattering

CLEMENS WENINGER AND NINA ROHRINGER

Introduction The experimental investigation of nonlinear and quantum optics in the X-ray regime is virtually uncharted territory. With the advent of X-ray free electron lasers (XFELs), a new opportunity arises to explore quantum optical effects involving X-ray interaction with core electrons. The most prominent example of quantum optics and electronics is the laser itself. Since its invention more than fifty years ago, scientists have striven to achieve amplification on atomic transitions of increasingly shorter wavelength. Here we present our theoretical studies and give a small summary of our experimental findings on atomic inner-shell X-ray lasers in neon [1], following two experimental campaigns at the LCLS XFEL at the SLAC National Accelerator Laboratory. We discuss two pumping schemes: The first scheme creates a population inversion by rapid photoionization in neon [1–3], a scheme first proposed in 1967 [4]. The second scheme is based on resonant stimulated X-ray Raman scattering [5] on isolated pre K-edge resonances in neon.

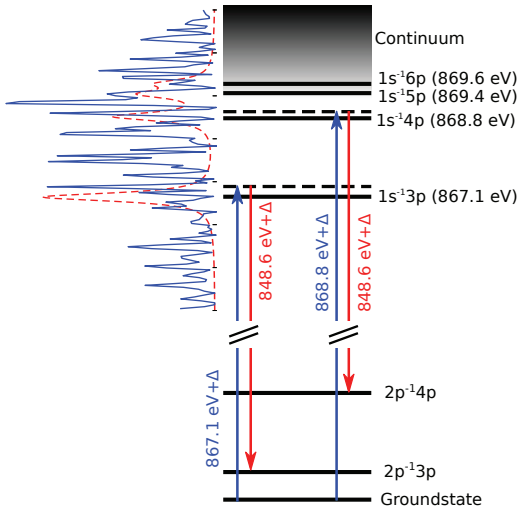

Figure 1: Level Scheme of the X-ray resonance Raman process in neon. The blue curve shows a simulated SASE pulse spectrum, the red dashed line shows the resonance oscillator strength in the pre K-edge region.

Experimental Results Focusing X-ray pulses of the LCLS XFEL with photon energies greater than 867 eV and pulse durations of 40 fs into a gas cell filled with neon at atmospheric pressure, a long, narrow plasma column of transiently core-excited neon atoms is created. The core excitation, resulting in a population inversion of the 2p versus 1s shell, can either be produced by rapid K-shell photoionization for photon energies above the K edge ($\omega > 870$ eV) or by a resonant core excitation, primarily to the electronic $1s^{-1}3p$ level at $\omega = 867$ eV (see level scheme in Fig. 1). On target, X-ray intensities of $\sim 10^{17}$ W/cm^2 are achieved for a focal radius of 1-2 μm, so that the creation of the core excited state happens on a fs timescale, i.e. comparable to the Auger-life time of the 1s hole (2.4 fs). Despite the small branching ratio of radiative versus Auger decay (0.018), a few seed photons at the frontend of the plasma column suffice to drive an avalanche of stimulated emission processes, resulting in saturated emission at the neon Kα transition at 849 eV photon energy (corresponding to a wavelength of 1.46 nm). For a typical number of $\sim 10^{12}$ incoming XFEL pump photons we measured $\sim 10^{10}$ photons in the amplified neon Kα line, emitted in a narrow cone of ~ 1 mrad angular divergence. This translates into a gain-length product of ~ 21 for the shot of highest intensity [1]. The emission spectra were recorded 4 m downstream of the interaction region with an X-ray spectrometer with ~ 1 eV energy resolution.

Measured spectra are shown in Fig. 2 as a function of the incoming photon energy varied across the K-edge region [6]. The transmitted XFEL pulse corresponds to the diagonal feature and has a spectral width of 6 eV FWHM, the amplified Kα emission corresponds to the vertical feature at 849 eV. Due to the spectrally broad XFEL pulse, the cross over from stimulated X-ray Raman scattering to amplified spontaneous emission is not discernable by merely looking at the signal strength as a function of central XFEL photon energy. A detailed analysis of the emission line shape, however, reveals the transition: For XFEL photon energies ω >870 eV, the line shape and peak position of the emitted radiation are reproducible from shot to shot, whereas for ω <870 eV the line profile and the peak position change stochastically. The shot-to shot energy shift results from the inherent spiky spectral structure of the incoming XFEL, which is based on the self-amplified spontaneous emission (SASE) process. Individual spectral spikes of the SASE pulse (having an average width of ~0.1 eV) are randomly detuned from the $1s\text{-}^1np$ core-excited resonances (width of 0.25 eV). The strongest spectral SASE spike situated on or close to a transition energy drives the resonant inelastic X-ray scattering process, which follows a well known linear energy dispersion [7] of emitted versus incoming photon energy. Since the position of the SASE spikes varies from shot to shot, the emitted photon energy shifts stochastically.

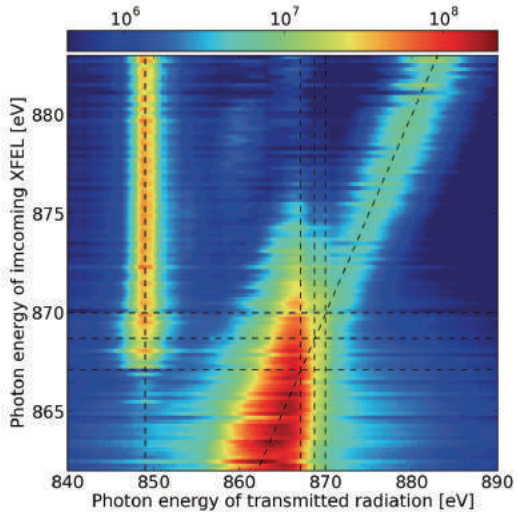

Figure 2: Spectra as a function of the average incoming XFEL photon-energy (y-axis) on a logarithmic false color scale, corresponding to the integrated CCD counts along the non-dispersive direction along the entrance slit of the spectrograph. The XFEL pump corresponds to the diagonal feature. Several absorption dips can be discerned in the structure of the XFEL pulse, corresponding to the position of the $1s^{-1}3p$ resonance (867.1 eV), the $1s^{-1}4p$ resonance (868.8 eV) and the K-edge (870.2 eV), marked as dashed lines. The Raman scattered / Kα emission line corresponds to the vertical feature at 848.6 eV.

Theoretical Results To corroborate our experimental findings we numerically solved generalized one-dimensional Maxwell-Bloch equations, to predict the emitted temporal and spectral X-ray laser intensity profiles. The equations were solved for an ensemble of numerically generated SASE pulses. To model the stimulated resonant Raman process, we take into account resonant excitation to the 3p, 4p, 5p and 6p levels. Despite pumping with a SASE XFEL source of limited temporal coherence, the produced atomic X-ray laser radiation is predicted to be nearly transform limited. Our calculations estimate the pulse duration of the emission ranging from sub fs to a few fs, but varying from shot to shot. Similar to the experiment, our numerically generated output spectra show a stochastic line shift (see Fig. 3). Moreover, the total yield of emitted X-ray photons as a function of XFEL pump energy is well reproduced by our simulations, so that in general an excellent agreement between theory and experiment is reported.

Conclusion Stimulated X-ray processes are accessible with present-day XFEL sources, as demonstrated by our recent experiments, realizing the first gain-saturated atomic inner shell X-ray laser based on rapid photoionization of inner-shell electrons. The X-ray amplification scheme can be extended to molecules [8–10], as corroborated by our numerical results on X-ray amplification and stimulated Raman scattering in N_2 [9] and CO [10]. Combined with the transmitted XFEL pulse, the generated atomic or molecular X-ray laser emission results in a novel, discretely tunable two-color X-ray source, which can be used in two-color X-ray pump probe experiments. Moreover, new opportunities arise, to stimulate inelastic X-ray scattering processes, resulting in an enhancement of the spontaneous scattering signal by several orders of magnitude. The limited spectral coherence of the broadband SASE XFEL pulses can thereby be exploited to achieve high energy resolution of the scattering process, in a statistical sense. Employing statistical analysis, such as covariance mapping on an ensemble of single-shot spectra high-resolution two-dimensional scattering spectra can be obtained.

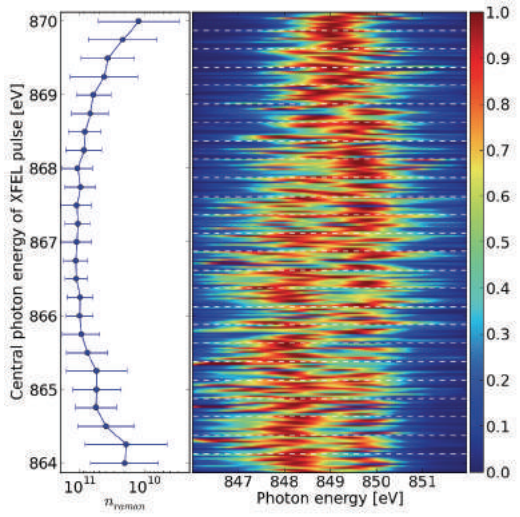

Figure 3: Theoretical Raman emission line shapes. Shown are the normalized Raman emission spectra as a function of central XFEL photon energy. For each of the 25 central photon energies (equally distributed between 864 eV and 870 eV, separated by the white dashed lines) 10 single-shot spectra are shown. The incoming SASE XFEL pulses are characterized by an averaged Gaussian spectrum of 6 eV bandwidth, a pulse duration of 40 fs and a pulse energy of 0.35 mJ. We assumed a propagation length of 10 mm and a gas density of 1.6×10^{19} atoms cm^{-3}. The left panel shows the geometric mean and standard deviation of the Raman signal strength (number of photons in the Raman line averaged over 100 SASE shots) as a function of central XFEL photon

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2.12 X-ray lasing in diatomic molecules

VICTOR KIMBERG AND NINA ROHRINGER

Since the invention of the first lasers in early 1960, a lot of efforts were made in order to achieve lasing of short wavelength VUV and soft X-ray transitions [1]. The main obstacles for lasing in that spectral range are the extremely short lifetimes of the electronic inner shell vacancies combined with relatively small transition dipoles of inner-shell transitions. To overcome this obstacle, the pump rate of the upper state must be higher than the Auger or fluorescence decay rate. For most cases in the soft X-ray range (100–1000 eV) this condition results in inverted pump rates on the femtosecond time scale. This pumping regime became possible with the recent invention of X-ray free-electron laser (XFEL) sources, which resulted in the first successful demonstration of an atomic inner-shell X-ray laser pumped by an XFEL [3]. Such a breakthrough in the field of X-ray quantum optics requires development of adequate theoretical tools for the prediction and analysis of the propagation and amplification of the short wavelength radiation. Special interest in that context is related to an accurate description of the interaction of X-rays and molecules taking into account the electronic and nuclear dynamics on the time scale of the ultrashort X-ray pulses (fs), which is the main goal of the present project.

The study of X-ray lasing in molecules is the first step towards development of advanced spectroscopic methods like stimulated resonant inelastic X-ray scattering (SRIXS). For realization of SRIXS schemes, two X-ray colors are necessary, separated by the typical excitation energies of the system of interest. Although schemes for seeded two-color XFEL sources in the hard X-ray regime have been proposed, the lack of a tunable two-color X-ray source with frequency separation beyond the SASE gain bandwidth seems to preclude SRIXS at present day XFELs. In that context, the molecular X-ray laser line combined with the tunable XFEL radiation results in a universal two-color X-ray radiation source. The amplified X-ray emission (AXE) from the molecules containing C, N, and O atoms is particularly important for studying organic molecules due to their typical atomic constituents. The element and site selective study of big molecules is possible in the X-ray range due to shifts of the atomic core-electron energies depending on the chemical surrounding.

Due to the additional nuclear degree of freedom, X-ray lasing in molecules offers new opportunities as compared to AXE in an atomic medium. The influence of vibrational dynamics on the X-ray amplification process is crucial: Depending on the nuclear dynamics, three different lasing scenarios can be discerned, as sketched in Fig. 1. The impinging XFEL pump beam prepares the molecules in an electronically core-excited state, either by resonant excitation or photoionization. This intermediary state is either a molecular bound state, or dissociative. In case of a dissociative core-excited state (a), radiative decay can either happen in the molecule (slowly dissociative state), or in the atom, if dissociation is fast in comparison to the lifetime of the upper state [2]. In the first case, a spectrally broad emission feature is expected. This is also expected in the case of a core-excited bound state coupled to a dissociative final state (b). In the present project, we study lasing between molecular bound states (c) and present calculations based on a generalized Maxwell-Bloch approach [4] in diatomic molecules. We treat both electronic and vibrational degrees of freedom, thereby revealing the importance of wave packet dynamics in stimulated X-ray processes.

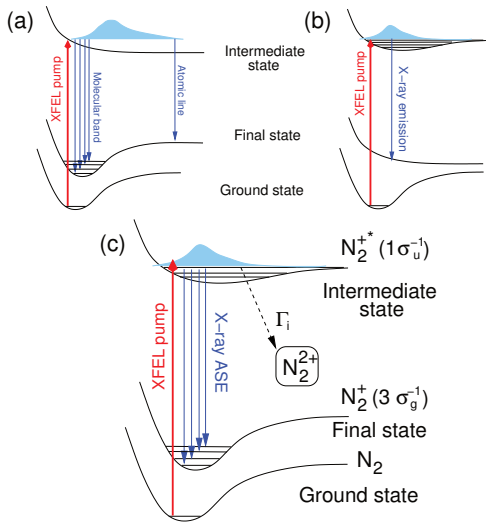

Figure 1: Lasing schemes in diatomic molecules. (a) Dissociative intermediate state: radiative decay in the molecule or in the atom, (b) dissociative final state, (c) bound-bound lasing. Here Γ_i is the Auger decay rate of the core-ionized state.

Let us discuss the dynamics of the AXE using N_2 as an example [4]. By tuning a focused XFEL beam above the K-edge of nitrogen (410 eV), a core-hole in N_2 is produced by K-shell ionization. This core-excited intermediate state has a short lifetime of ≈ 6.6 fs, dominated by the Auger decay. If core-ionization rates are comparable to the Auger rate, a sizeable population inversion in molecular nitrogen can be achieved. Despite the small fluorescence yield in nitrogen, spontaneously emitted X-ray photons can get exponentially amplified,

similarly to the atomic case [3]. The geometry of this single pass X-ray amplifier is determined by the focus properties of the pump source. A long (5-10 mm), narrow (1.5 μm) focus of the XFEL, creates an elongated plasma channel of core-inverted molecules. Fluorescence photons emitted at the entrance of the plasma channel stimulate radiative emission in direction of the propagating pump pulse and get exponentially amplified. Radiative decay of the core-ionized state proceeds mainly to the bound final states of the molecular ion (Fig. 1c). Since the transition to the lowest $3\sigma_g^{-1}$ state is the strongest, we restrict our analysis to the lasing on the $1\sigma_u^{-1} \rightarrow 3\sigma_g^{-1}$ transition ($\approx$ 395 eV), which shows the highest gain.

Our numerical results show, that X-ray lasing in diatomic molecules should be achievable at presently available XFEL sources. We assume a XFEL pulse duration of 50 fs, 3.6×10^{12} photons per pulse and a focus radius of 1.5 μm. Fig. 2a shows the average number of photons in the AXE pulse as a function of the propagation length, assuming a molecular density $N = 2.5 \times 10^{19}$ cm^{-3}. Before reaching saturation at a length of ≈ 2.5 mm, the number of photons in the AXE line grows exponentially with a gain of 72 cm^{-1}. At saturation, the rate of stimulated emission equals the Auger decay rate and the gain reduces, resulting in a bending of the gain curve. At the end of the medium, the AXE pulse contains $\approx 6 \times 10^9$ photons in the case of pre-aligned molecules with $\langle \cos^2 \theta \rangle = 0.8$. The corresponding conversion efficiency is $\approx 2 \times 10^{-3}$. The gain for an ensemble of unaligned molecules much lower (see dashed line in Fig. 2 (a)).Partial alignment of the molecular gain medium is therefore important to achieve gain saturation.

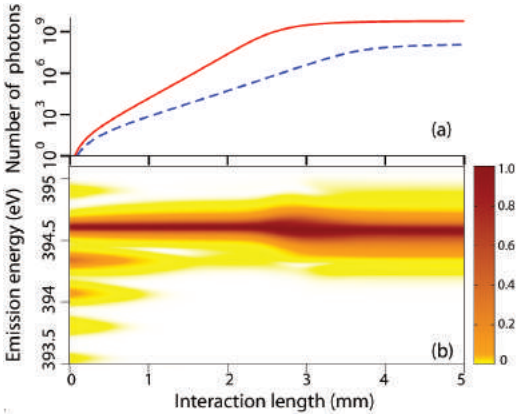

Figure 2: (a) Number of AXE photons for unaligned molecules (dashed line) and partially aligned ensemble (solid line). (b) Spectrum of the AXE pulse as a function of the interaction length z.

Fig. 2b shows the evolution of the emission spectrum as a function of the penetration depth. Below the onset of the linear gain region ($z \ll 1$ mm), the AXE spectrum consists of several emission lines of transitions between vibrational sublevels, similar to the X-ray fluorescence spectrum. In the linear gain region, a single transition energy picks up, suppressing the amplification of the other vibrational channels, so that at $z \approx 1.5$ mm, the spectrum transforms into a narrow line. The width of the line is determined by the natural lifetime broadening of the core-excited state Γ_i. At saturation ($z \gtrsim 2.5$ mm) the AXE line rebroadens (saturation broadening) and the line-shape is determined by non-linear effects. Deep in saturation ($z \gtrsim 4$ mm) the emission shifts towards lower energy and develops an asymmetric line-shape due to stimulated four-wave mixing of different vibrational transitions [4].

In general, the fluorescence spectrum depends on the nuclear wave packets of the ground and intermediate electronic states. Thus, by preparing the initial state in a specific vibrational state, for example by IR Raman excitation, the emission frequency of the AXE can be tuned within the fluorescence band. To demonstrate this effect, we run simulations for different vibrational initial states ($\nu_g = 0, 1, 2$). As it is shown in [4], the emitted AXE frequency coincides with the strongest peak of the fluorescence signal and can be fine-tuned by addressing specific vibrational levels. It is worth noting, that any initial vibrational wave packet which differs sufficiently from the vibrational ground state would result in a change of the AXE spectrum.

High AXE gain is also shown in the case of the CO molecule pumped at CK and OK edges [5]. We analyzed the dependence of the AXE intensity on the X-ray fluorescence spectrum, value and orientation of the electronic transition dipole moment, lifetime of the core-excited state and the duration of the pump pulse. Fine tunability of the molecular laser line in conjunction with the tunable XFEL radiation results in a universal two-color X-ray radiation source, enabling advanced all X-ray pump-probe experiments. The present scheme can be applied to other homo- and heteronuclear diatomic systems, thereby extending the spectral range of this molecular-based X-ray lasing scheme. Our theoretical predictions will be soon tested in an experiment at the FLASH XUV FEL in Hamburg [6].

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2.13 Collective Behaviors of Endosomes

JONATHAN DAWSON, LIONEL FORET, FRANK JÜLICHER

Ensodome networks are molecular transport and sorting systems Cells communicate with their environment by taking up and secreting many different types of molecules A fundamental problem in biology is to understand endosomal networks that organize the sorting and processing of molecules that enter the cell. Endosomal networks are not only cellular transport systems, but many signaling processes take place in endosomes. The endosomal network is therefore also an information processing system. Endosomes are small vesicular objects surrounded by a membrane that move and interact inside the cell. The function of endosomes in sorting and trafficking is governed by the dynamic assembly on the membrane of a multiprotein machinery organized by proteins of the Rab family. Early endosomes for example, in which cargo molecules enter after being internalized into a cell, are characterized by the protein Rab 5 [1, 2] Endosomes which possess the same protein coat can fuse with each other and thereby share the same pool of cargo molecules. The macroscopic kinetic properties, i.e., the properties of the endosomal network as a whole, result from the collective behaviors of many individual endosomes. To understand the collective behaviors of endosomes in a cell and the resulting transport properties of the endosomal network is a basic question that has remained largely undressed.

Individual endosomes move stochastically in the cell in a process mediated by molecular motors. When two endosomes meet, they can undergo fusion Endosomes may also emit smaller endosomes in a fission process. Furthermore, an endosome may leave the network by conversion to a different endosome type [1]. The collection of interacting endosomes therefore forms a distributed network in the cell in which cargo is sorted, transported and processes. Eventually, cargo leaves the network by the conversion of early endosomes to late endosomes or by recycling the cargo towards the cell membrane, Figure 1.

We have recently developed a general theory for the dynamics of cargo distributions in an endosomal network. We combined this theory with quantitative experiments to study how the macroscopic kinetic properties of the endosomal network emerge from microscopic processes at the level of individual endosomes. We compared our theory to experimental data in which dynamic distributions of endocytosed low-density lipoprotein (LDL) in endosomes were quantified. [4]

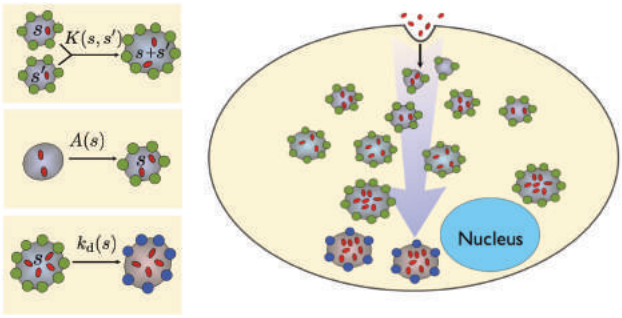

Figure 1: Schematic representation of endosomal processes (a-c) and endosomal trafficking (d). (a) Endosome fusion. (b) Formation of a cargo carrying early endosome. (c) Endosome conversion form early (green) to late (blue). (d) Cargo shown in red enters the cell via endocytosis and is distributed into a network of early endosomes (green). Cargo molecules can be recycled to the cell membrane or transferred to late endosomes (blue) from which they are transferred lysosomes for degradation.

Theory of cargo dynamics in endosome networks We denote by $n(s,t)ds$, the number of endosomes that carry an amount of cargo in the interval $[s, s+ds]$ at time t. The temporal evolution of $n(s)$ is described by [4]

$$\begin{aligned}\frac{\partial n(s,t)}{\partial t} &= \frac{K}{2}\int_0^s n(s')n(s-s')ds' \\ &- K\int_0^\infty n(s)n(s')ds' \\ &+ A(s) - k_{\rm d}n(s) \end{aligned} \quad (1)$$

Here, K is the fusion rate. A similar term accounting for fission has been omitted for simplicity. Endosome conversion to late endosomes is described by the rate $k_{\rm d}$. The generation of new cargo carrying endosomes occurs at a rate $A(s)$. The total cargo influx therefore is $J = \int_0^\infty sA(s)$Since cargo enters the network in small amounts, we choose a source function $A(s) = (J/s_0^2)e^{-s/s_0}$, where s_0 is a typical cargo amount. Note that the dynamic equation for endosome networks (1) is a generalisation of the Smoluchovsky equation for coagulation phenomena [3].

The equation (1) can be solved using Laplace transforms or by numerical methods [4]. Figure 2 shows the cargo distribution $n(s)$ at different times for a situation where at $t = 0$ no cargo is present, $n(s) = 0$ and the flux of cargo J is constant for $t > 0$.

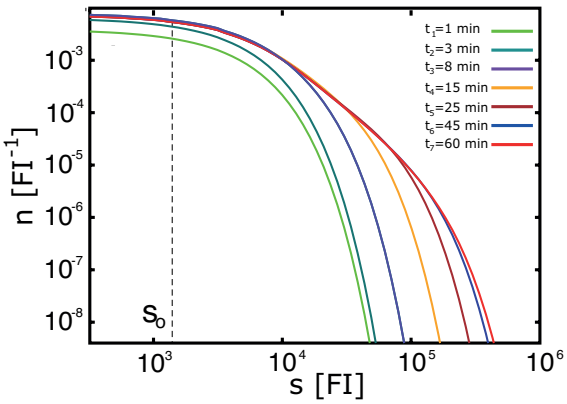

Figure 2: Cargo distribution for different times obtained as a solution of the kinetic equation (1). Times after cargo is added is given. At the initial time $t = 0$, the system contains no cargo $n(s, t = 0) = 0$. The endosomal network then fills up with cargo and eventually reaches a steady state.

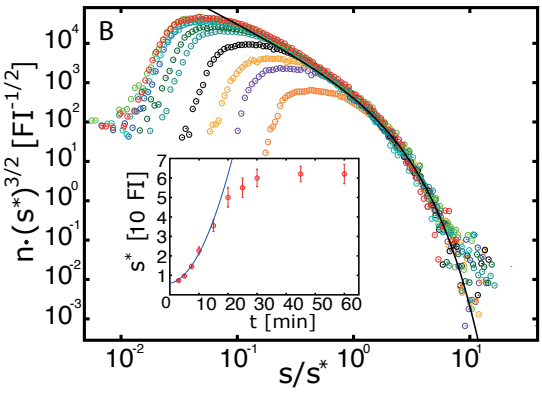

Figure 3: The density distribution $n(s)$ of Rab5-positive endosomes with total cargo intensity s quantified by automated image analysis at different times after addition of cargo. The characteristic cargo amount s^* is used for scaling of the axis, revealing collapse of the data for large s as predicted by the theory. The measured time dependence of s^* is shown in the inset.

At early times the cargo distribution $n(s)$ is narrow and peaked around s_0 with maximal value $n_{\max}$. This maximal value increases with time and saturates after a characteristic time $\tau = \left(JK/(2s_0)\right)^{-1/2}$, which depends on the rate of endosome fusion K and on the cargo influx J. Subsequently, endosome fusion leads to broadening of the distribution and the appearance of an increasingly large range of s in which the distribution follows a power-law decay $n(s) \sim s^{-3/2}$. This behaviour of the endosome network dynamics is well described for $s > s_0$ by

$$n(s) \simeq \left(\frac{J}{2\pi K}\right)^{1/2} s^{-3/2} \exp(-s/s^*(t)) \qquad (2)$$

where $s^*(t)$ is a time-dependent characteristic cargo amount. After a characteristic time k_{d}^{-1}, the distribution reaches the steady state profile of the form $n(s) \simeq s^{-3/2} e^{-s/s^*_\infty}$ with $s^*_\infty = 2JK/k_{\mathrm{d}}^2$ is the limit of $s^*(t)$ for large t. Note that this steady state profile and the time dependent profiles given by (2) are independent on the shape of the source function $A(s)$ for $s > s_0$.

Comparison of theory with experimental data Using quantitative image analysis of large numbers of fluorescence microscopy images at different times after addition of fluorescently labelled cargo to cultured cells, the time dependent cargo distributions $n(s, t)$ [4]. At each time point 1700 cells were imaged using automated microscopy.

The number of tracked endosomes containing LDL in each image (∼20 cells per image) ranged from about 50 (after 1 min of cargo uptake) to about 500 (60min cargo uptake). For each endosome, the total LDL fluorescence intensity was determined. Figure 3 shows the experimentally measured cargo distributions $n(s)$ at different times after addition of cargo. As predicted by our theory ((2)), this data collapses when plotted as $ns^{*3/2}$ versus $s/s*$, where $s^*(t)$ is the characteristic cargo amount in Eq. 2 shown in the inset. Our theory can quantitatively account for the full time-dependence of the cargo distribution over the time range of the experiment. Furthermore, we have used the theory to quantify changes of microscopic parameters that were influenced by specific genetic perturbations to the cells [4].

Conclusions Our theoretical framework predicts specific scaling properties of cargo distributions, which we confirmed in experiments in which endosomal parameters such as the number of endosomes and their cargo content were measured quantitatively. We could show that our approach is sensitive to weak perturbations and capable of quantifying changes of kinetic parameters. Because cargo distribution can vary in response to changes of the endocytic system, our analysis provides a powerful tool for the study of genetic and chemical perturbations that may alter parameters describing endosome kinetics. We could show that our theoretical framework can serve as a general tool for the quantitative analysis of intracellular transport between cellular compartments.

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2.14 Centering Microtubule Asters by Cortical Forces

NENAD PAVIN, RUI MA AND FRANK JÜLICHER

Role of pulling and pushing forces in cellular organization Microtubules play a key role in the spatial organization of cells and the positioning of organelles. Microtubules are stiff protein filaments that are highly dynamic and can reach over distances comparable to the cell size. The nucleation and growth of microtubules is coordinated by organizing centers such as centrosomes. As a result, microtubules in the cell form complex structures which include for example asters and spindles. Microtubules can exert forces on cell boundaries or on the cell nucleus. Such forces are particularly important for the positioning of microtubule organizing centers in the cell.

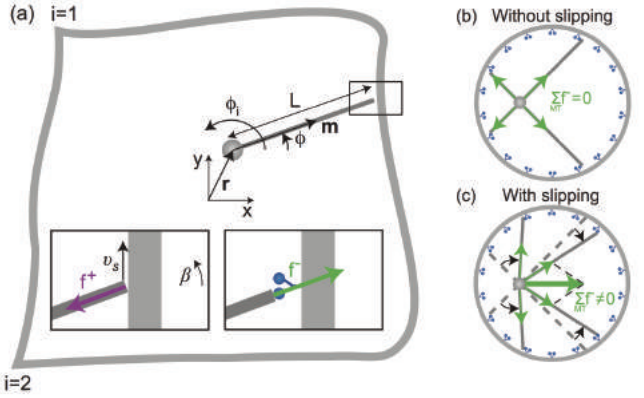

Figure 1: Schematic representation of microtubule asters in a confined two dimensional geometry. (a) General boundary shape with possible edges ($i = 1, 2$). The center is located to position $\mathbf{r}$. The microtubule orientation is denoted by $\mathbf{m}$, its length by L. Pushing forces of polymerising microtubules are denoted f^+, pulling forces mediated by motors are denoted f^-. The sliding velocity is v_s. (b) Pulling forces cancel for isotropically distributed microtubules in the absence of microtubule sliding. (c) If microtubules slide along the boundary, their orientation is modified and the distribution no longer isotropic. As a result a net pulling force is exerted on the organising centre.

Pushing forces on a cell boundary are generated by microtubule polymerization and growth and it has been proposed that pushing forces can ensure the positioning of asters at the cell center [1]. In addition to pushing forces, pulling forces can be generated at microtubule contacts with the cell boundary. Pulling forces have been implicated in processes in which the positioning of microtubule organizing centers in the cell is asymmetric [2]. Furthermore, they have been linked to the generation of spontaneous oscillations of the mitotic spindle during asymmetric cell division [3]. Such pulling force can be generated by the motor protein dynein.

We have studied the dynamics and mechanics of microtubule asters in different geometries to identify physical principles that govern aster positioning. We found that pulling forces play a key role for stable centering and they can lead to centering with higher reliability than pushing forces, contrary to what had been suggested previously [4,5].

Theory of microtubule mediated aster positioning We consider a microtubule aster, where microtubules are attached with one end at an organising center at position $\mathbf{r}$ in a two dimensional geometry, see Figure 1. We distinguish two populations of MTs that are in contact with a boundary such as the cell membrane: (i) growing microtubules that push on the boundary are distributed with angular density $n^+(\phi, t)$, (ii) shrinking microtubules that pull on the boundary with angular density $n^-(\phi, t)$. Here the angle ϕ describes the orientation of microtubules relative to the x-axis and t denotes time. These distributions obey the dynamic equations [4,5].

$$\frac{\partial n^+}{\partial t} = \frac{\nu}{2\pi} - k_{\rm cat} n^+ - k_{\rm b} n^+ - \frac{\partial}{\partial \phi} J_\phi, \qquad (1)$$

$$\frac{\partial n^-}{\partial t} = k_{\rm b} n^+ - k_{\rm off} n^-. \qquad (2)$$

Here, ν denotes the nucleation rate of microtubules, $k_{\rm cat}$ the catastrophe rate of pushing microtubules, $k_{\rm b}$ is the rate of MT binding to pulling motors and $k_{\rm off}$ is the detachment rate of pulling microtubules from motors. The flux of pushing microtubules along the boundary

$$J_\phi = v_\phi n^+ \qquad (3)$$

describes the microtubule reorientation due to slipping along the boundary at angular rate v_ϕ. In a situation where the aster position $\mathbf{r}$ is fixed, $v_\phi = (v_s/L)\cos\beta$, where $L(\mathbf{r}, \phi)$ is the distance between $\mathbf{r}$ and the microtubule contact with the boundary. The angle between the microtubule and the normal to the boundary is denoted β. The slipping velocity is $v_s = (f^+/\xi)\sin\beta$, where f^+ is the force exerted by a pushing MT on the boundary in the direction parallel to the MT, and ξ is the friction coefficient associated with slipping. The total force acting on the organizing center is given by $\mathbf{F} = \mathbf{F}^+ + \mathbf{F}^-$, where

$$\mathbf{F}^\pm = \mp \int_0^{2\pi} {\rm d}\phi n^\pm f^\pm \mathbf{m} \qquad (4)$$

is the net pushing and pulling force, respectively. Here $\mathbf{m}(\phi)$ denotes the unit vector in the direction of the microtubule at an angle ϕ, see Figure 1.

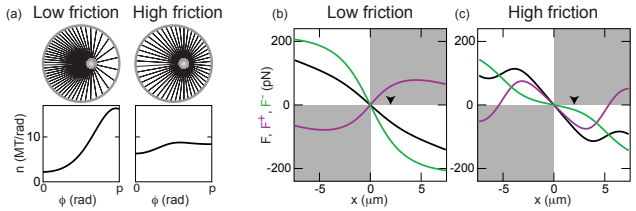

Figure 2: Net forces exerted on the center of an aster in circular geometry due to pushing and pulling of microtubules on the boundary. (a) Microtubule angular distributions in circular geometry for low friction (high slippage) and high friction (low slippage) for a displaced center position of the aster. (b) Pushing force (purple), pulling force (green) and total force (black) as a function of center position x for low friction. (c) Same plot for high friction.

Aster positioning in different geometries Solving the dynamic equations (1) and (2) for the angular microtubule distributions, we determine for given aster position $\mathbf{r}$ the net force $\mathbf{F}$ acting on the aster [4,5]. The force fields obtained include positions for which $\mathbf{F} = \mathbf{0}$ which correspond to stationary states. The stability of a stationary positions can be determined from the eigenvectors of the matrix $(1/2)(\partial_i F_j + \partial_j F_i)$ describing the effective centering stiffness, where $i, j = x, y$. Pulling and pushing forces play different roles in aster positioning. This can be illustrated most easily in a circular geometry. In the absence of microtubule slippage when the friction ξ is large and pulling forces are ineffective. In this case pushing forces can lead to stable centering. However, as slippage becomes more prominent (ξ small), pulling forces do lead to stable centering, while pushing forces in this case do not contribute to centering and reduce stability of the center position, see Figure 2 (a).

The centering effects of pulling forces can be understood as follows: in the absence of slippage, pulling forces cancel. However, after microtubules slip and reorient, pulling forces generate a net centering force, see Figure 2 (b) and (c). Pushing forces can mediate centering in the absence of slippage by their length distribution and by length dependent bucking. However as buckling occurs, the curved shape of microtubules leads to irregularities in the microtubule aster and centering becomes noisy and less reliable. In the presence of microtubule slippage, pushing forces can have a destabilising effect on centering. Therefore, pulling forces are perfectly suited for reliable and stable centering in two and three dimensions while pushing forces are less reliable [4]. In one-dimensional geometries, including very elongated systems, pulling forces are ineffective and centering only occurs mainly via pushing forces, see Figure 3.

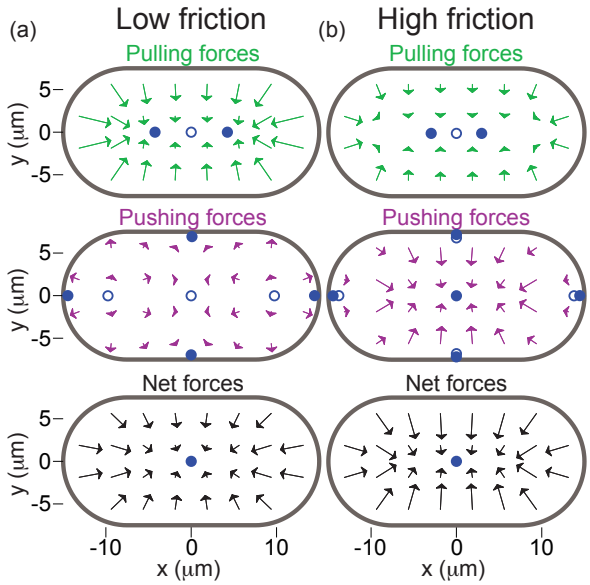

Figure 3: Force patterns as a function of the position x of the aster center in an elongated geometry. (a) Pulling forces, pushing forces and net forces for low boundary friction. (b) Same plot for high friction.

Microtubule slippage along the boundary can thus generate strong centering effects via pulling forces. For large sliding friction, slippage does not occur and only pushing forces contribute to centering. In a circular geometry, pulling forces induce stable and reliable centering while pushing forces tend to destabilise the centred position (see Figure 2). This is very different from a one-dimensional situation where pushing forces lead to stable centering. In our model we can move from a one-dimensional situation to the 2-d case by changing the aspect ratio of the geometry under study (Figure 3).

Comparison with experiments Our theory was tested by in vitro experiments in which artificially grown microtubule asters are moving in microfabricated chambers with walls coated by dynein motors [4]. These experiments demonstrated that in the absence of dynein motors centering occured in square geometries, albeit with some uncertainty because of microtubule buckling. In the presence of dyneins, centering was precise and reliable. This phenomenon which is explained by our work is expected to play a crucial role for the spatial organisation of the mitotic spindle during symmetric and asymmetric cell division.

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2.15 Shape oscillations of dividing cells

GUILLAUME SALBREUX

The actin cortex is a thin layer of actin filaments connected to the cell membrane and giving mechanical rigidity to the cell surface. Myosin molecular motors use the energy of ATP hydrolysis to generate stresses in the network of actin filaments, resulting in the establishment of a cell surface tension [1].

During cytokinesis, actin and myosin accumulate at the cell equator, resulting in the ingression of a furrow physically separating the cell into two daughter cells. A substantial actomyosin cortex however remains in the cell poles, outside of the equatorial ring. The dividing cell can therefore be roughly approximated by two spheres under tensions. This physical situation is reminiscent of two soap bubbles connected by a pipe, whose equilibrium position is an unstable one. This instability can be understood from the form of the law of Laplace, which states that the pressure inside a sphere under tension is inversely proportional to the radius of curvature of the sphere, $P = \frac{2T}{R}$. When one of the soap bubble decreases its volume, the radius R decreases, leading to an increase of the pressure favoring a further decrease of its volume. We were therefore wondering how the cell maintains a symmetric stable shape and whether cell shape symmetry could be spontaneously broken.

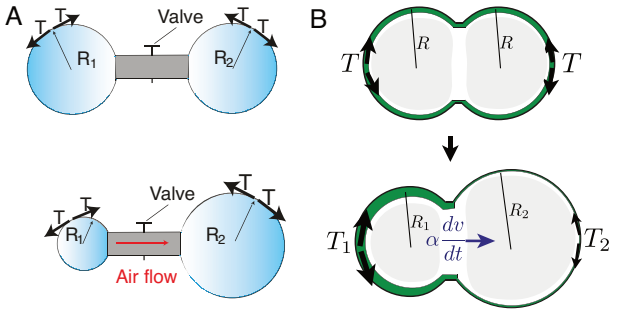

Figure 1: A. Schematic of an experiment demonstrating the instability of two soap bubbles connected by a pipe. B. Schematic of a mechanical model for a dividing cell.

Observations in the lab of E. Paluch of a large number of dividing Hela and L929 cells revealed that in about 20 % of the cells, cytoplasmic flows oscillating from one pole to the other could be detected. In about 2% of control cells and in a larger fraction of cells submitted to a treatment reinforcing the polar cortex, more dramatic cell shape oscillations could be observed, eventually resulting in division failure [2]. The two cell poles oscillate in phase opposition and the total cell volume appears to be conserved. Addition of a myosin-inhibiting drug stops the oscillations, indicating that forces generated in the cytoskeleton are involved in the process.

In addition, measurement of the fluorescence intensity of actin and myosin in the cortex shows that the actin density is also oscillating, with the density in one pole increasing when the pole is contracting (Fig. 2B, experimental data from E. Paluch lab). Actin and myosin were oscillating in phase and were proportional to each other during the oscillation.

These observations indicate that dividing cells can exhibit spontaneous symmetry-breaking instabilities but, contrary to soap bubbles, the instability results in shape and cortical oscillations. To understand this behavior, we have developed a minimal physical model of a dividing cell. The cell shape is represented by two portions of sphere with volumes V_1 and V_2 and radii of curvature R_1 and R_2 (Fig. 1B). Imbalance of pressure between the two halves result in a flow from one side to the other, such that the normalized difference of volume between the poles $v = \frac{V_1 - V_2}{V_1 + V_2}$ follows the mechanical equation

$$\alpha \frac{dv}{dt} = -\left[\frac{2T_1(c_1)}{R_1} - \frac{2T_2(c_2)}{R_2} + 2Kv + 2K_3 v^3\right] \quad (1)$$

where the term in brackets is the difference of pressure $P_1 - P_2$ between the two poles. α is a friction coefficient limiting volume exchange between the two halves of the cell. Permeation of cytosol through the poroelastic cytoplasm is a possible source of dissipation giving rise to this friction. Cortical tensions at the poles are denoted T_1 and T_2 and are functions of the myosin 2D densities c_1 and c_2. Because myosin is generating contractile stresses giving rise to cortical tension, we expect the cortical tension to be a monotonous function of the actomyosin density. The last two terms in Eq. 1 arise from bulk elasticity opposing cell deformation of the two future daughter cells. Such an elastic term could possibly arise from cytoskeletal and membrane structure with solid-like properties in the cytoplasm.

In addition, the actomyosin cortex is a dynamic structure turning over on a timescale of one minute [1]. We therefore postulated a simple equation for the evolution of the actomyosin density

$$\frac{dc_i}{dt} = \frac{1}{\tau}(c_0 - c_i) - \frac{c_i}{S_i}\frac{dS_i}{dt}\,, i = 1, 2 \quad (2)$$

where S_1 and S_2 are the surface area of the two cell poles. The first term in this equation corresponds to a first-order equation for binding and unbinding of actin to the cell surface, with binding rate $k_{on} = c_0/\tau$ and unbinding rate $k_{off} = 1/\tau$. The second term arises from matter conservation, as can simply be seen by taking the limit of no turnover, $\tau \to \infty$: Eq. 2 then reduces to

$\frac{d(c_i S_i)}{dt} = 0$, corresponding to conservation of the total amount of actin at each pole of the cell.

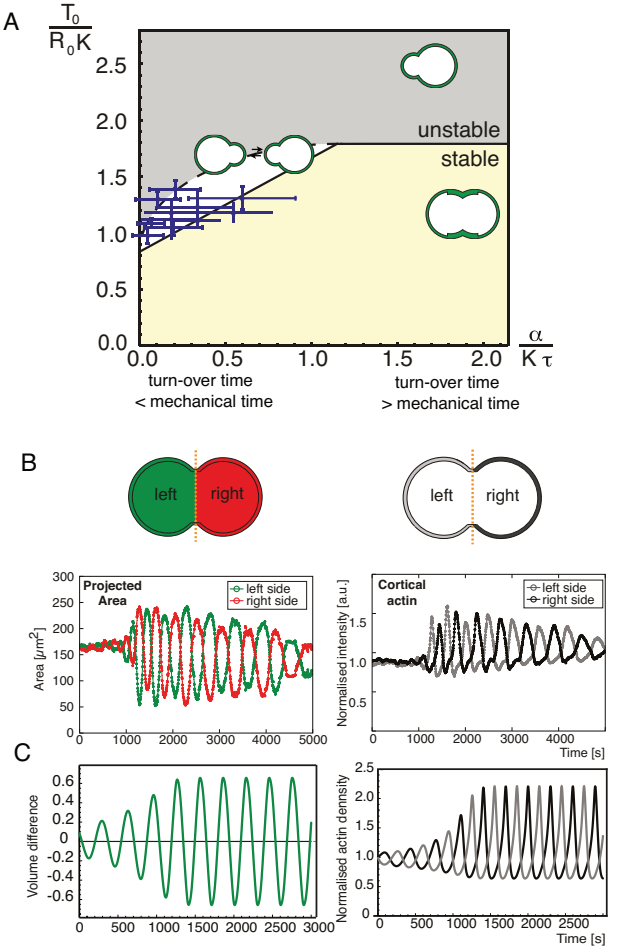

Figure 2: (A) Theoretical linear stability diagram of a symmetric cell. A Hopf bifurcation occurs from the yellow to white region, and a pitchfork bifurcation from the yellow to gray region. Blue crosses indicate cellular parameters extracted from a time series analysis of oscillating cells. (B) Experimental measurement of the projected left and right pole area (green and red curve), and left and right fluorescence intensity of cortical actin (gray and black curve) (C) Numerical solving of the driving equations 1 and 2 for parameters corresponding to the cell shown in B. The waveform and period of oscillations match experimental observations.

Eqs. (1) and (2) form a system of coupled equation for v, c_1 and c_2. A linear stability analysis of these equations shows that the symmetric steady state $v = 0$, $c_1 = c_2 = c_0$, with cortical tensions equal to $T_0 = T(c_0)$ and radii equal to R_0, becomes unstable for large enough values of the ratio of cortical tension to cell elasticity $\frac{T_0}{R_0 K}$. For small enough values of the ratio $\frac{\alpha}{K\tau}$, corresponding to slow actin turnover, the system undergoes a Hopf bifurcation (Fig. 2) and the model predicts that the cell starts to spontaneously oscillate. For fast turnover rate, the actin density is constant and a pitchfork bifurcation occurs for high value of the tension T_0, analogous to the soap bubble situation described above. The Hopf bifurcation occurs at smaller tension than the pitchfork bifurcation: indeed in addition to the destabilizing term in the law of Laplace previously mentioned, an additional instability occurs for slow turnover because a contraction of one pole leads to an accumulation of the actin density due to matter conservation and an increase in cortical tension, further driving contraction of the pole (Fig. 3).

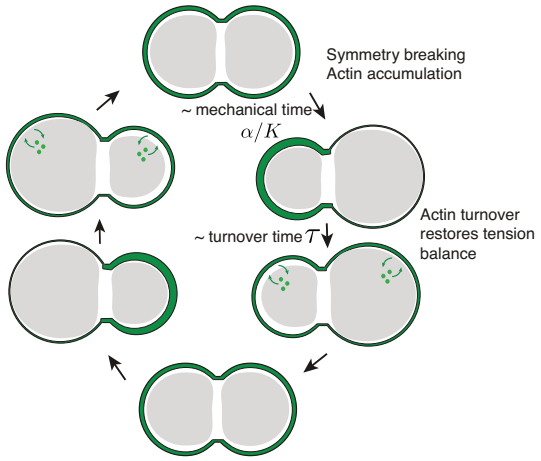

Figure 3: Schematic of the mechanism of cell shape oscillation.

To verify that cytokinetic oscillating cells are in the oscillating regime predicted by the theory, we have fitted the driving equations 1 and 2 to experimental measurements of cell shape and cortical density. Both driving equations could be fitted with good accuracy and the fitting procedure yielded values for the ratio T_0/R_0K and for the timescales $\alpha/K \simeq 30$s and $\tau \simeq 120$s, in accordance with measurements of turnover by FRAP experiments. This procedure allowed us to plot the cells in the theoretical phase diagram of Fig. 2A. Strikingly, all the studied cells fell in the unstable region of the diagram, near the Hopf bifurcation, showing that our analysis is self-consistent.

The oscillation mechanism we propose here is generic and could be relevant for other systems where cortical oscillations have been observed [3, 4]. The feedback loop generating the oscillation simply arises from matter conservation and a dependency of actomyosin tension on myosin density. Interestingly, the linear stability diagram in Fig. 2 indicates that cell elasticity is required to ensure the stability of the cell during cytokinesis, as the cell is always unstable for $\frac{T_0}{R_0 K} \to \infty$. It will therefore be interesting to further investigate the physical origin of cell elasticity during cytokinesis.

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2.16 Mechanism of actomyosin ring propulsion in zebrafish gastrulation

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How mechanical forces drive morphogenesis is a central question in developmental biology [1]. Quantitative descriptions are essential to understand how forces generated at the cytoskeleton level give rise to tissue-scale deformation. We have studied here the mechanics of epiboly, an event in the early development of the zebrafish where a superficial epithelial tissue, the enveloping layer (EVL), expands and spreads over the yolk of the embryo (Fig. 1). At the end of epiboly, the EVL completely engulfs the embryo and closes at the vegetal pole. Tissue spreading towards the vegetal pole is thought to be driven by an actomyosin structure located within the yolk cell and connected by tight junction to the EVL (Fig. 1). Intuitively, the actomyosin ring can possibly act through a purse-string mechanism, where actomyosin-generated tension favors contraction of the ring, leading to its motion to the vegetal pole due to the curvature of the embryo. A detailed analysis of the forces involved has however led us to propose a different physical picture.

Imaging of the actomyosin ring has revealed that the actin network does not appear significantly anisotropic and that a large region of the ring undergoes large retrograde flows, oriented towards the animal pole [2]. We have therefore developed a theoretical description of epiboly in which the EVL and actomyosin ring are modeled as layers of compressible viscous fluids under isotropic active internal tension (Fig. 1C). In such a description, the EVL and actin ring are described respectively by the following constitutive equations

$$t_{ij} = \eta_t \partial_k v_k \delta_{ij} + \eta_t^s [\partial_i v_j + \partial_j v_i - \partial_k v_k \delta_{ij}] + \zeta_t \delta_{ij} \quad (1)$$

$$t_{ij} = \eta_a \partial_k v_k \delta_{ij} + \eta_a^s [\partial_i v_j + \partial_j v_i - \partial_k v_k \delta_{ij}] + \zeta_a \delta_{ij} \quad (2)$$

where the tension in the material is the sum of a viscous tension proportional to the rate of deformation (with shear viscosities η_a^s and η_t^s and bulk viscosities η_a and η_s), and an internal isotropic tension proportional to ζ_a and ζ_s. The tension ζ_a is thought to arise from myosin molecular motors exerting forces in the actomyosin layer [3], while the tissue tension ζ_t could arise from cell interfacial tensions, cell elasticity or cell division and apoptosis [4]. In addition, we assume that polymerization and depolymerization of actin ensures that the actomyosin layer is undergoing fast turnover compared to the rate of flow [5]. This is consistent with the observation that a nearly uniform density of cortical actomyosin is maintained in the ring, despite the effect of material advection by the flow. Finally, we assume that the ring and EVL are mechanically connected at their interface.

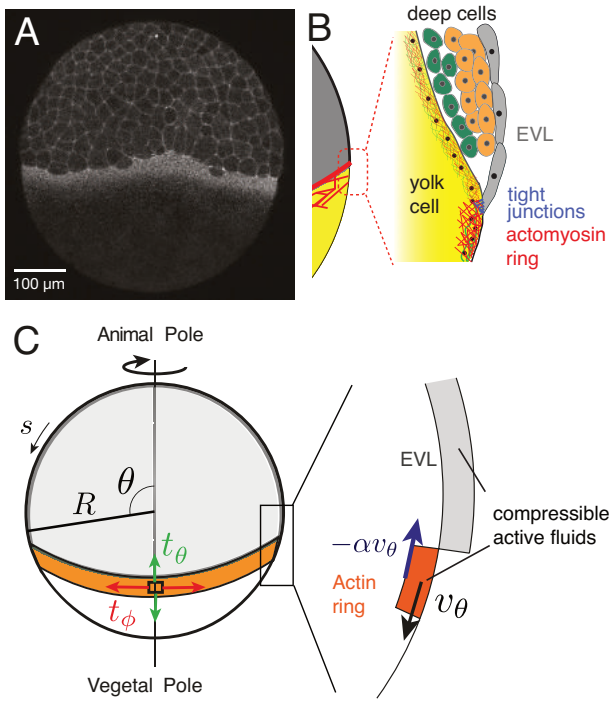

Figure 1: (A) Zebrafish embryo imaged at 60% epiboly. An actin ring forms at the margin of the enveloping layer epithelia (EVL), and drives the spreading motion of the EVL towards the vegetal pole. (B) Schematic of a cross section of the embryo. The actin ring is mechanically connected by tight junctions to the EVL through the membrane of the yolk cell. (C) Theoretical description of epiboly: the EVL and actin ring are represented by thin viscous layers of active fluid. The flow in the actin ring is resisted by friction against internal structures of the yolk.

We first computed theoretical flow profiles assuming that the EVL and actomyosin ring are flowing without friction. For sufficiently large active tension ratio ζ_a/ζ_t and provided that the EVL-actin margin is located sufficiently vegetally to the equator, flowing solutions can be found where the EVL expands vegetally, due to curvature of the embryo favoring contraction of the ring to the vegetal pole. The theoretical description also predicts that retrograde flow arise in the actin ring due to contractile tension exerted by myosin, as observed experimentally. One prediction of the zero-friction limit however contradicts experimental observations: because the ring has a free boundary and force balance imposes that the longitudinal tension t_θ is constant in the ring (up to a correction of order $\frac{h}{R} \ll 1$, with h the width of the ring), the viscous and active tensions have to balance each other in the longitudinal direction, resulting in a vanishing total longitudinal tension. Laser ablation experiments however led

to a significant recoil velocity along the animal-vegetal direction, suggesting that the total tension t_θ does not vanish in the ring (Fig. 3).

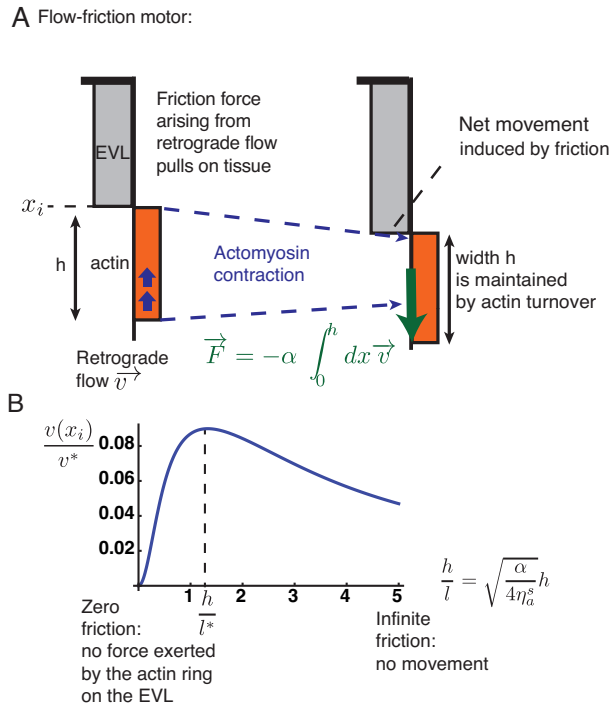

Figure 2: Flow-Friction motor. (A) Schematic for the flow-friction based motor: the actomyosin material contracts due to myosin active forces, giving rise to a retrograde flow. Its contraction is resisted by friction, resulting in a positive force on the EVL for sufficiently large retrograde flow $v_x < 0$. (B) Ring advancement velocity as a function of friction, with velocity normalized to a reference velocity $v^* = \frac{\zeta_a h}{\eta_a^s}$. For infinite friction, the ring can not move relative to the substrate. For zero friction, no resistance is exerted by the substrate and no movement is generated. For intermediate friction, a maximal velocity is reached.

We have therefore modified our initial description to include a possible role for friction acting on the actomyosin ring. Including this external force, the force balance in the ring reads

$$\partial_\theta t_\theta + \cot\theta(t_\theta - t_\phi) = \alpha R v_\theta \qquad (3)$$

with α a friction coefficient. A possible candidate giving rise to this friction is a network of microtubules spanning the surface of the yolk cell and presumably mechanically linked to the actomyosin layer [2]. The presence of non-zero friction gives rise to a qualitatively new picture of how the actomyosin ring can drive the motion of the EVL. Indeed, the retrograde flow generated by myosin contractility is resisted by an external friction force oriented opposite to the retrograde flow, towards the vegetal pole. Provided that actomyosin turnover maintains a constant width of the actomyosin ring in front of the EVL, a stationary pulling force is then generated on the EVL. Interestingly, a maximal velocity is reached for an intermediate value of friction (Fig. 2B). The mechanism can be compared to the motion of a caterpillar, which moves backward to generate forward motion (Fig. 2A). Importantly, the curvature of the embryo is not required for this process, consistent with observations that deformation of the embryo shape into a cylinder does not affect epiboly movements [2].

To further verify the validity of the proposed description, we have performed a fit of the theoretical expressions for the tensions and flow profiles in the EVL and actomyosin ring to the experimental flow profiles and relative total tensions in the ring obtained from laser ablation experiments, measured at 4 different stages of epiboly from 40% to 80%. Experimental data including both kinetic and mechanical properties can be accurately fitted with a small number of free parameters, over the whole course of epiboly (Fig. 3).

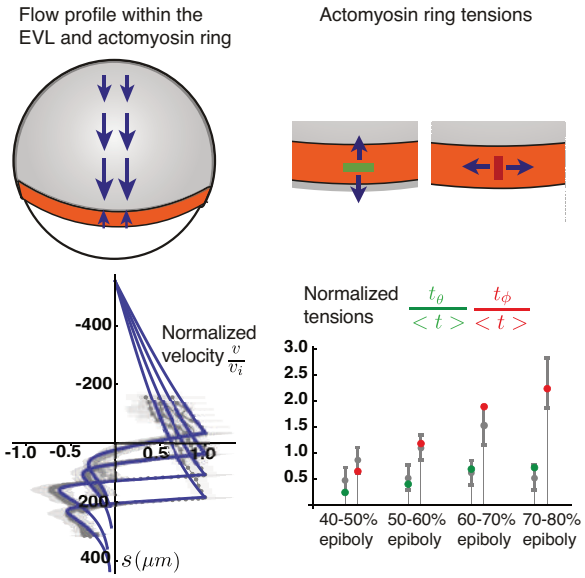

Figure 3: Global fit of the model predictions for flows (blue curves, left) and tensions (green and red dots, right) compared to the experimentally measured flow profiles and actomyosin ring relative tensions obtained from laser ablation (gray curves and dots in the respective panels), at successive epiboly stages.

The theoretical description we have developed therefore quantitatively accounts for a morphogenetic process at the scale of an entire embryo. By identifying the few key physical parameters invlved in the process, we were able to make theoretical predictions allowing to distinguish between two distinct driving mechanisms of zebrafish epiboly.

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2.17 Space-time velocity correlations in random walks

VASILY ZABURDAEV

Introduction The concept of the continuous time random walks is a powerful tool of statistical physics with applications truly breaking the borders across disciplines. It successfully describes diverse diffusion-like processes in physics, economics, biology and social sciences. Interestingly, a large part of those problems exhibits anomalous behavior [1, 2]. Regimes of diffusion are usually characterized by the scaling of the mean squared displacement of diffusing particles $\langle x^2 \rangle \propto t^\alpha$. Very long jumps of walkers lead to a faster superdiffusive behavior with $\alpha > 1$, whereas traps holding particles for a long time at the same point result in slower subdiffusion with $\alpha < 1$. By its nature a random walk belongs to the class of single-particle processes. Recently, however, it was shown that a model of superdiffusive random walks could successfully describe the energy perturbation spreading in complex, nonlinear many-particle systems [3]. In many-particle systems, other quantities can be used to characterize a transport process. One of them is the space-time velocity autocorrelation function which relates the velocities of particles at a certain distance in space and at different times. Since there was a clear benefit of applying a random walk approach to many-particle systems we tried to reverse this path and transfer the notion of such a correlation function to a single-particle random walk process. Note, however, that the standard temporal velocity autocorrelation function of a random walk cannot last longer than the time between two consecutive re-orientation events of a random walker.

We would like to find out whether more extended correlations can be detected by unfolding the velocity correlation function into the *spatial* domain. We define the space-time (*s-t*) velocity auto-correlation function for single-particle random walks and, for models yielding normal and superdiffusive dynamics, we show that this function helps to uncover long-lived velocity correlations that extend beyond the horizon dictated by the standard temporal correlation function. We argue that the process-specific generalized correlation function can be accessed experimentally.

Model and deifinition of the s-t velocity correlation function We consider a random walk performed by a particle moving ballistically with a fixed velocity v_i between two turning events. The duration of the i-th 'flight', τ_i, is governed by a probability density function (PDF) $\psi(\tau)$. At the end of each flight the particle changes its velocity to a new random value v_{i+1}, sampled from the PDF $h(v)$, and then starts a new flight. Two random variables, τ_i and v_i, are statistically independent but the spatial and temporal evolution of the walker during the flight is coupled, $x_{i+1} - x_i = v_i \tau_i$. This general setup is able to reproduce normal and anomalous diffusion by a proper choice of PDF's of flight-times and velocities [4]. There is a multitude of real-life systems and processes whose evolution can be described by this model. Examples range from the dynamics of tracers in turbulent flows and cold atoms in optical potentials to foraging animals and migrating T-cells.

The key property of this model is a well-defined velocity of a walker at any instant of time. This feature allows us to introduce a space-time velocity autocorrelation function for a walker's velocity by redefining the conventional expression

$$C(x,t) = \langle v(0,0) v(x,t) \rangle \,, \tag{1}$$

for a single-particle process. Namely, a particle starts its random walk with velocity $v_0 = v(x=0, t=0)$. After time t the particle is found at a point x with some velocity $v(x,t)$. Then the product of two velocities is averaged over all possible realizations of the random walk process and all possible initial velocities, v_0, sampled with $h(v_0)$. The definition can be rewritten in integral form,

$$C(x,t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} v v_0 P(v,x,t|v_0,0,0) h(v_0) dv_0 dv, \tag{2}$$

where $P(v,x,t|v_0,0,0)$ is the probability density function of finding a particle in (x,t) with velocity v, provided it has started with velocity v_0 at time $t=0$ and $x=0$. After integration with respect to x, Eqs. (1,2) yield the standard velocity auto-correlation function $C(t) = \langle v(0) v(t) \rangle$. Similarly to the derivation of transport equations for the PDF of particles' positions, we can derive and solve equations for $P(v,x,t|v_0,0,0)$ by applying the Fourier and Laplace transforms. After substituting it in the definition of the correlation function (2) we obtain the general answer for our problem [5].

Some results for normal and anomalous diffusion The general answer for $C(x,t)$ contains two terms. The first term describes the particles which are still in their very first flight. Their spatial density is represented by two ballistic delta peaks with a height decaying according to the survival probability $\Psi(t) = 1 - \int_0^t \psi(\tau) d\tau$. The second term represents particles which experience several collisions before the observation time and these particles can be found between the ballistic peaks. A universal feature of the central part described by the second term is that its integral with respect to x is equal to zero. Therefore only particles which are in the state

of their first flight contribute to the temporal correlation function.

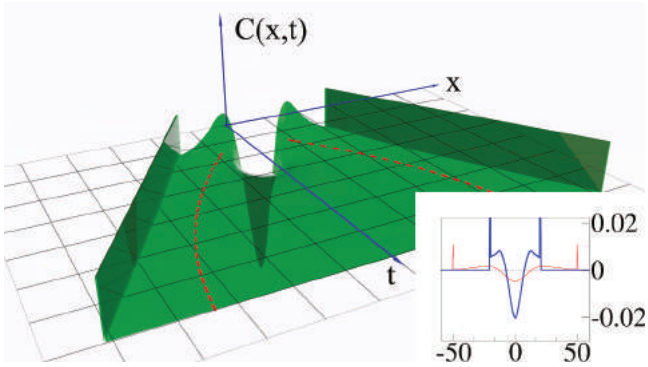

Figure 1: Space-time velocity auto-correlation function $C(x,t)$ for the superdiffusive Lévy walk, with $\gamma = 3/2$ as a function of x and t. The red dashed lines indicate the positions of local maxima $x_{\rm m}^{\pm}$ on the $x-t$ plane which follow the power-law scaling $x_{\rm m}^{\pm} \propto \pm t^{1/\gamma}$, while the height of the maxima decays as $t^{-1-1/\gamma}$. The inset depicts spatial profiles of $C(x,t)$ at two different instants of time, $t = 20$ (heavy blue line) and 50 (light red line).

We now assume that particles move with a fixed speed v_0 and the flight time is distributed according to a power law: $\psi(\tau) = \gamma/[\tau_0(1+\tau/\tau_0)^{1+\gamma}]$, where τ_0 sets the time-scale of the process (so-called Lévy walk model). When $\gamma > 2$, the mean square of the flight time is finite and inside of the casual cone, the density obeys the standard diffusion equation,

$$\frac{\partial P(x,t)}{\partial t} = D\triangle P(x,t); \quad D = \frac{v_0^2\tau_0}{\gamma-2}. \tag{3}$$

In this case, the corresponding central part of the correlation function reduces to a remarkably simple result:

$$C_{\rm centr}(x,t) = v_0^2\frac{D\tau_0}{\gamma-1}\triangle P(x,t) = v_0^2\frac{\tau_0}{\gamma-1}\frac{\partial P(x,t)}{\partial t}. \tag{4}$$

The above expression reveals an interesting relation between the PDF of the process and the corresponding *s-t* correlation function, namely that $C(x,t)$ is proportional to $\partial P(x,t)/\partial t$. The results presented by Eqs. (3, 4) are valid for an arbitrary choice of $\psi(t)$ that has a finite second moment, $\int_0^\infty \tau^2\psi(\tau)d\tau < \infty$, including the most generic form, an exponential function $\psi(\tau) = e^{-\tau/\tau_0}/\tau_0$. In this case $C(t) = v_0^2 e^{-t/\tau_0}$ while the space-time velocity correlations, for example, at the point $x = 0$ scale like $t^{-3/2}$. This example highlights the fact that the *s-t* velocity correlation function provides access to long-lived correlations and therefore increases the chance of their detection in experiments.

For $1 < \gamma < 2$ the mean squared flight-time diverges. It induces a superdiffusive behavior with the density of particles obeying a generalized diffusion equation,

$$\frac{\partial P(x,t)}{\partial t} = -K(-\triangle)^{\gamma/2}P(x,t), \tag{5}$$

where $K = \tau_0^{\gamma-1}v_0^\gamma(\gamma-1)\Gamma[1-\gamma]\cos(\pi\gamma/2)$ and $\triangle^{\gamma/2}$ is the fractional Laplacian operator. Note that this description is valid in the inner part of the casual cone only. In there $C(x,t)$ is proportional to the fractional Laplacian of the density of particles, or to the first time derivative of the density:

$$C_{\rm centr}(x,t) = \frac{v_0^2\tau_0}{\gamma-1}\frac{\partial P(x,t)}{\partial t}. \tag{6}$$

As in the case of normal diffusion, the velocity autocorrelations are negative near the point $x = 0$, see Fig.1. Upon departure from the origin the correlations become positive and produce two local maxima. As before, the integral of the central part of the *s-t* function with respect to x vanishes, and only ballistic peaks contribute to $C(t)$ in this case alike. The cases of even faster diffusion where the mean flight time diverges can also be considered and give rise to even slower decaying correlations [5].

Discussion In all considered regimes there is a region of negative correlations at the vicinity of the starting point of the random walk. This means that the majority of particles found there is flying in the direction opposite to that of their initial motion, which we call an *echo effect*. The shape of the echo region, the time-scaling of its width and height are model-specific characteristics. Remarkably, simulations of a stochastic process described by a system of Langevin equations show analogous results, which strongly suggests that our theoretical findings are applicable to generic stochastic transport phenomena with a finite velocity of moving particles. The spatiotemporal velocity autocorrelation function can be also generalized to the case of two-dimensional random walks, and thus provides another level-of-detail for the analysis of the transport phenomena from different areas of physics and real life.

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2.18 Intermittency model for $1/f$-noise

ELI BARKAI, MARKUS NIEMANN, HOLGER KANTZ

A signal is called $1/f$ noise [1,2], if its power spectrum $S(f)$ exhibits a power law at low frequencies,

$$S(f) \sim \frac{\text{constant}}{f^\gamma} \text{ where } 0 < \gamma < 2\,. \tag{1}$$

Starting with Bernamont [3] many models of these widely observed phenomena were put forward. Indeed, $1/f$ noise is practically universal, ranging from voltages and currents in vacuum tubes, diodes and transistors, to annual amounts of rainfall, to name only a few examples. A closer look at the phenomenon reveals several themes which demand further explanation.

• A $1/f$ type power spectrum is not integrable: $S_{tot} := \int_{-\infty}^{\infty} S(f)\,\mathrm{d}f = \infty$, due to the low frequency behavior, when $\gamma \geq 1$. This violates Parseval's theorem, which states that the total power in the frequency domain, i.e. S_{tot}, equals the power in the time domain, which is given by the time integral over the square of the signal. For finite time series length, the latter is always finite.

The standard explanation why nonetheless one finds $1/f$ noise in nature is that below some cutoff frequency f_0 the $1/f$ behaviour is replaced by some non-singular behaviour. Experimentalists have therefore carefully searched for this cutoff, increasing the measurement time as far as reasonable: three weeks for noise in MOSFET and 300 years for weather data. No cutoff frequency is observed even after these long measurement times. This is one of the outstanding features of $1/f$ noise.

• Mandelbrot [4] suggests that models of $1/f$ noise for $\gamma \geq 1$ should be related to non-stationarity processes, though the nature of this non-stationarity is still an open question [5,6].

• Experiments find that at least in some cases the amplitude of the power spectrum varies among identical systems measured at different times, but the shape and in particular the value of the exponent γ is quite consistent [1,2]. This means that a $1/f$ spectrum is a non self averaging observable, at least in some systems.

Recent measurements of blinking quantum dots, liquid crystals in the electrohydrodynamic convection regime and nanoscale electrodes shed new light on the nature of $1/f$ noise. These systems, while very different in their nature, reveal a *power law intermittency route* to $1/f$ noise. This means that power law waiting times in a micro-state of the system are responsible for the observed spectrum. This approach was suggested as a fundamental mechanism for $1/f$ noise in the context of intermittency of chaos and turbulence, with the work of Manneville [7].

Model. Motivated by the above, we consider a stochastic process $I(t)$ with only two states, $I(t) = I_0$ or $I(t) = -I_0$. The sojourn times τ in these states are independently identically distributed random variables with PDFs $\psi(\tau)$. Thus after waiting a random time in any state (called *epoch*), the particle chooses the next state to be *up* or *down* with equal probability. The waiting times PDFs have long tails $\psi(\tau) \propto \tau^{-(1+\alpha)}$ with $0 < \alpha < 1$, hence the averages of *up* and *down* times are infinite. This is a simple stochastic model of a blinking quantum dot. This model is known to exhibit weak ergodicity breaking [8,9], i.e., time averages do not converge to a single number but remain random variables even in the infinite time limit. The intuitive reason for that is that in every finite time signal, there is one epoch which is of the order of the total observation time, and the value $I(t)$ during this epoch influences the value of the time average.

Statement of the main results. For our model, we can compute all relevant features of the power spectrum [11] and thereby resolve all three issues raised in the introduction. For $\alpha < 1$ the expectation value of the spectrum is not constant, but decreases with measurement time $\langle S_t(\omega)\rangle \simeq t^{\alpha-1}\sigma_\alpha(\omega)$. Expanding the t-independent function $\sigma_\alpha(\omega)$ for small frequencies ω, one finds a typical non-integrable $1/f$-noise

$$\langle S_t(\omega)\rangle \simeq C\frac{t^{\alpha-1}}{\omega^{2-\alpha}}. \tag{2}$$

In general, the value $S_t(\omega)$ of the spectrum is a fluctuating quantity even in the $t \to \infty$ limit. The statistical behavior for large t (for pairwise disjoint $\omega_i \neq 0$) is fully described by the convergence in distribution of

$$\left(\frac{S_t(\omega_1)}{\langle S_t(\omega_1)\rangle}, \ldots, \frac{S_t(\omega_n)}{\langle S_t(\omega_n)\rangle}\right) \to Y_\alpha \cdot (\xi_1, \ldots, \xi_n), \tag{3}$$

where Y_α is a random variable of normalized Mittag-Leffler distribution with exponent α whose moments are $\langle Y_\alpha^n\rangle = n!\Gamma(1+\alpha)^n/\Gamma(1+n\alpha)$. The ξ_i are independent exponential random variables with unit mean. For $\alpha = 1$ the Mittag-Leffler random variable becomes $Y_1 = 1$, so that the powers $S_t(\omega_i)$ of different frequencies become independent exponentially distributed random variables - a result known for several ergodic random processes [10]. In the case of weak ergodicity breaking ($\alpha < 1$), the whole spectrum has a common random pre-factor Y_α which shifts the complete observed spectrum. However, being a common pre-factor, it does not affect the shape of the estimated spectrum so that fea-

tures as $1/f$-noise can be detected independently of the realization.

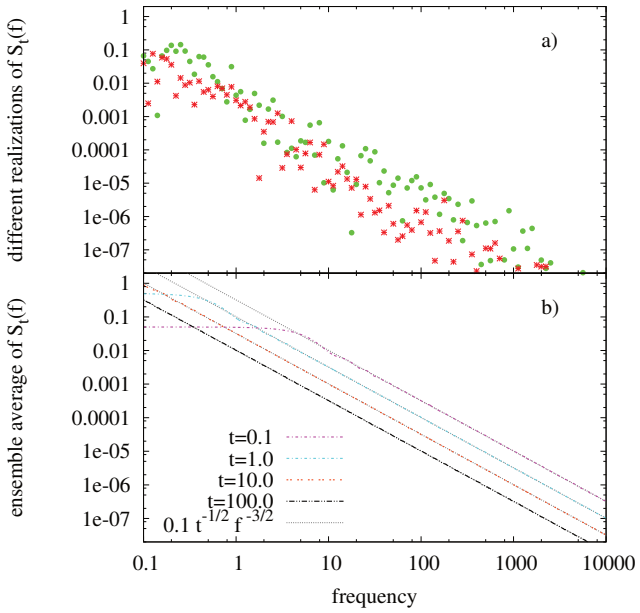

Figure 1: a) $S_t(f)$ plotted for two different realizations ($\alpha = 0.5$, $t = 10^2$). Inside each realization the fluctuations follow exponential distributions. Different realizations are shifted with respect to each other due the random pre-factor Y_α. b) Ensemble average of $S_t(f)$ plotted for different lengths t of the time series. One sees the decay of the spectrum $\langle S_t(f)\rangle \propto t^{-1/2} f^{-3/2}$ both in time and frequency. The crossover frequency is around $f_c \propto 1/t$. The simulations perfectly match the theory Eqs. (2,3).

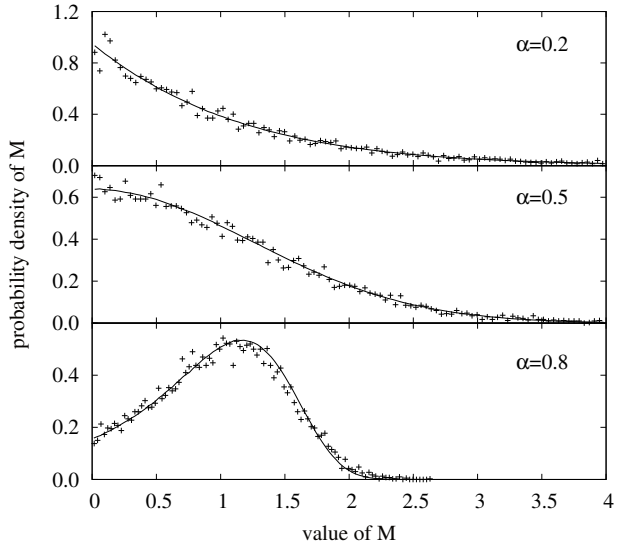

Figure 2: Distributions of the frequency averaged spectra representing Y_α in Eq.(3). The lines are the analytic probability densities of the Mittag-Leffler distributions ($t = 10^4$)

Numerical results. We simulated the two state model with $I_0 = 1$ for different time series lengths and different α. The waiting times were generated by using a uniformly distributed random number $0 < X \leq 1$ and setting $\tau = c_\alpha X^{-1/\alpha}$. The constant c_α was chosen such that $\langle n(1)\rangle \simeq 10\,000$. The ensemble consists of 10 000 realizations of the time series.

In Fig. 1a we show different realizations of $S_t(f)$. The stochastic fluctuations inside and between the realizations are clearly observable. In Fig. 1b the ensemble average of the power spectrum for different lengths is plotted. The $1/f$ spectrum and its decay with observation time is clearly visible. Note that at very low frequencies we find $S_t(\omega) \simeq \text{const}$ independent of frequency - an effect we explain below.

The histograms of estimates of the common pre-factor Y_α in Eq.(3) which should be Mittag-Leffler distributed are shown in Fig. 2. The good agreement with the theory is apparent.

Removing the non integrability paradox of $1/f$ noise. As mentioned in the introduction, the $1/\omega^{2-\alpha}$ noise is non integrable, $\int_0^\infty \langle S(\omega)\rangle \mathrm{d}\omega = \infty$, due to the low frequency behavior. This in turn violates the simple bound due to Parceval's theorem. To resolve this, notice that the random phase approximation employed to derive the results of Eq.(2) and Eq.(3) breaks down when $\omega = 0$. Hence the distribution of the power spectrum in Eq.(3) is not valid for $\omega = 0$ and this case must be treated separately. Indeed, we find [11] that $S_t(0)$ is determined by a random variable that diverges linearly in t with infinite observation time t. Hence, the spectrum at zero frequency does tend to infinity, but for any finite measurement time it is finite. So indeed *theoretically* there is a low-frequency cut-off of the divergence of the $1/f$ spectrum. We define the crossover frequency ω_c for the transition between the zero frequency limit and higher frequencies where the Mittag-Leffler statistics takes control, by merging the two behaviours. The result shows that the crossover frequency depends on the measurement time as $1/t$. Evidently, this is the only way how such a cross-over can take place in the absence of a characteristic time scale for dynamics: measurement time itself sets the time scale for crossover. Increasing measurement time merely stretches the domain of frequency where the $1/f$ noise is observed (see Fig.1b). Thus we conclude that the power spectrum is integrable as it should.

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2.19 A fluctuation relation for a deterministic hydrodynamical flow

JULIA GUNDERMANN, JOCHEN BRÖCKER, HOLGER KANTZ

Within the framework of stochastic thermodynamics, non-equilibrium fluctuations have been characterized by fluctuation relations, starting with the famous integral relation by Jarzynski [1]. A detailed version of this relation is given by Crooks [2]. By the change of some external control parameter, a thermodynamic system in equilibrium with a heat bath of inverse temperature $\beta = 1/(k_B T)$ in a macrostate A is brought into some other macroscopic state B at the same temperature. This non-equilibrium transition requires some mechanical work W. Its average exceeds the difference in free energy ΔF by the average amount of dissipated work. However, the precise amount of work needed in a single realisation of this process depends on the microstate in which the system is when starting the process. Repeating this many times, one finds a distribution for the work W. Then the probability $P_{A\to B}(W)$ that on the forward process an amount W of work is required is related to the probability that on the backward process the very same amount $-W$ of work will be released by Crooks' relation:

$$\frac{P_{A\to B}(W)}{P_{B\to A}(-W)} = e^{\beta(W-\Delta F)} \,. \qquad (1)$$

A typical example would be the isothermal compression of some gas.

We study here whether Crooks theorem is also valid for fluctuations in a dynamical system. Here, the fluctuations are dynamically generated and hence they persist even in the limit of infinite system size, where thermal fluctuations disappear.

We consider a two dimensional inviscid fluid, governed by the Euler equations, on a rectangular domain of size $L \times 1/L$. In terms of vorticity ω, its equation of motion reads

$$\partial_t \omega = \frac{1}{g}\left(-\partial_x\psi\partial_y\omega + \partial_y\psi\partial_x\omega\right), \qquad \Delta\psi = \omega. \qquad (2)$$

Here, ψ is the stream function, which gives the velocity as $v^i = g^{-1}(-\partial_y\psi, \partial_x\psi)$, $i = 1, 2$. This guarantees $\mathrm{div}(v) = g^{-1}\partial_i(gv^i) = 0$. Further, g is the Riemannian volume, and Δ is the Laplacian with respect to the Riemannian metric. The external control parameter to be varied is the edge length $L(t)$ of this domain, and our protocol is a deformation from a square into a rectangle. $L(t)$ enters the metric tensor in the equations of motion. For any fixed value of the control parameter, the energy and the enstrophy of the system are conserved. Under the change of this control parameter, the change of energy depends on details of the velocity field, even if the initial energy is the same, through

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\frac{\dot{L}}{L}\int \mathrm{d}x\mathrm{d}y \left(\frac{\partial_x^2\psi}{L^2} - \partial_y^2\psi L^2\right)\psi. \qquad (3)$$

To recall, the stream function ψ contains the full information of the velocity field.

We study this process numerically by solving Eq.(2) with time-dependent $L(t)$ with $L(0) = 1$ (macrostate A) and $L(t_{final}) = 1.5$ (macrostate B). We use a pseudospectral method with a truncated Fourier series of the vorticity with $N \times N$ complex Fourier amplitudes Ω_{kl}, for details see [3].

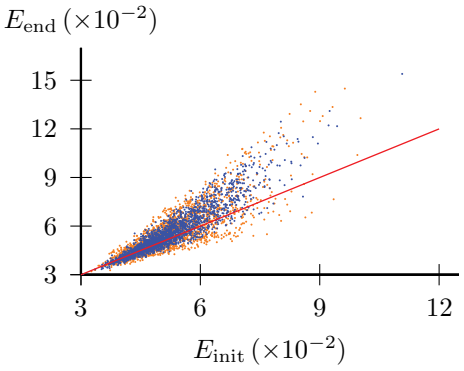

Figure 1: Scatterplot of each field's final energy over its initial energy (sample size: 2000) for a fast (orange) and a slow (blue) process. Fields are sampled from a canonical distribution with $\alpha = 3$, $\beta = -60$, The red line indicates equal initial and final energy.

Picking the initial conditions from a generalised canonical ensemble with Lagrangian multipliers α for enstrophy and β for energy [4] gives a very good description of the equilibrium state and furthermore allows us to introduce the inverse temperature β. Actually, realistic velocity fields are sampled for β being negative, which will be our choice here. However, the results do not depend on the sign of β. Nonetheless, this shows that the analogy to thermodynamics is a rather formal one. The final versus the initial energy of such an ensemble of simulations is shown in Fig.1 for two different speeds for the change of $L(t)$. As claimed, velocity fields with identical initial energy lead to a variety of different final energies. Secondly, this spread is the larger the faster the change of the control parameter is performed. This is in analogy to non-equilibrium thermodynamics: The faster the process, the more the system is driven out of equilibrium. To study Crooks' relation, the backward process has to be performed as well. For that, we initialize velocity fields from the canonical distribution of the macrostate B and then tune the control parameter $L(t)$ back to state A.

Typical distributions $P_{A\to B}(W)$ and $P_{B\to A}(-W)$ for two different values of β are shown in Fig.2. Different from similar studies for thermodynamic systems, we find highly non-Gaussian distributions. As Fig.2b shows, these distributions possess the property that $\log(P_{A\to B}(W)/P_{B\to A}(-W))$ lie on a straight line in agreement with Eq.(1). A quantitative verification of Crooks' theorem requires to define the difference in free energy between macrostates A and B. We do this in the natural way as

$$\Delta F = \frac{1}{\beta}\log\left(\frac{Z_A}{Z_B}\right) , \qquad (4)$$

where Z denotes the partition function associated with the Boltzmann distribution for inverse temperature β and the control parameter values $L(A)$ and $L(B)$. With the numerical values of ΔF and β, Eq.(1) has no free parameters any more. It is represented by the straight line in Fig.2b. Evidently, there is excellent agreement between Eq.(1) using these values, and the numerical data. The systematic deviations of the dots from the line for very small and very large values W is due to sampling errors of very low probabilities.

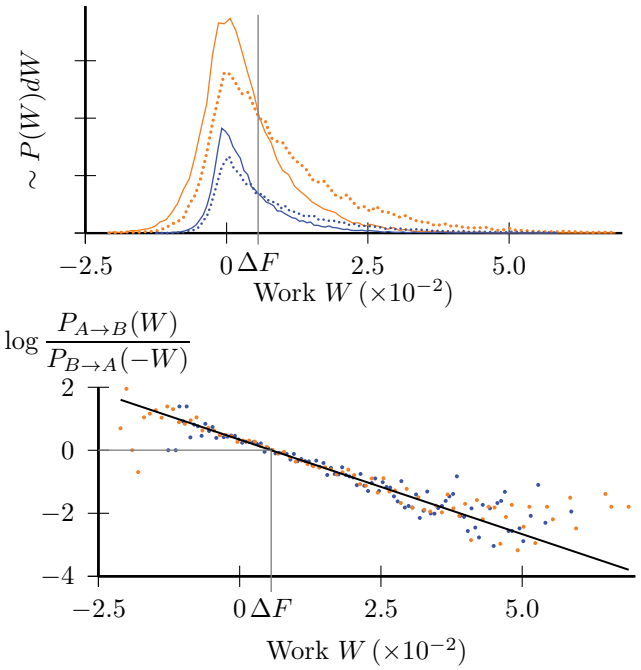

Figure 2: Crooks' relation for a double periodic domain with fields chosen from a canonical distribution. (a) upper panel: Work distributions obtain for the forward processes (solid lines) and the distributions $P_{B\to A}(-W)$ for the backward processes (dotted lines) (the ordinate has different scales for the blue and the orange distributions for better visibility). (b) lower panel: Ratio of the numerically sampled work distributions, plotted on a logarithmic scale (dots). Solid line: RHS of Eq.(1) for parameters as given above. Parameters: $\alpha = 3$, $\beta = -60$, blue = slow process, orange: fast process, $\Delta F = 5.6 \times 10^{-3}$.

Calculating the expectation value of the work distributions shown in Fig.2a, see Fig.3, one finds that it is actually *smaller* than ΔF (or resp. $\langle W\rangle \leq -\Delta F$ in the backward process), thus apparently violating the second law. The reason for this abnormal behavior is the negative temperature. In fact, using Crooks' relation and Jensen's inequality one gets $0 \leq \beta(\langle W\rangle - \Delta F)$ for any β. This gives $\langle W\rangle \geq \Delta F$ for positive temperature but $\langle W\rangle \leq \Delta F$ in our case. The difference is usually referred to as the dissipated work $W_{\rm diss} = W - \Delta F$. Figure 3 shows that the absolute value of the mean dissipated work decreases for slower processes. This supports the analogy to "ordinary" thermodynamic systems, where the mean dissipated work decreases when slowing down the protocol in order to reach the reversible limit $\langle W_{\rm diss}\rangle = 0$ for an infinitely slow process.

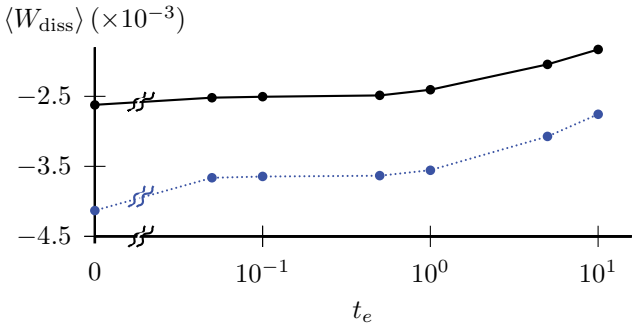

Figure 3: The average dissipated work in the forward (black) and backward (blue) process, versus the total time of the protocol t_{final}.

Relying on the quasi-Hamiltonian structure of the equations of motion and on specific conservation laws, we are indeed able to prove that Crooks' relation should hold [3]. Since the parameter change from A to B is done in finite time, energy is, as expected, dissipated. However, and this stresses again that the analogy to thermodynamics is purely formal, the dissipated work is negative, and there is neither dissipation nor a heat bath in these deterministic equations of motion.

In summary, we have verified that Crooks' theorem holds in a deterministic turbulent fluid on macroscopic length scales (i.e., outside the regime of nanosystems). This might be of high relevance for the estimation of probabilities of extreme events. An extreme event in this process would be the increase of the kinetic energy by some exceptionally large amount, which, in atmospheric physics, would be a storm caused by sheer imposed on some velocity field. Such a large gain of energy has a very low probability, too low to be estimated from a finite observation time series. However, since the decrease of the same amount of energy is much more probable, a statistical estimate of the latter together with the right hand side of Eq.(1) might yield the desired very low probability. Hence, we will explore whether Crooks' theorem might be a useful alternative to extreme value statistics.

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2.20 Stochastic processes leading to anomalous vocabulary growth

MARTIN GERLACH, EDUARDO G. ALTMANN

In this work we model the usage of language by stochastic processes. Our goal is to understand the sub-linear growth of the vocabulary with database size. We obtain generative models which not only account for empirical observations in large databases, but also yield (i) a mechanistic understanding of the origin of such a behaviour, and (ii) predict the size of the vocabulary of arbitrarily large databases.

Statistics of word usages share remarkable similarities with other social, physical, and biological systems, in particular the appearance of fat-tailed distributions. With the recent availability of large datasets in digital form (e.g. texts from the Internet) we are now able to quantitatively test theoretical models explaining these emergent phenomena. One practical problem is the estimation of the vocabulary growth, i.e. the dependence of the number of different words, N, on the size of the database (total number of words), M. The classical result for this relation is the empirical Heaps' law of anomalous (sub-linear) growth, which states that $N \sim M^{\lambda}$ with $\lambda \in [0, 1]$. Apart from an interest in fundamental properties of language, this problem is motivated by applications in search engines. We address it through two related but different stochastic models as described below. We compare their predictions with data from the google-ngram database [1], a collection of several millions of books published in the past 5 centuries.

Ensemble of Poisson Processes In the simplest approach we assume that the occurrence of each word is governed by an independent Poisson process with an intensity (rate) proportional to the frequency F of the word. Thus, the relationship between the ranked frequency distribution of all words, $F(r)$, and the expectation of $N(M)$, can be established as:

$$\mathbb{E}\left[N(M)\right] = \sum_{r} 1 - e^{-F(r)M}. \tag{1}$$

In Ref. [2] we have shown that the frequency of occurrence of a word with rank $r = 1, 2, \ldots$ can best be described by a double power-law (dp):

$$F_{\mathrm{dp}}(r; \gamma, b) \sim \begin{cases} r^{-1}, & r \leq b \\ r^{-\gamma} & r > b, \end{cases} \tag{2}$$

where the two free parameters γ and b hardly change with database and vary among different languages, e.g. in English $\gamma = 1.77$, and $b = 7873$. Introducing Eq. (2) into Eq. (1) we obtain for the expectation of $N(M)$:

$$N_{\mathrm{dp}}(M; \gamma, b) \sim \begin{cases} M, & M \ll M_b \\ M^{1/\gamma}, & M \gg M_b, \end{cases} \tag{3}$$

where M_b is the number of words such that $N(M_b) = b$.

In Fig. 1 we show that the google-ngram database obeys the scalings of Eq. (3) for different languages. The data of different years lie in a relatively narrow region of the plot which resembles a single curve compatible with the double scaling of Eq. (3). This curve is well described by the $N(M)$ curve obtained from the combination of the double power-law distribution (2) with fixed parameters (γ, b). On closer inspection, the fine details of the $N(M)$ curve are not compatible with the fluctuations expected from the strongly simplifying assumptions of Poisson usage of words. It is, nevertheless, remarkable that the agreement between the two-parameter model and the data remains within 50% for different databases and over 9 orders of magnitude in size. The fact that the same distribution (2) accounts not only for the observation across all years, but also among different languages, shows that the vocabulary rise is driven mainly by the database size and not by a historical variation in vocabulary richness.

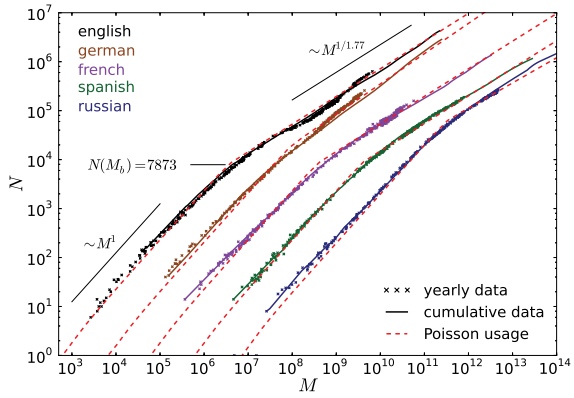

Figure 1: Vocabulary N as a function of database size M for yearly (x-symbols) database, cumulative (solid) database, and the ensemble of Poisson processes (dashed) assuming the rank-frequency distribution (2) with $b = 7873$ and $\gamma = 1.77$ for English. Other languages show the same scaling behaviour. In order to increase visibility, the curves for German, French, Spanish, and Russian were shifted, respectively, by one, two, three, and 4 decades with respect to their x-values

Yule-type Process In this section we propose a simple generative model which recovers and allows for an improved interpretation of the double scalings in our empirical findings – Eqs. (2) and (3). This approach goes beyond the ensemble of Poisson processes considered in the previous section, because it does not *a priori* assign fixed frequencies of occurrence to words. In line with the tradition of stochastic growth models explaining fat-tailed distributions, we consider an extension of

Yule's model [3] which contains two classes of word-types: a finite core vocabulary and an infinite noncore vocabulary. At each step a word (i.e. word-token) is drawn and attributed to one of the distinct words (i.e. word-type), see Fig. 2.

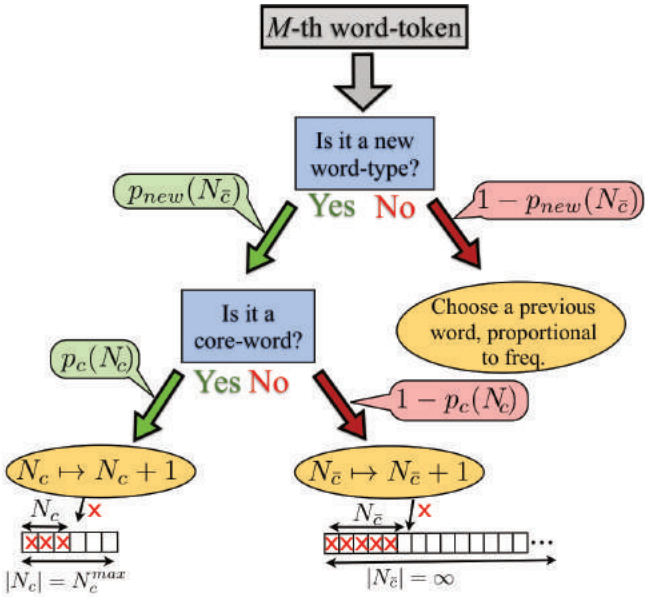

Figure 2: Illustration of our generative model for the usage of new words. At each step a word-token is drawn ($M \mapsto M+1$). The new word-token can either be a new word-type ($N \mapsto N+1$) with a probability $p_{\rm new}$ or an already existing word-type ($N \mapsto N$) with probability $1-p_{\rm new}$. In the latter case, a (previously used) word-type is attributed to the word-token at random with probability proportional to the number of times this word-type has occurred before. In the former case, the new word-type can either originate from a finite set of $N_c^{\max}$ core-words ($N_c \mapsto N_c+1$) with probability p_c or come from a potentially infinite set of noncore-words ($N_{\bar{c}} \mapsto N_{\bar{c}}+1$), where $N = N_c + N_{\bar{c}}$. We consider p_c to be a constant, i.e. $p_c^0 \lessapprox 1$, which becomes zero only if all core-words were drawn. Further we assume that $p_{\rm new} = p_{\rm new}(N_{\bar{c}})$ and propose as an update rule $p_{\rm new} \mapsto p_{\rm new}\,(1-\alpha/(N_{\bar{c}}+N_c^{\max}))$. The latter is a direct consequence of an unlimited non-core vocabulary [2].

We now show how the model in Fig. 2 recovers Eqs. (2) and (3). Notice that our model can be considered a biased random walk in N, which, as an approximation, can be mapped onto a binomial random walk by the coordinate transformation $N(M)$ such that $p_{\rm new}\,(N) = p_{\rm new}\,(N(M))$. The resulting Poisson-Binomial process can be treated analytically [2], e.g., the transformation $N(M)$ is then given by the average of the vocabulary growth:

$$\begin{aligned} N(M) &= \int_0^M \mathrm{d}M' p_{\rm new}\,(M') \\ &= \int_{N(0)}^{N(M)} \mathrm{d}N' \left|\frac{\mathrm{d}M'}{\mathrm{d}N'}\right| p_{\rm new}\,(N')\,. \end{aligned} \tag{4}$$

Considering the limiting cases $N \gg N_c^{\max}$ ($N \ll N_c^{\max}$), where $p_{\rm new} \sim N^{-\alpha}$ ($p_{\rm new} \approx$ const.), Eq. (3) yields a self-consistent solution, where the relation $\gamma = 1+\alpha$ is established. Furthermore, we identify the following relation between the parameters of our generative model and the fitting parameters of Eq. (2): $N_c^{\max} = b$ and $\alpha = \gamma - 1$, which can thus be interpreted as: b is the size of the core vocabulary and γ controls the sensitivity of the probability of using a new word to the number of already used words. Since the probability of usage for already used word-types is assumed to be proportional to the number of times it occurred before, we guarantee that Eq. (3) implies Eq. (2) [2, 3], meaning that the double scaling in the ranked frequency distribution $F(r)$ is also recovered from our generative model. Direct simulations of the model can reproduce the empirical results of the google-ngram data for the ranked frequency distribution $F(r)$ and the vocabulary growth $N(M)$ over the whole range of observation (more than 7 orders of magnitude) [2].

Conclusion We have shown that simple stochastic models are able to capture the details of empirical observations of word frequencies, in particular the double scaling in the anomalous vocabulary growth. From our proposed Yule-type process this vocabulary growth can be interpreted as a consequence of the existence of two classes of words: a finite core-vocabulary and a virtually infinite noncore-vocabulary. On the other hand, assuming Poisson usage of words with fixed frequencies, we are able to calculate the expected number of different words simply knowing the database size and using the two language dependent parameters in Eq. (2). This is crucial for search engines and data mining programs because it allows for an estimation of the memory to be allocated prior to the scanning of an unknown database. However, the simplifying assumption of Poisson usage typically underestimates the fluctuations around the expected number of different words. In future studies we, therefore, aim at including the effects of correlations [4] into the model.

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2.21 Monte Carlo sampling in open chaotic systems

JORGE C. LEITÃO, EDUARDO G. ALTMANN

We show that a suitably modified Monte Carlo method allows for an efficient sampling of chaotic dynamical systems. By combining an efficient random-walk with a Monte Carlo framework, we are able to unveil extremely fine fractal structures of complex systems. By extending the Wang-Landau algorithm [1] to this extreme case of rough landscape, we reduce the computational time scaling for sampling open chaotic systems from exponential to polynomial.

Introduction Monte Carlo methods arguably provide the most used framework for numerical and statistical investigations in Physics. The traditional field of application of Monte Carlo methods is many body systems (e.g., spin systems, proteins, and fluids). The computation of any macroscopic observable involves performing averages over all the degrees of freedom. The high dimensionality of many body systems makes it impossible to enumerate all states and leads to the failure of analytical methods in generic systems. In Monte Carlo methods, averages are estimated based on a finite sample generated by a random walk on the phase-space. The power of Monte Carlo methods comes from the ability to perform non-uniform sampling of the phase-space and re-weight accordingly using importance sampling techniques. A major development is the Wang-Landau algorithm [1], which allows to perform flat-histogram simulations without a priori knowledge of the sampling distribution. However, the applicability of this and any importance sampling method is ultimately dependent on an efficient random walk able to reach unlikely regions of the phase-space. This is only possible if the random walk is designed to take advantage of some characteristic property of the phase-space.

Another class of physical systems which are typically investigated through numerical and statistical methods are non-linear dynamical systems. This happens even in low-dimensional chaotic systems because of the exponential divergence of initial conditions. We focus on systems on which the chaotic regime occurs on finite time scales, as typically observed in open systems (e.g., scattering, fluid mechanics, chemical reactions) or in closed systems with leaks [2]. Transiently chaotic systems are characterized by invariant properties (e.g. Lyapunov exponents, escape rate κ) calculated on the set of trajectories which remain for a long time inside it. A typical picture of the complex dependence of the escape time t on the phase space coordinate is shown in Fig. 1. It exhibits a complex landscape with infinitely many fractally distributed singularities (initial conditions on the stable manifold of the chaotic saddle). The difficulty in performing an efficient sampling in such a phase space is twofold: (i) the distribution of escape times decays exponentially $\rho(t) \sim \exp(-\kappa t)$, being thus difficult to find the trajectories with large t; (ii) due to the fractality of singularities, there is no typical size σ which guarantees locality of the Monte Carlo random walk. We showed [2] that a modified version of the Wang-Landau algorithm which cures problem (ii) by exploring the order of the fractal landscape results in an efficient sampling method which avoids the exponential difficulty of problem (i).

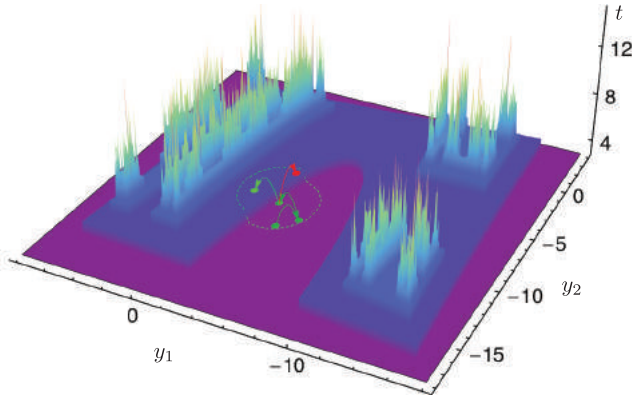

Figure 1: Fractal landscapes observed in transiently chaotic systems. The initial conditions with infinite escape time build an infinite, zero-measure, and non-integer dimension set. The circles and arrows illustrate our random walk, which consists of proposals (arrows) and acceptances (green)/refusals (red). This example corresponds to the escape time function of two of the four phase-space coordinates of 4-Dimensional coupled Hénon maps [3].

Our method uses an importance sampling technique based on the Metropolis-Hastings algorithm. The algorithm performs a random walk (a Markov process) on the phase-space Γ that asymptotically generate states from a distribution $P(\boldsymbol{r})$. The random walk starts from a random initial point $\boldsymbol{r} \in \Gamma$. From it, a state $\boldsymbol{r}' \in \Gamma$ is proposed from a conditional probability $g(\boldsymbol{r} \to \boldsymbol{r}')$ and it is accepted or rejected according to a conditional probability $A(\boldsymbol{r} \to \boldsymbol{r}')$. If the state is accepted, the random walk transits $\boldsymbol{r} \to \boldsymbol{r}'$. The efficiency of the random walk is controlled by $g(\boldsymbol{r} \to \boldsymbol{r}')$, and $P(\boldsymbol{r})$ is the sampling distribution (for importance sampling). In the Metropolis-Hastings, $A(\boldsymbol{r} \to \boldsymbol{r}')$ is uniquely defined by the choice of $g(\boldsymbol{r} \to \boldsymbol{r}')$ and $P(\boldsymbol{r})$ in such a way that the random-walk generates states according to $P(\boldsymbol{r})$. We first focus on the choice of $P(\boldsymbol{r})$. If the phase-space is uniformly sampled, $P(\boldsymbol{r}) = 1/V(\Gamma) = \text{const}$, the histogram of escape times is $\rho(t)$. We avoid this by choosing $P(\boldsymbol{r}) = 1/\rho(t(\boldsymbol{r}))$ (called flat-histogram), which implies a uniform histogram on the escape time variable. Since $\rho(t)$ is unknown but resembles a density of states

(now on the variable t instead of the traditional energy), we employ the Wang-Landau algorithm to compute it [1]. We now focus on the proposal distribution $g(\boldsymbol{r} \to \boldsymbol{r}')$. If the proposal is a uniform distribution, $g(\boldsymbol{r} \to \boldsymbol{r}') = 1/V(\Gamma)$, on average, the histogram of escape times of the proposed state $\boldsymbol{r}'$ is $\rho(t)$. This is undesirable since most states would end up being rejected. Our main result is that, in transient systems, we can also avoid this and propose a state $\boldsymbol{r}'$ with high locality, $|t(\boldsymbol{r}') - t(\boldsymbol{r})| \sim 1$. We have shown that this is the case only when the characteristic width σ of the proposal distribution $g(\boldsymbol{r} \to \boldsymbol{r}')$, centered at $\boldsymbol{r}$ (e.g. a Gaussian distribution centered at $\boldsymbol{r}$ width width σ) decays exponentially in t with the maximal Lyapunov exponent of the system λ_L [3],

$$\sigma(t) = e^{-\lambda_L t} \ . \tag{1}$$

This was shown through analytical calculations on the open tent map and through detailed simulations in a chain of coupled Hénon maps. The tent map was chosen because the escape time function $t(\boldsymbol{r})$ is the construction of the paradigmatic Cantor set. Our calculations resided on the fact that, at each t, the typical length scales with the Lyapunov exponent of the correspondent system. Our result was confirmed by Monte Carlo simulations in both the tent map and other systems with phase-spaces up to 30 dimensions. This result has a simple interpretation in light of exponential divergence of initial conditions. In order to provide $t(\boldsymbol{r}') \sim t(\boldsymbol{r})$, the states $\boldsymbol{r}$ and $\boldsymbol{r}'$ have to be exponentially closer according to Eq (1), as each iteration makes them diverge, on average, by λ_L. Like $\rho(t)$, $\sigma(t)$ is also generally unknown, but there is no way of obtaining it as the Wang-Landau was designed to compute density of states. We overcame this by generalizing the Wang-Landau algorithm to compute the proposal function [3].

The fundamental consequence of our result is that, because the steps are local on the variable t and the time-histogram is uniform, a random walk on the variable t behaves as a purely diffusive process. This means we are able to reach any t in polynomial time, with number of steps proportional to t^2. This should be compared with the required computational effort of a uniform sampling. We numerically compute the number of map iterations required to obtain an independent state with $t = t_{max}$, and see how this increases with t_{max}. Because each random walk step costs t map iterations to compute $t(\boldsymbol{r})$, our approach scales as t_{max}^3, while a uniform sampling scales exponentially, $\exp(\kappa t_{max})$. In Fig. 2 we confirm this dramatic improvement of our approach. It allows to reach increasing times in polynomial time, allowing to sample states with probabilities as low as 10^{-100}. Moreover, our approach is not restricted by the number of dimensions, as shown in the inset of Fig. 2. This outperforms other tools to study transiently chaotic systems, such as methods to compute the chaotic saddle, which so far were limited to 4 and, in some cases, 8 dimensional systems.

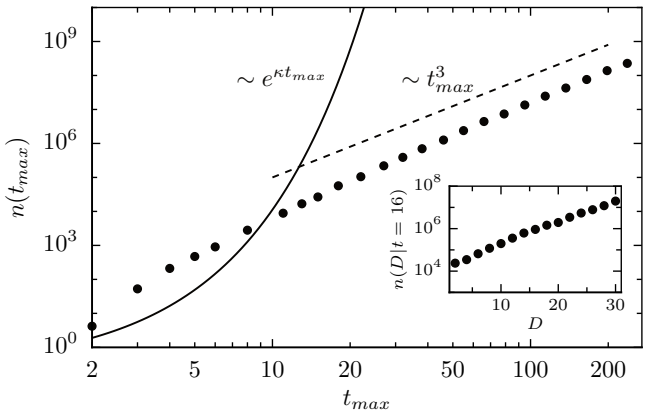

Figure 2: Power-law scaling of our approach in comparison to the exponential scaling of an uniform sampling. Log-Log plot of the number of map iterations n required to sample a state with $t = t_{max}$ as a function of maximum escape time t_{max} for a 4-dimensional coupled Hénon map [3]. A t_{max}^3 scaling is shown in dashed line and the exponential scaling of a uniform sampling in black line. Inset shows an exponential increase of n with D, measured for $t_{max} = 16$ in up to 30 dimensions.

In summary we applied a Monte Carlo method in transiently chaotic systems to obtain long-living trajectories and compute averages over the phase-space. We showed that a local random walk (in respect to the escape time) on the continuous phase-space is only obtained when the characteristic width of the random walk steps decays exponentially in time with the maximal Lyapunov exponent of the system. As a consequence, we avoid the exponential scaling and reach increasing escape times in polynomial time.

Future perspectives of this project include the extention of this Monte Carlo framework to study other chaotic systems. The intersection of both subjects comes from the exponential divergence of initial conditions, which imposes a statistical approach to study chaotic systems. Our perspectives include numerous problems in transient chaos, and possible non-hyperbolic, spatially extended, and other classes of chaotic systems.

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2.22 Disorder-driven non-Fermi liquid behavior and magnetism in Germanium-based filled skutterudites

S. KIRCHNER, M. NICKLAS, R. BORTH, R. GUMENIUK, W. SCHNELLE, H. ROSNER, A. LEITHE-JASPER, YU. GRIN, F. STEGLICH

Filled Skutterudites are materials of general composition MT_4X_{12} that condense in a cubic structure where M is a member of the alkaline, alkaline earth, lanthanide, or actinide series, T is an element of the iron group, *i.e. Fe*, *Ru*, or *Os* and *X* stands for either *P*, *As*, or *Sb*. The host T_4X_4 forms a rigid structure with two icosahedral voids per unit cell in which the filler or guest element *M* is located. These systems display a wide variety of possible ground states, including unconventional superconductivity, itinerant magnetism [1], non-Fermi liquid behavior, polar ordering and possibly even topological insulating states. The name for this material class derives from a village in Norway where minerals of this crystal structure where discovered. In recent years, filled skutterudites have also attracted interest as potential alternatives for the technologically important high-ZT materials lead telluride and bismuth telluride (ZT refers to the dimensionless thermoelectric figure of merit which characterizes the efficiency of thermoelectric heat engines).
Recently, germanium-based filled skutterudites, MPt_4Ge_{12} have were synthesized, where the cage is formed by Pt_4Ge_{12} and the filler atom is an element of the lanthanide, or actinide series [2, 3]. Possible ground states include superconductivity for *e.g. M=Sr,La,Pr,Th*, antiferromagnetism for *M=Nd, Eu* and heavy fermion behavior for *M=Sm* whereas $CePt_4Ge_{12}$ is weakly intermediate-valent *i.e.* close to Kondo lattice behavior, with a moderate mass enhancement of 2.6 and a coherence temperature of about 80K.

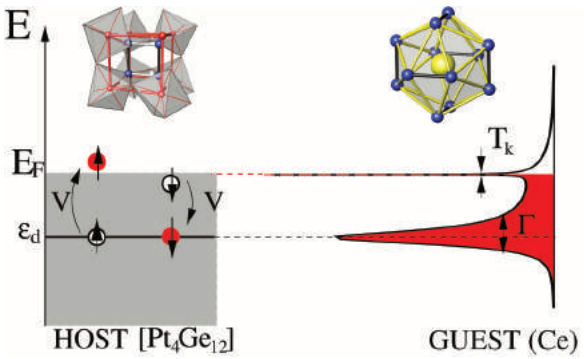

Figure 1: Local density of states (DOS) on the cerium ion (guest). For simplicity, the host DOS is assumed to be featureless. Detailed band structure calculations of the host DOS can be found in [4]. The Kondo exchange interaction J_K is proportional to $|V|^2$, where V is the hybridization determined by the wave function overlap between the cerium $4f$ orbital and the conduction electron wavefunction of the cage. J_K decreases when ϵ_d, the distance of the 4f state from the Fermi energy, increases. T_K is the Kondo temperature.

This raises the question if one can tune $CePt_4Ge_{12}$ from intermediate valence behavior into the local moment regime and induce magnetic order. A reduction in intermediate valency of Ce in $CePt_4Ge_{12}$ is equivalent to increasing the weight of the $4f^1$-state in the ground state and thus corresponds to an increase in the red area in the sketch shown in Fig. 1. Replacing a Ge atom by the much larger Sb atom reduces $|V|^2$. Sb substitution also provides an additional electron which results in an increase of $|\epsilon_d|$. Both effects reduce the Kondo exchange interaction and thus the Kondo temperature. As the Kondo temperature is reduced, the effective mass of the electrons due to electron-electron interaction increases. This is indeed observed in $CePt_4Ge_{12-x}Sb_x$ which shows an increase of the low-temperature limit of the specific heat over temperature (C/T) ratio as x increases as long as $x < 1.5$, see Fig. 2.

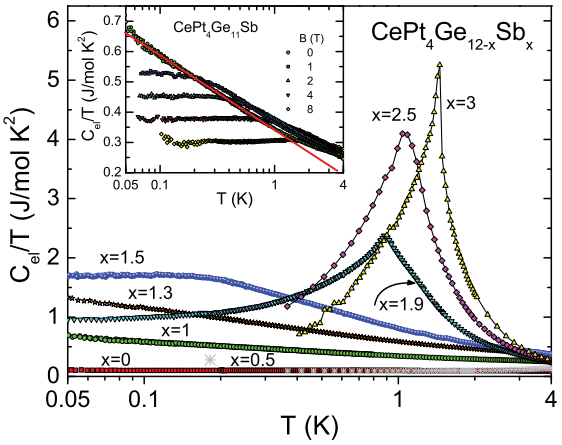

Figure 2: The low-temperature limit of $C_{\rm el}(T)/T$ increases with increasing antimony content for $x < 1.5$ signaling the increase in electron-electron interaction. For $x > 1.5$ a phase transition into a magnetically ordered state occurs. The magnetic entropy associated with the transition approaches Rln2 per *Ce* as x increases. The inset shows the logarithmically diverging $C_{\rm el}(T)/T$ found for $CePt_4Ge_{11}Sb$ and the crossover to Fermi liquid behavior in applied magnetic fields. (Figure taken from Ref. [4].)

The decrease in J_K weakens Kondo singlet formation and increases the tendency towards magnetism. As a result, $CePt_4Ge_{12-x}Sb_x$ orders magnetically for $x \geq 1.9$. This phase transition into an antiferromagnetic state is clearly visible in the specific heat data, see Fig. 2. The associated magnetic entropy and the size of the ordered moment are in line with local-moment magnetism. The Néel temperature, T_N, increases with increasing x and decreasing J_K. A pronounced maximum in the resistivity at temperature

T_{max} with $T_{max} > T_N$ is seen for $x \geq 1.5$. Both energy scales, $T_{max}(x)$ and $T_N(x)$, appear to extrapolate to zero within the region $1 \leq x < 1.5$. The specific heat coefficient of $CePt_4Ge_{11}Sb$ diverges logarithmically at lowest temperatures as

$$C_{\rm el}/T \sim \ln(T_0/T), \qquad (1)$$

as shown in the inset of Fig. 2 which points to a non-Fermi liquid ground state.

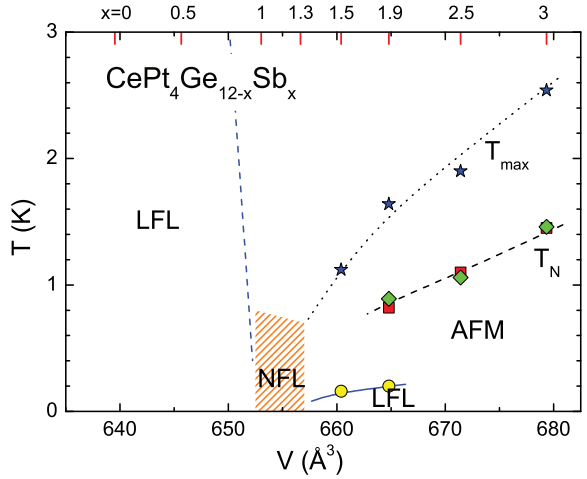

Figure 3: Antimony-doping of $CePt_4Ge_{12}$ tunes the system from intermediate-valence behavior through a disorder-driven non-Fermi liquid phase into a local moment magnet. LFL marks the Landau Fermi liquid phase, NFL is the non-Fermi liquid region. Below T_N, antiferromagnetism (AFM) is found. T_{max} marks the position of resistivity maximum.

At first glance, the overall phase diagram of $CePt_4Ge_{12-x}Sb_x$, shown in Fig. 3 thus resembles closely the phase diagram of quantum critical heavy fermion systems, where a paramagnetic Landau Fermi liquid undergoes a continuous zero-temperature phase transition into a magnetically ordered phase with Fermi liquid quasi-particles [5]. The absence of magnetic long-range order for $x = 1.5$, however, rules out such an interpretation. Understanding the phase diagram of $CePt_4Ge_{12-x}Sb_x$ requires the consideration of disorder effects. As the change in the hybridization is local, J_K will vary depending on the positions $\vec{y}$ of the *Sb* atoms, $J_K(\vec{y}) = \langle J_K \rangle + \delta J_K(\vec{y})$ resulting in a distribution of Kondo temperatures reflecting the disorder in J_K. A possible distribution is shown in Fig. 4, which can be approximated as

$$P[T_K] \approx A_0 + A_1 T_K + A_2 T_K^2 \text{ for } T_K < \Omega. \qquad (2)$$

For the disorder-averaged specific heat one therefore finds

$$\langle C_{el} \rangle = C_0 \int_T^\Omega dT_K \, P[T_K] \frac{T}{T_K} \sim A_0 C_0 T \ln(\Omega/T). \qquad (3)$$

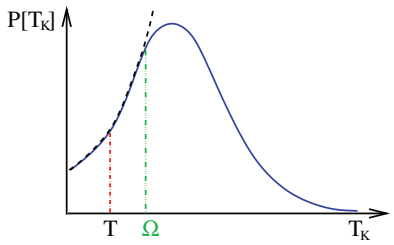

Figure 4: Possibe disorder distribution of the local Kondo scales in $CePt_4Ge_{12-x}Sb_x$: The Sb content leads to a position-dependent variation of the exchange interation between Ce-4f and itinerant electrons and a distribution of Kondo temperatures T_K. T marks the temperature of a measurement and Ω marks the scale at which the low-energy fit deviates from $P[T_K]$.

An analysis of the transport properties is more involved but it can be shown that the low-temperature resistivity ρ is $\rho(T) = \rho_0 - aT$, where ρ_0 is the residual resistivity and a is a positive prefactor [6, 7]. A magnetic field removes the A_0 term and therefore induces Fermi-liquid behavior, see Fig. 2, and a negative magnetoresistence [4]. The presence of Landau Fermi liquid behavior in $CePt_4Ge_{12-x}Sb_x$ for $x \geq 1.5$ and thus the absence of the A_0-term in $P[T_K]$ despite the x-dependence of $J_K(x)$ is therefore the result of an effective magnetic field due to short- or long-range order between the Ce-moments. The maximum in resistivity at T_{max} marks the decrease in electron scattering due to short-range order.

In conclusion, the antimony-doped germanium-based filled skutterudite $CePt_4Ge_{12-x}Sb_x$ has a unique phase diagram that connects intermediate-valence behavior with local moment magnetism and displays a Kondo-disorder driven non-Fermi liquid phase [4].

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2.23 Nonlinear thermoelectric transport through confined nanostructures

STEFAN KIRCHNER, ENRIQUE MUÑOZ AND FARZANEH ZAMANI

Non-linear transport through single-electron devices has recently attracted interest. At the linear-response level, strong electron-electron interaction in these confined nanostructures leads to enhanced conductance close to twice the quantum of conductance. This has been observed in semi-conductor heterostructures as well as in single-molecule devices. It therefore came as a surprise that the non-linear conductance did not display a similar degree of universality [1,2]. Transport studies in semi-conductor heterostructures resulted in $\alpha_G = 0.1$ and $\gamma_G = 0.5$ [1] whereas a similar experiment yielded $\alpha_S = 0.05$ and $\gamma_S = 0.1$ [2] for single-moelcule devices where the transport coefficients α and γ are defined through

$$\frac{G(T,0)-G(T,V)}{c_T 2e^2/h} = F(T/T_K, eV/k_BT_K) \quad (1)$$
$$\approx \alpha\left(\frac{eV}{kT_K}\right)^2 - c_T\gamma\left(\frac{T}{T_K}\right)^2\left(\frac{eV}{kT_K}\right)^2,$$

where $G(T,V)$ is the conductance at temperature T and applied bias voltage V and T_K is a dynamically generated low-energy scale and c_T is defined through $G(T,0)/G(0,0) = 1 - c_T(T/T_K)^2$ for $T \ll T_K$. A *standard model* for transport through confined nanostructures is

$$H = \sum_{k,\delta=L,R,\sigma} \epsilon_{k,\delta} c^\dagger_{k,\delta,\sigma} c_{k,\delta,\sigma} + H_{loc} + \sum_{k,\delta,\sigma} V_\delta c^\dagger_{k,\delta,\sigma} d_\sigma + \text{h.c},$$

where V_δ describes the coupling strength between lead $\delta = L, R$ and lead δ and $H_{\rm loc}$ is given by

$$\hat{H}_{loc} = U\left(\hat{d}^\dagger_\uparrow \hat{d}_\uparrow - \frac{1}{2}\right)\left(\hat{d}^\dagger_\downarrow \hat{d}_\downarrow - \frac{1}{2}\right) - \frac{U}{4} + \sum_\sigma E_d \hat{d}^\dagger_\sigma \hat{d}_\sigma.$$

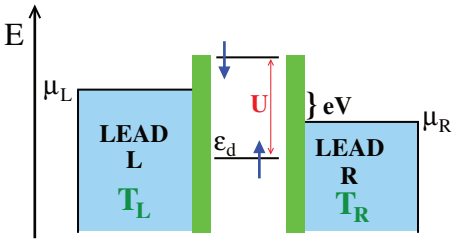

Figure 1: An interacting quantum dot with single-particle state at ϵ_d and intra-dot Coulomb repulsion of strength U attached to (non-interacting) metallic leads. The left/right lead is held at chemical potential μ_L/μ_R and temperature T_L/T_R. Here, $E_d = \epsilon_d + U/2$

Fig. 1 shows a sketch of the model. The applied bias voltage is given by the difference of chemical potentials, *i.e.* $eV = \mu_L - \mu_R$. For $E_d = 0$, *i.e.* at particle-hole symmetry, $\alpha \approx 0.15$ has been obtained independently of the amount of asymmetry in the lead-dot coupling between the two leads [3]. Experimental devices, however, usually lack particle-hole symmetry. A calculation of α and γ in a strongly interacting system away from particle-hole symmetry in a non-thermal steady state is difficult. In Ref. [7] we developed an expansion for $G(T,V)$ in E_d around the strong-coupling fixed point where the particle-hole symmetric system is solved using renormalized PT [4,5]. This is accomplished by adopting a functional integral description on the Keldysh contour,

$$Z = \int \mathcal{D}[\hat{\psi}^\dagger, \hat{\psi}]\mathcal{D}[\hat{\Phi}^\dagger, \hat{\Phi}] e^{iS[\hat{\psi}^\dagger,\hat{\psi},\hat{\Phi}^\dagger,\hat{\Phi}]} \quad (2)$$

where $\hat{\psi}^\dagger$ are Grassmann fields associated with the leads and $\hat{\Phi}^\dagger, \hat{\Phi}$ encodes the dynamics of the dot and Z is the generating functional on the Keldysh contour. The leads are non-interacting and can be integrated out. A fermionic Hubbard-Stratonovic decoupling allows a systematic expansion around the fully interacting $E_d = 0$ system in terms of dual fermions [6]. As the expansion builds on the reducible 4-point vertex of the refernce system ($E_d = 0$), Ward identities are ensured. An important consequence is that our approach is current-conserving. It has recently been generalized to finite magnetic field B and used to fit transport experiments [8].

At the equilibrium level, the method can be compared to numerical renormalization group calculations [9]. This is shown in Fig. 2, where a comparison between the two methods is made for c_B defined through

$$G(T=0,B)/G(0,0) = 1 - c_B\left(\frac{B}{T_K}\right)^2 \quad (B \ll T_K). \quad (3)$$

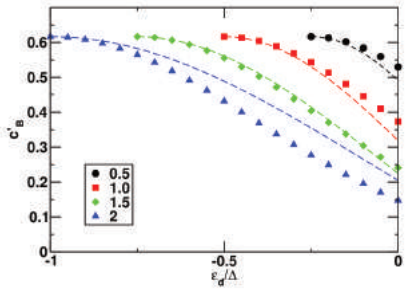

Figure 2: A comparision between renormalized dual fermion perturbation theory and numerical renormalization group for c_B vs. ϵ_d of the linear response conductance for several U. The points furthest to the left correspond to $E_d = 0$.(The figure is taken from [9].)

Details of the method and its generalization for the finite-field case can be found in Refs. [7,9].

Non-linear thermoelectric transport through confined nanostructures has not received much attention despite considerable current interest in nanopatterning as a way of increasing phonon-scattering and thus the thermoelectric figure of merit, $ZT \sim \sigma S^2/\kappa$, a dimensionless number characterizing the efficiency of thermoelectric heat engines. Here, σ is the electrical conductivity, S is the thermopower coefficient and κ is the thermal conductivity. ZT of a metal at low temperatures is small as S is related to a logarithmic derivative of σ with respect to energy and $\frac{\kappa_{el}}{T\sigma}\Big|_{T\to 0} = L_0$ according to the Wiedemann-Franz law (L_0 is the Lorenz number and κ_{el} the electronic contribution to κ). Results derived from the renormalized dual fermion PT for the linear-response thermopower is shown in Fig. 3(a), where an enhancement of $S_{\text{lin.res.}}$ is found away from $\tilde{u}$ due to the Kondo effect. Further results can be found in Ref. [10]. In the non-linear regime, *i.e.* beyond linear-response, the Wiedemann-Franz is not expected to hold and S may not be small [10]. Transport coefficients as *e.g.* κ, S etc. are defined at the linear response level through

$$\boldsymbol{I} = L_{11}\boldsymbol{\nabla} V + L_{12}\boldsymbol{\nabla} T \quad (4)$$

$$\boldsymbol{I}_Q = L_{21}\boldsymbol{\nabla} V + L_{22}\boldsymbol{\nabla} T, \quad (5)$$

where I is the charge and I_Q is the heat current and the coefficients are evaluated at vanishing gradients in V and T. Then, S is given by $S = L_{12}/L_{11}$ and $\kappa = L_{12}L_{21}/L_{11} - L_{22}$. A generalization to the non-linear regime requires knowledge of the entropy current J_S and the entropy production rate $\mathcal{P} > 0$ defined by

$$\frac{dS}{dt} + \nabla \cdot J_S = \mathcal{P}. \quad (6)$$

The method of Ref. [7] can be extended to the energy current J_E [10]. In addition, In steady state and for non-interacting leads, *i.e.* the situation sketched in Fig. 1, one can show that

$$\mathcal{P} = \frac{J_E}{T_L} - \frac{J_E}{T_R} - \frac{\mu_L}{T_L} I + \frac{\mu_R}{T_R} I, \quad (7)$$

which allows to generalize Eqs. 4, 5 to the non-linear regime [10, 11]. This allows to apply the renormalized dual fermion perturbation theory to the non-linear thermopower coefficient and to the Wiedemann-Franz ratio $L(T) = \frac{\kappa(T,V)}{TG(T,V)}$. The enhancement of the non-linear thermopower over its linear response result is shown in Fig. 3(b) and the Wiedemann-Franz ratio at $T = 0$ vs. bias volage is shown in Fig. 3(c) We thus find that a considerable enhancement of the figure of merit, ZT, at low temperatures and finite bias voltage is in principle possible. Details can be found in Refs. [10,11].

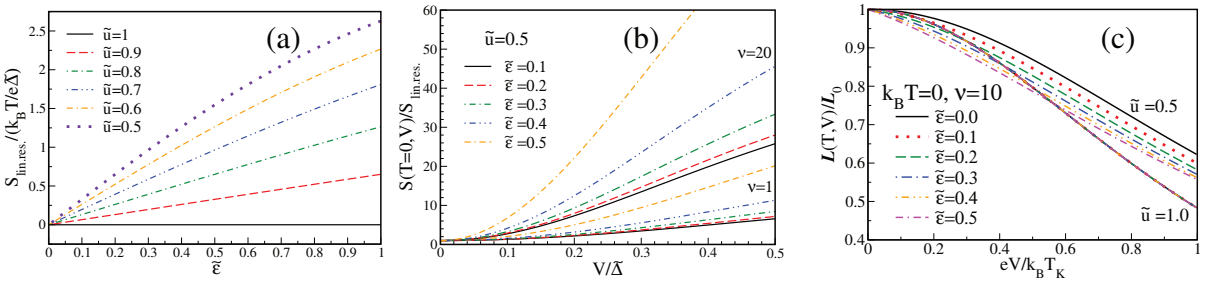

Figure 3: Renormalized dual fermion PT results from Refs. [10, 11]. For simplicity, we have set $\tilde{\epsilon} = E_d/T_K$; ν is the asymmetry of the lead-dot-coupling to left/right lead. (a) Thermopower at the linear response level vs. particle-hole asymmetry for various renormalized Coulomb interactions calculated with renormalized dual fermion PT. The thermopower vanishes in the particle-hole symmetric case *i.e.* at $\tilde{\epsilon}$ and at the strong-coupling fixed point $\tilde{u} = 1$. (b) Enhancement of the non-linear thermopower coefficient over the linear-response result vs. bias voltage. A huge enhancement is found. (c) The Wiedemann-Franz ratio $\kappa_{el}/(T\sigma)$ in units of L_0 vs. bias voltage at $T = 0$. The Wiedemann-Franz law is recovered at $V = 0$.

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2.24 Self-induced transparency in extreme intensity laser-plasma interaction

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Contemporary laser systems reach intensities high-enough ($I \gtrsim 10^{18}\,\mathrm{W\,cm^{-2}}$ for $1\,\mu\mathrm{m}$ wavelength) to accelerate electrons to relativistic velocities within a laser cycle. In this so-called *relativistic intensity regime*, the basic optical properties of a plasma are profoundly affected by nonlinearities in the corresponding laser-plasma interaction.

An ordinary laser pulse can propagate in a plasma if the electron density n_0 is lower than the critical density $n_c = \epsilon_0\, m_e\, \omega_L^2/e^2$, where m_e is the electron mass, $-e$ is the electron charge, and ϵ_0 is the permittivity of free space. For relativistically intense laser pulses, the electron mass has to be corrected by the relativistic factor $\gamma = \sqrt{1+\mathbf{p}^2/m_e^2c^2}$, where $\mathbf{p}$ is the electron momentum. For a plane wave, γ can be related to the normalized amplitude of the wave vector potential $a_0 = eA_0/(m_e c)$, $\gamma \simeq \sqrt{1+a_0^2/2}$. Therefore, one is forced to introduce an intensity dependent effective critical density [1]

$$n_c^{\mathrm{eff}} = \sqrt{1+\frac{a_0^2}{2}}\, n_c\,. \tag{1}$$

Thus, a relativistically intense laser pulse can propagate in a nominally overdense plasma, a phenomenon known as *relativistic self-induced transparency* (RSIT). Apart from its role as a fundamental process in laser-plasma interaction, RSIT is also of interest in applications. In the context of ion acceleration, for instance, RSIT can prevent efficient radiation-pressure-acceleration.

In writting Eq. (1) one assumes linear response of an infinite, homogeneous plasma to an infinite plane wave. Therefore, this simple relation is no longer valid for typical experimental settings in which the pulse is incident on a steep vaccuum-plasma interface. To overcome this difficulty, a theory which treats the plasma as a cold fluid with a sharp interface with vacuum has been developed [2–4]. For circularly polarized (CP) pulses, normal incidence, and immobile ions, stationary solutions which correspond to total reflection (standing wave formation) at the plasma boundary have been predicted to exist above a certain threshold density $n_{\mathrm{th}}(a_0)$, see Fig. 1(b). These solutions express the balance of radiation pressure and electrostatic force (due to charge seperation) on electrons at the plasma boundary. Typically, the density at the plasma boundary becomes much higher than n_c^{eff} and pulse propagation is inhibited for $n_0 > n_{\mathrm{th}}(a_0)$.

Although this level of description of a plasma as a cold fluid has been shown to capture the essential phenomenology in some cases [3, 5], its assumptions can still break down if the laser-plasma interaction triggers kinetic effects, such as electron heating. As we have shown [6], such effects can lead to pulse propagation by disturbing the equilibrium of ponderomotive and electrostatic forces at the edge of the plasma. In order to understand this point we study the dynamics of electrons in the fields predicted by the cold-fluid model.

The equations of motion for an electron in the region $x \le x_b$, in the case of full reflection, can be derived from the Hamiltonian $H(x,p_x) = \gamma(x,p_x) - \phi(x)$, where the electron γ factor reads $\gamma = \sqrt{1+a^2(x)+p_x^2}$, p_x is the electron's longitudinal momentum, and the electrostatic $\phi(x)$ and vector potential $a(x)$ can be calculated by matching boundary conditions for the standing wave and evanescent fields at the plasma-vacuum interface [3, 4, 6]. Then, using conservation of $H(x,p_x)$, we can plot portraits of the single-electron phase space, as in Fig. 1(d).

Of greatest importance in the following are the separatrices labeled Γ and Δ, as they determine the region within which motion close to the equilibrium point $\mathrm{Q}_b \equiv (x_b, 0)$ is oscillatory. The point on separatrix Γ at position x_b (at the plasma boundary) defines a momentum $p_x^{\mathrm{cr}} \equiv p_x(x_b)$, which can be calculated explicitly [6]. If a test electron at the edge of the CEL, x_b, is given an initial momentum $-|\Delta p_x|$, with $|\Delta p_x| < |p_x^{\mathrm{cr}}|$, it will move within the limits set by separatrices Γ and Δ, returning back to the plasma. If on the other hand $|\Delta p_x| > |p_x^{\mathrm{cr}}|$, the electron's motion will be unbounded and it will escape to the vacuum. It can be shown that $|p_x^{\mathrm{cr}}| \to 0$ as $n_0 \to n_{\mathrm{th}}$, for a fixed a_0.

It thus becomes clear that finite perturbations of initial conditions of electrons at the edge of the plasma, for example due to heating, could lead to electrons escaping towards the vacuum, even though the equilibrium $\mathrm{Q}_b \equiv (x_b, 0)$ is stable in the linear approximation.

To verify the importance of such kinetic effects on the threshold between total reflection and RSIT, we perform Particle-In-Cell (PIC) simulations using the one-dimensional in space, three-dimensional in velocity (1D3V) code SQUASH. The plasma extents from $x = 0$ to $x = L_p$, with a step-like density profile of constant density n_0 and temperature $T_0 \simeq 5 \cdot 10^{-4}$ (in units of $m_e c^2$). The circularly polarized laser pulse is incident from $x < 0$ onto the plasma. The laser pulse profile is trapezoidal, i.e. the intensity increases linearly within a rising time τ_r, up to a maximum value $a_0^2/2$. The numerically determined threshold for RSIT is shown in Fig. 1(a) for different τ_r.

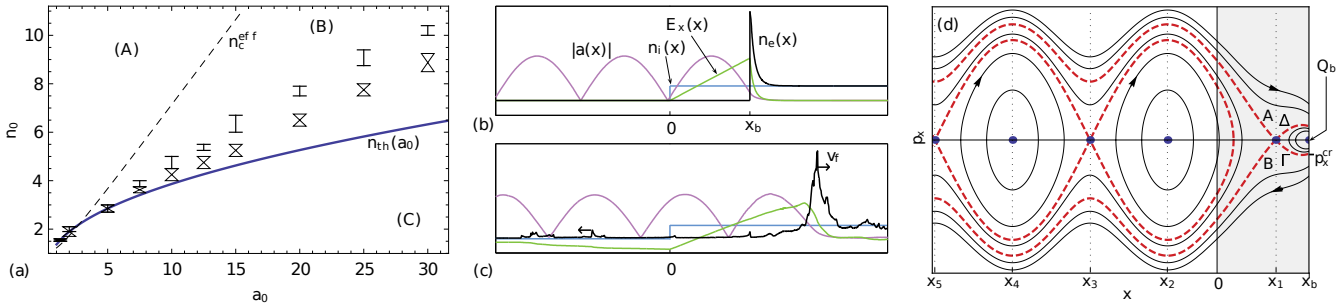

Figure 1: (a) Effective critical density as a function of the laser field amplitude a_0 as predicted by the simple relation (1) (dashed, black line). Threshold density $n_{\rm th}(a_0)$ below which, according to the cold-fluid theory, no standing wave solutions exist (solid, blue line). RSIT threshold as extracted from our PIC simulations with two different pulse rise times: $0.25\tau_L$ (errorbars) and $4\tau_L$ (triangular errorbars), where $\tau_L = 2\pi/\omega_L$ is the laser period. (b) Schematic representation of the stationary solution predicted by the cold-fluid theory for the case of total reflection [regions (A) and (B) of panel (a)]. Shown are the electric field $E_x(x)$, vector potential of the standing wave $|a(x)|$, and ion (electron) density $n_i(x)$ [$n_e(x)$]. (c) Schematic representation of a typical case of pulse propagation in PIC simulations [for RSIT in region (B) or (C) of panel (a)]. Arrows indicate the direction of electron motion. (d) Typical single electron phase-space portrait for electrons in the CEL and vacuum. Equilibria are shown as blue dots, separatrices as red, dashed lines and some typical trajectories as black, solid lines.

For a typical case of full reflection, the phase space portraits of Fig. 2(a)-(d), show that the minimum momentum, $p_x^{\rm min}$, attained by electrons is smaller in absolute value than the momentum required to move beyond the limits set by the separatrices of bounded and unbounded motion, $|p_x^{\rm min}| < |p_x^{\rm cr}|$. Thus, electrons which cross the plasma boundary x_b do not escape into the vacuum but rather re-enter the plasma. On the other hand, in a typical case of pulse propagation [Fig. 2(e)-(f)] the minimum electron momentum satisfies $|p_x^{\rm min}| > |p_x^{\rm cr}|$ and electrons move outside the separatrix of bounded and unbounded motion, eventually reaching the vacuum. As the electrostatic field decreases in magnitude the pulse can propagate deeper in the plasma. This mechanism of triggering RSIT by electron expulsion is valid for a wide range of a_0 [6]. As can be seen in Fig. 1(a), the exact threshold of RSIT depends on the pulse temporal profile, since a steeper pulse will induce stronger electron heating [6].

In conclusion, we have connected the cold-fluid and kinetic levels of RSIT description through a study of single-particle phase space. Deviations of kinetic simulations from cold-fluid theory predictions are explained as a longitudinal heating effect induced by the incident laser pulse. The reported dependency of the RSIT threshold on the pulse profile could provide a versatile tool for high-contrast CP laser pulse characterization.

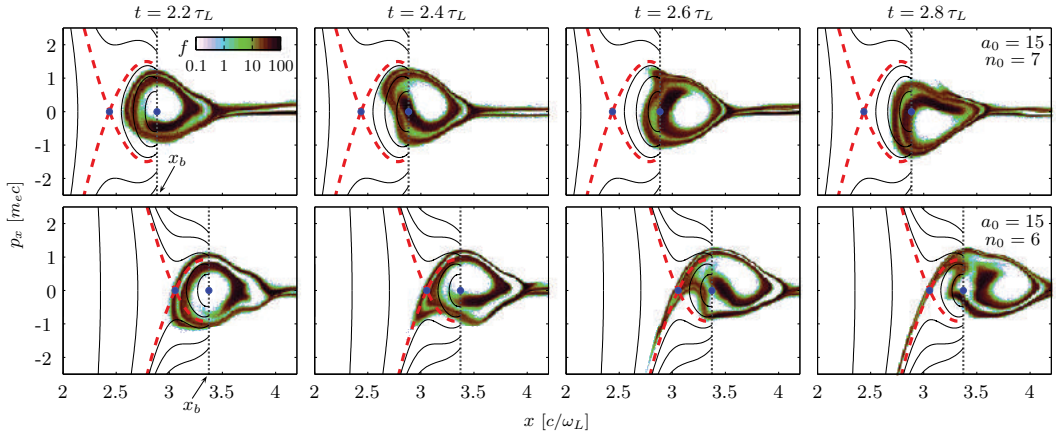

Figure 2: Comparison between phase space separatrices as predicted by the stationary, cold-fluid model, and electron distribution function $f(x, v)$ from PIC simulation results for $a_0 = 15$ and $n_0 = 7$ (top panel), $n_0 = 6.0$ (bottom panel) and rising time $\tau_r = 0.25\,\tau_L$. The plasma boundary ($x = x_b$), as predicted by the cold-fluid model, is indicated by a gray, dotted, vertical line.

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2.25 Solitary waves in random nonlocal nonlinear media

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The nonlinear Schrödinger equation (NLS) appears in diverse physical settings, among them, for instance, nonlinear optics, Bose-Einstein condensates (BEC), and water waves. A particular class of solutions to the NLS equation are solitons, particle-like wave packets that do not change their shape upon temporal evolution or spatial propagation. Solitons appear due to the compensation of diffraction or dispersion, respectively, which naturally tends to spread the wave, by the nonlinearity. In realistic settings nonlinear systems supporting solitons are often subject to random perturbations. It has been well appreciated that randomness in the linear or nonlinear potential supporting solitons may have dramatic consequences on their stability and dynamics depending on the strength of disorder. In fact, it has been shown that disorder is equivalent to the presence of an effective loss in the nonlinear system [1]. On the other hand, it appears that the interplay between nonlinearity and weak randomness can lead to diverse interesting phenomena, such as random walk of solitons in the transverse plane [2]. Up to now, mostly local nonlinear interaction has been considered in studies of solitons in nonlinear random systems. This amounts to Kerr-type nonlinear optical response and contact boson interaction in BEC. Recently however, a few works appeared dealing with random systems that exhibit spatially nonlocal nonlinearity [3].

Nonlocality of the nonlinear response appears to be common to a great variety of nonlinear systems. Physically speaking, nonlocality means that the nonlinear response of the medium in a specific location is determined by the wave amplitude in a certain neighborhood of this location. The extent of this neighborhood is often referred to as the degree of nonlocality. Nonlocality is common to media where certain transport processes such as heat or charge transfer, diffusion and/or drift of atoms are responsible for the nonlinearity. It also occurs in media with long-range interparticle interaction. This is the case of nematic liquid crystals where nonlinearity involves the reorientation of induced dipoles and in the context of BECs with noncontact long-range interatomic interaction. Nonlocality of nonlinearity and its impact on solitons has been studied extensively in the last decade. One of the most important features of nonlocality is its ability to arrest catastrophic collapse of multidimensional waves and stabilize complex solitonic structures. These stabilizing properties of nonlocality have also been identified in the presence of randomness, i.e., Folli *et al.* [3] have shown that the soliton random walk can be efficiently suppressed in highly nonlocal media.

Here we will report on the effect of nonlocality on the stability of fundamental solitons in nonlinear random media [4]. While many previous papers consider only "longitudinal" random perturbations [i.e., a situation where the randomness is only a function of the longitudinal (propagation) coordinate, we will deal here with the general case when randomness is a function of both propagation and transverse coordinates. We will consider a random nonlocal system where the randomness contributes additively towards the nonlinear response of the medium. For sake of simplicity, we will restrict ourselves to a prototypical Gaussian nonlocal model, which is widely used in the literature. We will consider the evolution of the wave function $\psi(x,t)$ with x and t denoting generalized transverse and longitudinal (propagation) coordinates, respectively. The function ψ may represent the main electric field component of a linearly polarized light beam or the wave function of a quantum object such as BEC. We assume that ψ is governed by the following model equations:

$$i\partial_t\psi(x,t) + \partial_{xx}\psi(x,t) + \rho(x,t)\psi(x,t) = 0 \tag{1a}$$

$$\int_{-\infty}^{\infty} G(x-x')\left[|\psi|^2(x',t) + \epsilon(x',t)\right]\mathrm{d}x' = \rho(x,t). \tag{1b}$$

Here, the Gaussian nonlocal response function

$$G(x) = \frac{1}{\sqrt{\pi}\sigma}\mathrm{e}^{-\frac{x^2}{\sigma^2}} \tag{2}$$

was introduced, and ρ represents the resulting nonlinear response of the medium. In the context of nonlinear optics, ρ is usually identified with a nonlinear refractive index change, while it would account for the effective two-body interaction potential in the case of a BEC. The stochastic term ϵ in Eq. (1b) is assumed to be a δ correlated Langevin noise in both longitudinal and transverse coordinates. Then, the noise fulfills $\langle\epsilon\rangle = 0$ and $\langle\epsilon(x,t)\epsilon(x',t')\rangle = n^2\delta(t-t')\delta(x-x')$, where

$$\langle f\rangle = \lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N} f_j$$

denotes ensemble averaging over different stochastic realizations f_j, and n is the so-called coupling strength.

Because the noise term $\epsilon(x,t)$ is additive in the constituent equation (1b), it acts as a source term affecting the medium independently of whether the actual signal (e.g., the optical beam) is present or not. Therefore, in the nonlocal NLS Eq. (1) noise plays the role of a random background potential and is not affected by the nonlinearity itself. The parameter σ represents the extent of the nonlocality of the nonlinear response and hence defines different nonlocal regimes. Without the noise term, Eq. (1) supports stable nonlocal solitons.

In Eq. (1), the nonlocality parameter σ leads to both nonlocal nonlinearity and finite correlation length. To separate the effect of each of these two constituents, it is useful to discuss the effective noise function

$$\eta(x,t) = \int G(x-x')\epsilon(x',t)\mathrm{d}x'. \tag{3}$$

Since the noise term ϵ is δ correlated, we find

$$\langle \eta(x,t)\eta(x',t')\rangle = C(x-x')\delta(t-t'). \tag{4}$$

For our Gaussian nonlocal model, $C(x)$ reads

$$C(x) = \frac{n^2}{\sqrt{2\pi}\sigma} e^{-\frac{x^2}{2\sigma^2}}, \tag{5}$$

and describes the effect of nonlocality on the noise. Namely, while the actual random source is represented by a white noise the nonlocal character of the nonlinearity transforms it into an *effective colored noise*. As a result, the effective noise η exhibits a finite correlation length determined by the degree of nonlocality σ.

Let us now focus on the weakly nonlocal regime, where the degree of nonlocality σ is small compared to typical transverse length scales of the wavefunction ψ. For the fundamental bright soliton ψ_S this means that its width σ_S is large compared to σ. Then, let us assume that the noise term $\eta\psi$ in Eq. (1) acts perturbatively (of the order $\delta \ll 1$) on the soliton ψ_S, and the total wavefunction ψ can be written as the sum

$$\psi = (\psi_\mathrm{S} + \chi)\exp(i\lambda t), \tag{6}$$

where $\chi(x,t)$ is of the order $\delta \ll 1$ as well, and λ is the propagation constant or soliton parameter. When the correlation length σ of the noise is much smaller than the width of the soliton σ_S, the perturbation $\tilde{\chi}$ is spectrally much broader than the soliton $\tilde{\psi}_\mathrm{S}$. Therefore, we can assume that χ will essentially describe radiation, or, in other words, the part of the total wave function which is completely alien to the soliton. If we further assume that the radiation, once produced, does not interact anymore with the soliton and disperses quickly, it is possible to write down an evolution equation for the so-called mean field ψ_MF, which fulfills

$$\begin{aligned} &i\partial_t\psi_\mathrm{MF}(x,t) + \partial_{xx}\psi_\mathrm{MF}(x,t) + i\frac{C(0)}{2}\psi_\mathrm{MF}(x,t) \\ &\quad + \int G(x-x')|\psi_\mathrm{MF}(x',t)|^2\mathrm{d}x'\psi_\mathrm{MF}(x,t) = 0, \end{aligned} \tag{7}$$

and can be connected to the wave function ψ via $|\psi_\mathrm{MF}(x,t)|^2 \approx \langle|\psi(x,t)|^2\rangle$ [4]. We will see below that predictions of the mean field equation (7) are particularly useful as long as both random phase shifts and random walk play no role, i.e., when differences between ensemble average and single realization are small and therefore $\langle|\psi(x,t)|^2\rangle \approx |\psi(x,t)|^2$.

Let us now test the applicability of Eq. (7) to *single* realizations in the limit $\sigma \to 0$. If no perturbing noise is present, the fundamental bright soliton is given by

$$\psi_\mathrm{S}(x,t) = \frac{\sqrt{2\lambda}}{\cosh(\sqrt{\lambda}x)} e^{i\lambda t}, \tag{8}$$

where λ is the soliton parameter already introduced earlier in Eq. (6). In Fig. 1(a,b,c), the evolution of the fundamental soliton Eq. (8) for $\lambda = 1$ is shown for two different noise strengths, and compared to the mean field prediction Eq. (7) in Fig. 1(d,e,f). Of course, the mean field equation does not describe the stochastic fluctuations of the peak intensity [see Fig. 1(a) vs. (d)]. Moreover, the soliton in Fig. 1(c)] performs a random walk in the transverse plane [3], which is absent in Fig. 1(f) because Eq. (7) is an entirely deterministic equation. Otherwise, both the evolution of peak intensity as well as the soliton power are captured correctly.

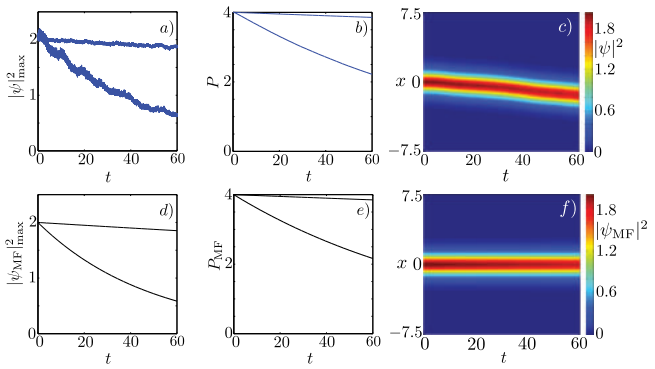

Figure 1: Soliton evolution under the influence of white noise ($\sigma \to 0$) according to Eq. (1) in the upper row (a,b,c) and mean field prediction Eq. (7) in the lower row (d,e,f) for two different noise strengths $C(0) = 6.4\times10^{-4}$, $C(0) = 1.024\times10^{-2}$ and initial soliton parameter $\lambda = 1$. (a) shows the evolution of the peak intensity, which is compared to the mean field prediction in (d) given by $|\psi_\mathrm{MF}|^2_\mathrm{max} = 2e^{-2C(0)t}$. (b) illustrates the loss of power due to radiation, where the mean field prediction in (d) is given by $P_\mathrm{MF} = 4e^{-C(0)t}$. (c) illustrates the dynamics of the intensity of the randomly perturbed soliton for the realization $C(0) = 6.4\times10^{-4}$, and (f) shows the corresponding mean field prediction. The fluctuations of the peak intensity as well as the random walk of the soliton according to Eq. (1) cannot be captured by the simplified Eq. (7).

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2.26 The X-ray edge problem in graphene

MARTINA HENTSCHEL AND GRIGORY TKACHOV

Motivation and introduction The X-ray edge problem comprises many-body effects that have been studied in detail for metals in the 1970ies and 1980ies, see Ref. [1] and references therein. The Emmy-Noether group "Many-body effects in mesoscopic systems", headed by Martina Hentschel (at the mpi**pks** 2006-2012), picked up this subject based on her Postdoc work with Harold Baranger at Duke University [2] on the X-ray edge problem in chaotic mesoscopic systems. The regular case is part of the PhD thesis of Georg Röder (defended 2011). Extension of the investigations to graphene [4] was natural and deepened our understanding of the topic with interesting results that we review here.

Our studies focus on the system's many-body response entailed in the photoabsorption spectra taken after an X-ray has excited a core electron of the material into the conduction band, here graphene. Such a sudden perturbation causes the non-adiabatic Anderson orthogonality catastrophe response that deforms the Fermi edge of the absorption signal into a so-called rounded edge. However, there can be an additional, counteracting many-body effect known as Mahan's exciton or Mahan-Nozières-DeDominici response that leads to a peaked edge. Both effects together are known as the X-ray edge problem and give rise to Fermi-edge singularites (FES) well studied in theory in experiment for metals.

Graphene appears to be of special interest for a number of reasons: The density of states (DOS) varies such that the well-known Dirac points are formed where the DOS vanishes. This causes the Anderson catstrophe response to be suppressed at the Dirac points, see e.g. [3]. Consequently, one expects a dependence of the photoabsorption signal on the filling of the band. Another interesting option is to vary the DOS using edge states. They are naturally present at the edge of zig-zag terminated graphene, such that the DOS varies between the bulk and the edge of the sample which will eventually cause different photoabsorption spectra depending on the position of the perturbation. At armchair terminated graphene edges we expect to recover the bulk behaviour as there exist no edge states here.

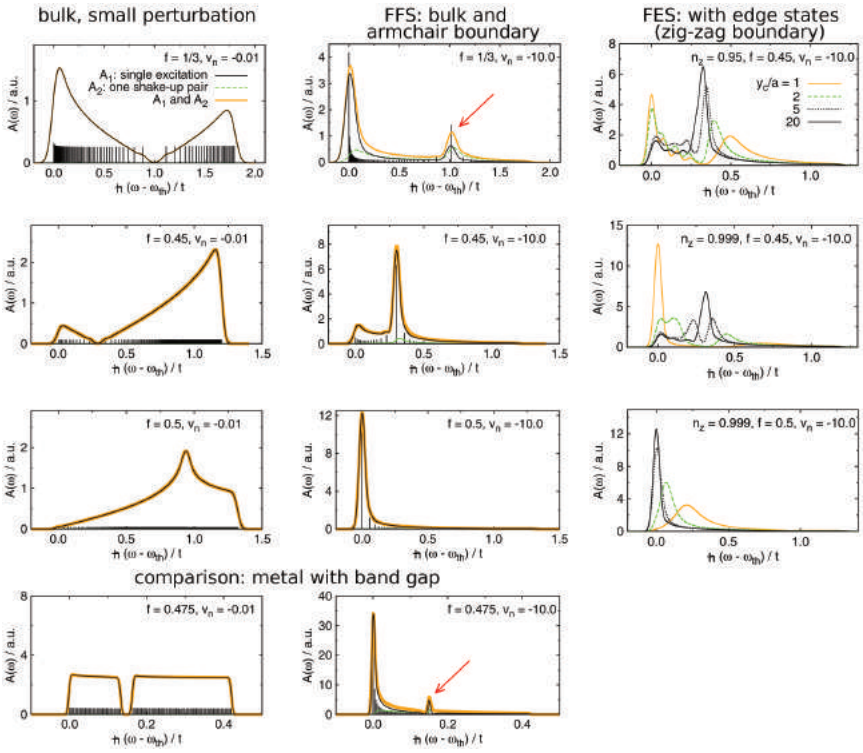

Figure 1: Photoabsorption cross section vs. excitation energy in graphene in the absence and presence of edge states. See text and Ref. [4] for details. Left: Absorption signal of bulk graphene for different filling factors f and a very small perturbation v_n. Center: Same, but for a strong perturbation such that FES become visible. Right: Photoabsortion near a zig-zag boundary. The different lines correspond to different contributions to the photoabsorption signal (left and central column) and to varying distance from the system boundary (right column), respectively.

Model and Results The model we use is based on the generalized Fermi golden rule method introduced by Ohtaka and Tanabe [1]. The character of the graphene boundary and the resulting local edge DOS is described by a parameter n_z [5,6] that determines deviation from the ideal zig-zag boundary $n_z = 1$.

Our results are summerized in Fig. 1. The left column shows the photoabsorption cross section in bulk graphene for a very small perturbation parameter $v_n = -0.01$ and increasing filling factor f (from $1/3$ via 0.45 to 0.5 corresponding to the Dirac point), the lowest panel shows the situation of a metal with band gap for comparison. At such small perturbation strengths, the photoabsorption signal closely resembles the DOS: The Dirac cone is clearly visible especially in the uppermost panel for one third filling.

The central panels capture the same situation, but now for a large peturbation strength such that the X-ray edge physics is revealed and Fermi edge singularities become visible. We observe, contrary to the metallic case, actually two of them: One at the Fermi energy (directly related to the filling factor) and another one at the Dirac energy (marked by the arrow). At half filling (third panel), both singularities coincide. The toy model of a metal with band gap, shown in the lowest panel, illustrates that the vanishing DOS at the Dirac point is the origin of the second peak in the photoabsorption cross section.

In the right column, edge states as present at a zigzag boundary are taken into account. The different lines illustrate the photoabsorption signal under variation of the position y_c/a (with lattice constant a) of the perturbation w.r.t. the system boundary. Corresponding changes in the photoabsorption signal are evident, note that the bulk values (discussed in the previous two columns) are reached for sufficient distance from the edge, y_c/a=20. Fillings near half filling and strong perturbations are considered. The upper two panels differ only in the value of n_z, i.e., in the degree of the boundary's "zigzagness", that is, the local edge DOS. The differences in the photoabsorption cross section underline the importance of edge states for this observable when the signal is taken near the graphene boundary.

Conclusion We have computed the X-ray edge problem for graphene. Our results indicate that the Dirac point shows up in the photoabsorption spectra as a second Fermi edge singularity for band fillings below one half. This information could be useful for the typically difficult determination of the Dirac point in experiments. Edge states play an important role at zigzag terminated graphene, and their similarity to those found in topological insulators indicates the relevance of our findings for this emerging system class as well as for band-gap engineered graphene where edge states are crucial as well [7].

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2.27 Understanding opinion formation in humans and animals

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Over the past two years one of the main research themes in the BioND group was collective opinion formation. Many species of animals exhibit so-called swarm intelligence, where a group of animals process information collectively. The most widely known examples are perhaps found in social insects, such as bees, which have evolved mechanisms for making democratic decisions on nesting sites, and certain species of ant, who collectively decide on the timing and target area of foraging expeditions. Also for flocks of birds, schools of fish, and herds of quadrupeds it is known that they can often locate food sources better and avoid predators more efficiently as a group than any member of the group on its own. Nevertheless, arguably, the most impressive examples of social decision making are found in humans.

Among all animals only humans have developed the ability and means to share opinions, knowledge, and insights beyond their circle of direct acquaintances. Our culture, including all of science, would be unthinkable without a process of accumulation of knowledge where bits of information are shared, tested, and selectively passed on. Among others, democratic government relies crucially on the ability of humans to process information collectively. However, collective information processing in humans is not always beneficial. While there is no evidence of adverse effects in animals, exchange of opinions between humans can sometimes lead to detrimental dynamics, with examples ranging from the comparatively harmless propagation of counter-factual myths and rumors, via youth violence, fueled by intra-group reinforcement, to large-scale radicalization and fascism.

Because of the crucial dependence of human society and culture on opinion formation processes, it is meaningful to ask which factors influence the outcome of these processes. In particular, when will collective information processing lead to the discovery of factually true and meaningful insights, and when will it lead to propagation of counter-factual beliefs? Answering these questions is all the more pressing, since we are radically altering the way in which we communicate. Population-wide access to the internet could conceivably lead to a well-informed and politically interested and active electorate, or, equally conceivably, to a fragmented society where people select their news sources to confirm and reinforce their beliefs and superstitions.

A paradigmatic model for social opinion formation processes is the adaptive voter model [1]. This model describes the social opinion formation process, by a network, where nodes represent individual agents and links represent social contacts. Each node has an internal variable, representing the agents opinion, which is chosen from a finite set of opinions. In the most common variant of the model the set comprises only two opinions. Starting from some initial random configuration the system evolves due to processes: *social segregation* the tendency to distance oneself from those holding contrary opinions, and *social adjustment* the tendency to adopt the opinion of acquaintances. In the network model, social segregation is realized through the rewiring of links. So-called active links, connecting agents who hold conflicting opinions are rewired stochastically at a rate p, such that after rewiring they connects agents holding identical opinions. Social adjustment is modeled through the copying of opinions: On any given active link, one of the agents copies the other opinion at the rate $1 - p$. A key question is then how the value of p, which can be interpreted as a rewiring rate affects the outcome of the opinion formation process.

From previous works it was known that for large p, the network undergoes fragmentation, which results in the formation of disconnected components that are internally in consensus but hold different opinions from each other. At low values of p the system approach a dynamic stead state, where an active discussion is maintained and nodes continually agents their opinions. In a finite system stochastic fluctuations can eventually drive the system to an absorbing global consensus state. These active and fragmented regimes are separated by a continuous phase transition, the *fragmentation transition*.

While conceptually simple, the adaptive voter model is a difficult model for which well-established theoretical tools fail. In particular moment expansions, that yield good results in other adaptive network models overestimate the critical value of p by up to 80%. To gain intuition, we applied all previoulsly proposed approximation schemes for adaptive networks to the adaptive voter model [2]. Among others, we showed numerically that even the active neighborhood approximation (a sophisticated approach that describes the dynamics by an infinite-dimensional equation system) yields only unsatisfactory results, which we recently confirmed by an excact solution [8]. Through a detailed analysis of the failures of other approxiamtion schemes, we were able to propose a new type of approximation that predicts the fragmentation point with excellent accuracy [2, 4, 5].

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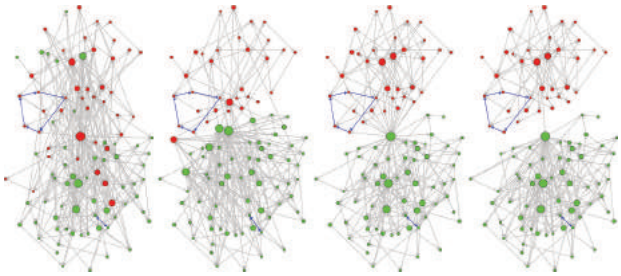

Figure 1: Two state-homogeneous attracting components (blue/dark gray) nucleate self-stabilizing structures leading to early fragmentation.

We moved on to study a variant of the model that is reminiscent of social media such as twitter [7]. Here, links are directed such that one party can transmit its opinion (the followed influences the followed) whereas the other party can rewire the link (the follower can unfollow the followed). In this model we found that fragmentation can already occur at arbitrarily low rewiring rates, which could potentially explain the strong fragmentation observed in social media. Moreover, fragmentation in this model is initiated by a nucleation process, suggesting that the underlying phase transition is in this case discontinuous.

A common criticism of the voter model is that is overly simplified and thus cannot provide insights into real world opinion formation processes. Indeed, real world data and even laboratory experiments with humans tend to be too complicated to be directly comparable to the voter model. We therefore focused on the conceptually simpler setting of collective opinion formation in animals. All animals that live in groups and migrate, necessarily have to reach a consensus on the direction of migration and thus undergo a social opinion formation process. In contrast to humans which are exposed to a multitude of different sources of information, the informational status of animal agents is often directly dependent on their sensory modalities and thus easy to determine. We can thus consider two indivduals as linked if they are mutually aware of their relative position and heading direction.

We focused first on a previous experiment in which groups of locust nymphs were left to march freely in a ring-shaped arena [6]. It was found that at low locusts densities the motion was random, whereas at high locust densities collective motion in a preferred direction (clockwise or counter-clockwise) was observed. At medium densities intermittent collective motion with occasional switches of direction was observed. We where able to explain this transitions analytically using a variant of the adaptive voter model [3]. Notably, this model also reproduced the correct distribution of switching times in the intermittent phase.

In a second step, we used the model proposed for the locust to predict the outcome of a binary opinion formation experiment with fish that was carried out in parallel at the lab of Iain Couzin at Princeton University. The experimental setting involved mixed schools of fish in which some individuals were trained to head to a blue target, whereas others were trained to head to a yellow target. The latter group was much more strongly opinionated, such that mixed schools could be created in which the collective movement was controlled by a minority of yellow seeking fish. However, if additional fish are added to such a school that do not have a preference, the control can be returned to the blue-seeking majority. This phenomenon that was first predicted in detailed fish simulations, and subsequently also in the network model and demonstrated experimentally [9]. Moreover, the analytically tractable network model reveals the bifurcation structure underlying this phenomenon.

Our results show that even very simple models of opinion formation can be used opinion formation experiments with animals. However, more importantly these models provide important benchmark systems on which theoretical tools can be refined to ultimately tackle more complicated models that can realistically describe and predict opinion formation processes in humans.

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2.28 Chiral flows in the actomyosin cell cortex

S. FÜRTHAUER, S. NAGANATHAN, F. JÜLICHER, S.W. GRILL

Introduction The actomyosin cortex is a thin film of a gel-like material enriched in filamentous actin and myosin which drives many of the morphogenetic rearrangements which are seen during the development of an organism from a fertilized egg. Examples are dorsal closure in fruit flies, epiboly in Zebrafish, and polarizing cortical flow in the one cell stage *C. elegans* embryos. In all these cases myosin motor proteins cause the cortex to contract, which drives flows from regions of lower towards regions of higher myosin concentration [1]. In *C. elegans*, these flows are involved in polarity establishment and are important for the subsequent asymmetric cell division.

Since cytoskeletal filaments are chiral, systems of cytoskeletal filaments can display chiral properties. Specifically, the interaction between actin and myosin is chiral [2]. We therefore asked if large-scale rearrangements in the actomyosin cortex can display chiral asymmetries. For this we investigated flows which occur during polarity establishment in *C. elegans* embryos. We show that these flows are chiral, demonstrating that the actomyosin cortex in the early embryo has a broken chiral symmetry. This precedes the chiral symmetry breaking of the entire organism.

On large lengths and times the actomyosin cortex can be described as a thin film of an active gel [3]. To describe chiral flow, we have developed an extension of active gel theory which incorporates the effects of active chiral processes [5]. Our work shows that active torque dipoles in a thin film of fluid can generate flows which break chiral symmetry [6]. We find that the chiral flows in *C. elegans* can be described in this framework.

Observation of chiral flows We measured cortical flows in the *C. elegans* embryo closely following the methods outlined in [1]. The embryo is plated between a glass cover slip and an agar substrate, and the bottom surface of the embryo is imaged (Fig 1). The motor protein Non-Muscle-Myosin II (NMY II) is fluorescently labeled and the cortical plane is recorded at regular time intervals using a spinning disc confocal microscope. We use these images to extract the flow velocity field $\mathbf{v}$. We observe a small flow component in the direction orthogonal to the anterior-posterior (AP) axis (y-direction). Even though the y-velocity of the flow field is smaller than the velocity of flows along the AP-axis (x-direction) it is reproducible and subsists when averaging over many embryos (Fig. 1). Since the embryo is azimuthally symmetric, the existence of a y component of the flow field shows that chiral symmetry is broken. We define a clockwise rotation around the AP-axis when viewed from the anterior pole as left-handed. Thus, flows perform a left handed rotation around the AP-axis in the posterior of the embryo and a right handed rotation in the anterior (Fig 1).

Physical origin of chiral flows Since actin filaments are chiral, the interaction between actin and myosin is chiral. This has been demonstrated in sliding assays where myosin motors attached to a surface made actin filaments rotate around their long axis [2]. Thus, a myosin mini-filament that couples two actin filaments is a torque dipole, see Fig. 2 (a). The handedness of this torque dipole is set by the chirality of the actin-myosin interaction. Torque dipoles in a fluid generate an intrinsic rotation rate [5], see Fig. 2 (b). Close to a surface the intrinsic rotation rate couples to the velocity field [6]. Specifically, if the density of torque dipoles is non-homogeneous a flow in the direction orthogonal to the gradient torque dipole density is generated, see Fig. 2 (c).

Closely following the logic outlined in [5,6], we obtain an equation of motion for a thin active chiral film of viscous fluid. Motions in the film are driven by an active torque density τ and an active tension T according to

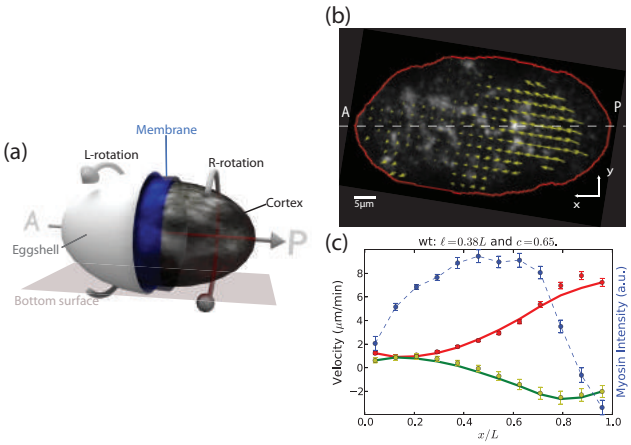

Figure 1: (a): Sketch of a *C. elegans* embryo. Anterior (A), posterior (P). Curved arrows represent clockwise (L) and counter-clockwise rotations (R). Bottom surface indicated by red plane. (b): Cortical flow (arrows) on the *C. elegans* bottom surface. (c): Profiles of myosin fluorescence intensity (blue), v_x (red) and v_y (green) averaged over the entire period of flows and $N = 25$ wildtype embryos. Errorbars represent standard error of the mean. Solid lines represent fits to Eqns. 2 and 3.

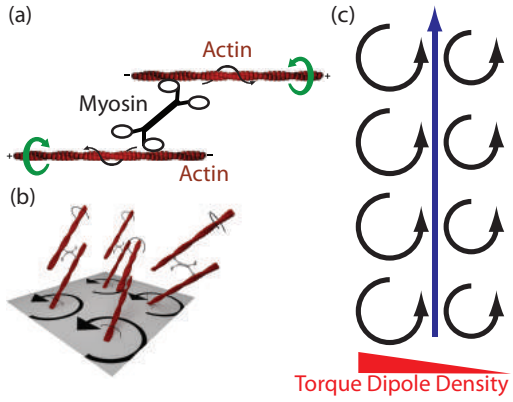

Figure 2: Cartoon of the active chiral processes in the actomyosin cell cortex. (a): Torque dipole. Black arrows denote the path of the myosin motor heads, curved green arrows denote torques. (b): Torque dipoles on a surface. Black curved arrows denote the torque exerted on the surface. (c): Active torque densities (black arrows) generate a flow (blue arrow) in the direction orthogonal to the gradient.

$$\eta(\partial_j^2 v_i + \partial_i\partial_j v_j) - \gamma v_i = \partial_i T - \epsilon_{ij}\partial_j \tau \quad , \qquad (1)$$

where the indices i, j take the values x, y and a summation convention is implied. The Levi-Civita symbol ϵ_{ij} takes the values $\epsilon_{xx} = \epsilon_{yy} = 0$ and $\epsilon_{xy} = -\epsilon_{yx} = 1$. Since the cell is azimuthally symmetric, the x and y components of the equation of motion decouple such that

$$\ell\partial_x^2 v_x - \frac{1}{\ell} v_x = \alpha\partial_x m \quad \text{and} \qquad (2)$$

$$\frac{1}{2}\ell\partial_x^2 v_y - \frac{1}{\ell} v_y = \beta\partial_x m \quad . \qquad (3)$$

Here we have introduced the hydrodynamic length $\ell = \sqrt{2\eta/\gamma}$. We use $T/(2\eta\gamma) = \alpha n$ and $\tau/(2\eta\gamma) = \beta m$, with m denoting the local concentration of myosin. The ratio $c = \tau/T$ quantifies the relative magnitude of isotropic to chiral active tension. Eqns. 2 and 3 can be used quantitatively relate the distribution of myosin with the flow field (Fig 1 (c)). The best fit between the predicted and measured flow field is obtained for the hydrodynamic length $\ell/L \simeq 0.38$ and $c \simeq 0.65$.

Perturbation experiments To challenge our theory we performed perturbation experiments. We use RNA mediated interference to modify myosin regulation. Figure 3 shows that Eqns. 2 and 3 reproduce the flows observed under two modifying conditions. Importantly we find that the chirality c is actively regulated by proteins which affect the interaction between actin and myosin. Most notably we find that reducing the concentration of casein kinase one ($csnk1$), a serine-threonine kinase and a regulator of signal transduction pathways, leads to increased chirality ($c \simeq 1.24$, Fig. 3 (a)). In contrast, reducing the concentration of $ect2$, an exchange factor of Rho GTPases, decreases it ($c \simeq 0.04$, Fig. 3 (b)). Interestingly, both these proteins are involved in the non-canonical Wnt signaling pathway. This pathway has been shown to be involved in a shifting of the *C. elegans* midline away from the AP-axis at the 4 to 8 cell stage, which is the determining event for left-right symmetry breaking of the *C. elegans* worm [4]. Because actomyosin participates in this midline shift, our results suggest that the chirality of the actin-myosin interaction that we have revealed at the one cell stage is also important for LR-symmetry of the entire organism.

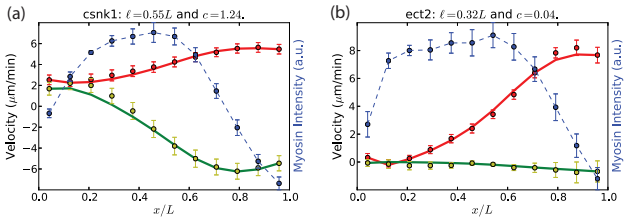

Figure 3: (a),(b): Perturbations of the myosin-actin interaction change the chirality of flows. v_x (red), v_y (green), and myosin density (blue) for $csnk1$ (a) and $ect2$ (b) are shown. Note the different scaling of the y-axes. Solid lines represent fits to Eqns. 2 and 3. We conclude that chiral flows are inihibited by $csnk1$ (a) and enhanced by $ect2$ (b).

Conclusion We have discovered that cortical flows in the *C. elegans* one cell stage embryo are chiral. We have presented a theoretical description of the cell cortex as an active chiral gel, which is in good agreement with the experimental data and provides a mean to quantify the physical effect of perturbations of the cell cortex. Importantly, affecting cortical composition by RNAi leads to phenotypes with perturbed chiral flows. We have shown that two proteins of the non-canonical Wnt pathway ($ect2$ and $csnk1$) are involved in regulating the active torque and cortical chirality. Interestingly the non-canonical Wnt pathway is involved in LR symmetry breaking of the entire organism, which leads us to speculate that active chiral processes in the actomyosin cell cortex are of general developmental importance.

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2.29 Forces and flows for actomyosin ring propulsion in zebrafish gastrulation

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Introduction The actomyosin cytoskeleton is responsible for driving most of the deformations and rearrangements that occur when an embryo develops. However, how these rearrangements are driven by force generation in the actomyosin cytoskeleton is unclear in many instances. For example, in zebrafish epiboly, the epithelial enveloping layer (EVL) of cells spreads from the animal cap of the gastrula over the yolk cell to completely engulf it at the end of gastrulation [1]. This developmental rearrangement requires contact between the EVL and a thin cytoplasmic layer on the surface of the yolk cell to which the EVL is connected at its margin [2–4] (Fig. 1A). It has been proposed that an actomyosin structure within this thin layer acts as a contractile ring that drives epiboly by pulling on the edge of the EVL [4–6]. The aim of this work was to investigate the mechanism of propulsion of this actomyosin ring [7].

Tension in the ring One possible mechanism is that myosin motor protein activity generates tension along the circumference of the actomyosin ring, which due to the spherical geometry of the embryo gives rise to a force pulling on the EVL margin once the ring has past the equator. To test for the presence of circumferential tension within the actomyosin ring, we utilized a UV lasercutter [8] to sever the actomyosin network along a 20 μm long line close to the EVL margin in an orientation perpendicular to the margin (Fig. 1B). Perpendicular cuts resulted in rapid initial recoil velocities of the actomyosin network that increased over the course of epiboly (Fig. 1C, red), suggesting that circumferential tension within the actomyosin ring increases during EVL epiboly progression.

Due to the spherical geometry of the yolk cell, circumferential tension will result in a net force pulling on the EVL margin, which is zero when the ring is at the equator and grows as the ring approaches the vegetal pole. As a consequence, tension in the animal-vegetal (AV) direction is expected reach at most 20% of circumferential tension at 80% epiboly [7]. We tested this by performing lasercuts parallel to the EVL margin (Fig. 1B). Contrary to our expectations, we found that the initial recoil velocity of the actomyosin network for parallel cuts was approximately half of the initial recoil velocity for perpendicular cuts at 60-70% epiboly and remained constant during epiboly progression (Fig. 1C, green). We conclude that AV tension is much larger than expected if the actomyosin ring were acting as a constricting ring only.

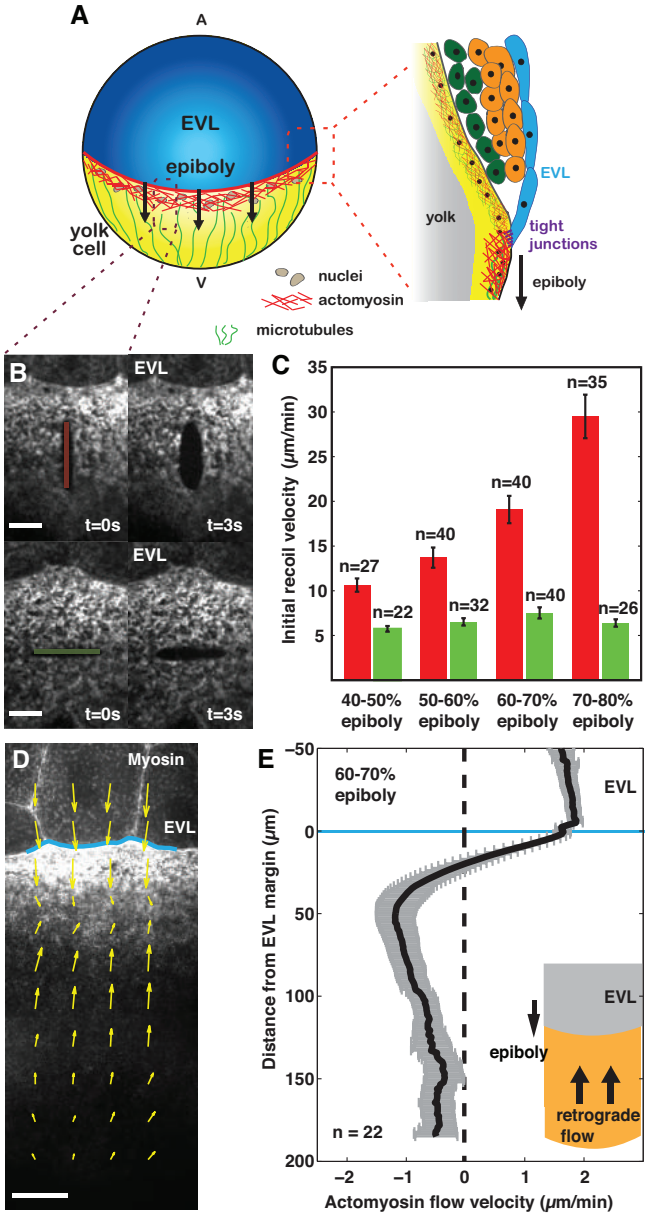

Figure 1: (A) Sketch of zebrafish embryo geometry during epiboly. Red structures indicate the actomyosin ring, which moves from the animal (A) towards the vegetal (V) pole (arrows). (B) Embryos at 65% epiboly where the actomyosin ring was cut along a 20 μm line perpendicular (red) and parallel (green) to the EVL margin. Scale bars, 10 μm. (C) Initial laser cut recoil velocities at different stages of epiboly for perpendicular (red) and parallel cuts (green). (D) Cortical flows within the actomyosin ring at 60% epiboly. The EVL margin (blue line) and actomyosin flow (yellow arrows) are shown. Scale bar, 20 μm. (E) Average profile of cortical flow in embryos at 60-70% epiboly (N = 22).

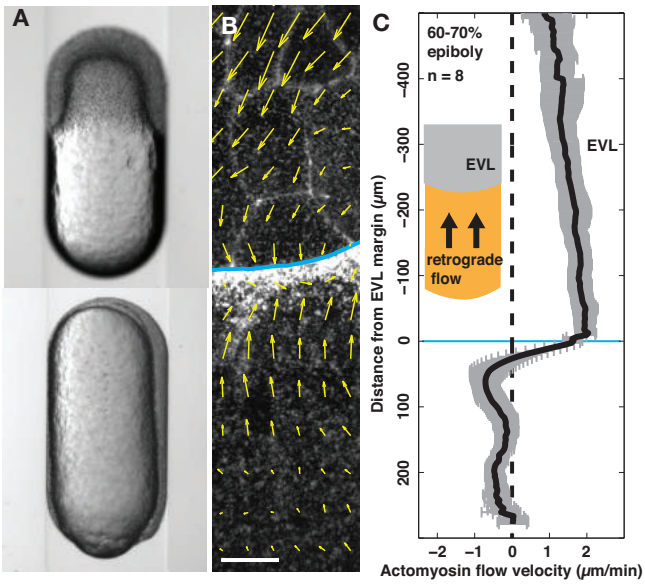

Figure 2: (A) Brightfield images of cylindrical embryos at 30% (top) and 100% epiboly (bottom). Embryo width, 500μm. (B) EVL margin (blue line) and the flow field (yellow arrows) in cylindrical embryos at 60% epiboly. Scale bar, 25 μm. (C) Average actomyosin flow profiles of cylindrical embryos at 60-70% epiboly.

We next sought to investigate where the additional tension in the AV direction comes from. Formation of the actomyosin ring was accompanied by flows of actin and myosin into the ring from the vegetal side (Fig. 1D). These retrograde actomyosin flows were slow (0.3 μm/min) at the onset of EVL epiboly, but increased their retrograde velocity as epiboly proceeded, reaching maximal flow velocities of 1.2 μm/min at the 60-70% epiboly stage (Fig. 1E).

Crawling mechanism, flow-friction motor To investigate if retrograde actomyosin flows could give rise to additional tension in the AV direction, we developed a theoretical description of actomyosin dynamics within the framework of thin films of active fluids [7]. This description revealed two contributions to the total force exerted by the ring upon the EVL - one from circumferential tension coupling to geometry, and one from retrograde cortical flow. In the absence of friction between the actomyosin ring and adjacent components of the yolk cell, total force on the EVL arises through a ring-contraction mechanism that couples to the spherical geometry of the yolk cell. This mechanism can drive epiboly only once the actomyosin ring has passed the equator. In contrast, when friction is present, total force on the EVL has a geometry-independent contribution. Here, actomyosin retrograde flow is resisted by friction with the yolk cell membrane and the underlying cytoskeletal structures, and the ring self-propells in a crawling fashion (also referred to as 'flow-friction motor'). Importantly, flow provides additional tension in the AV direction, consistent with the degree of tension anisotropy observed in the laser ablation experiments (Fig. 1C). Furthermore, experimentally measured flow profiles within the EVL and the actomyosin ring, as well as the relative tensions obtained from laser ablation, are accurately predicted [7]. To conclude, we identified two distinct modes of ring propulsion: a cable-constriction and a crawling mechanism.

Cylindrical embryos We next asked if the flow-based propulsion is sufficient to drive EVL epiboly. Since cable-constriction does not exert a net force on the EVL when the ring is positioned right at the equator, propulsion by this motor would be hindered when the yolk cell is deformed from its original spherical geometry into a cylindrical shape. We thus deformed the yolk cell into a cylindrical shape by aspirating pre-gastrula stage embryos (2.5 hpf) into agarose tubes of a diameter smaller than that of the embryo and analyzed resulting changes in EVL movements. We found that EVL epiboly movements are largely unaffected in cylindrical embryos and proceed with velocities similar to those of spherical control embryos ($2.0 \pm 0.2\mu$m/min compared to $1.9 \pm 0.1\mu$m/min at 60-70% epiboly; compare Figs. 2C and 1E). This shows that cable-constriction is not essential for EVL actomyosin ring propulsion, and indicates that the crawling mechanism achieved by actomyosin flow is sufficient to drive EVL epiboly during zebrafish gastrulation.

Conclusion Actomyosin ring propulsion during epiboly in zebrafish gastrulation proceeds in a crawling mechanism driven by actomyosin flow. Our findings have major implications for the function of actomyosin rings in morphogenesis, and raise the possibility of a more general role of actomyosin cortical flows for driving developmental rearrangements.

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2.30 Linking genomic changes to phenotypic differences

MICHAEL HILLER

Finding which genomic differences or more generally which genomic regions underlie a specific phenotypic difference between species is hard because there are both countless genomic and phenotypic changes between any pair of species. Thus, the comparison of two genomes has no power to infer such associations.

However, evolutionary theory suggests that phenotypes that are repeatedly lost in independent species should lead to a genomic signature with high specificity. We developed a novel computational approach that attempts to detect this specific signature for a given independently lost phenotype [1]. Vitamin C synthesis is an example of a phenotype with independent losses. While the majority of mammalian species can synthesize their own vitamin C, humans and a few other primates, the guinea pig and bats have lost this ability and require a dietary source of vitamin C to prevent the disease scurvy [2]. Theory about selection and neutral evolution predicts that the loss of this phenotype will eventually lead to loss of the genomic regions that encode the ability to synthesize vitamin C due to neutral evolution. This should happen only in the phenotype-loss species. In all other mammals that retain this ability, the genomic information for this phenotype will also be retained by selection. Consequently, such repeated phenotypic losses result in a specific evolutionary signature in these genomes. Our approach searches for exactly this signature by detecting genomic regions that are absent in species lacking a given phenotype (in this case, vitamin C synthesis) and that are present in those species possessing this phenotype. Conceptually this approach is similar to forward genetics, where researchers map the mutation underlying a given phenotypic difference by crossing and mapping experiments, therefore we term our approach "forward genomics".

To apply forward genomics to the vitamin C phenotype, we firstly had to overcome issues related to the incompleteness of genomic data. Certain regions in the genome are currently not fully sequenced or have an elevated sequencing error rate. As this perfectly mimics the real loss of genomic regions (which we are searching for), we had to rigorously distinguish these artifacts from real losses. Secondly, theory suggests that complete absence of a once-functional genomic region will only occur after long evolutionary time. For more recent phenotypic losses, these once-functional regions would still be visible in the genome but have accumulated more mutations. Therefore, genomic regions that are likely to be related to the loss of this phenotype will have accumulated more mutations in exactly those species lacking this phenotype. To detect such regions, we computationally reconstructed the DNA sequence of the mammalian ancestor using maximum likelihood to quantify the number of mutations that occurred in every species for every genomic region (Figure 1).

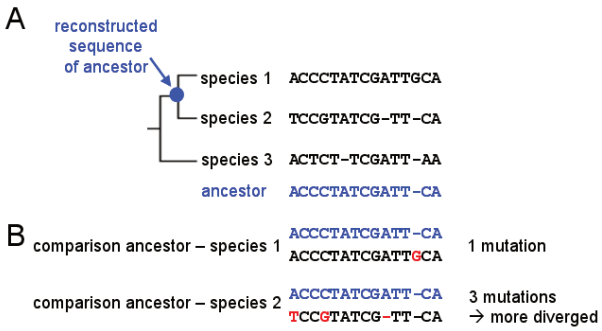

Figure 1: Ancestral sequence reconstruction:
(A) For the given sequence alignment, species 3 is used as the outgroup to infer the most likely sequence of the ancestor of species 1 and 2. Insertions and deletions are shown by a dash.
(B) For this genomic regions, we can compare the reconstructed sequence of the ancestor to species 1 and 2 to quantify the number of mutations. In this example, species 2 has accumulated more mutations and is therefore more diverged at the sequence level.

We used forward genomics to screen the genomes of 27 mammals and found a single genomic locus that perfectly matches the vitamin C phenotype. This genomic locus overlaps the *Gulo* gene that encodes a key enzyme responsible for vitamin C synthesis (Figure 2). Interestingly, we also found that *Gulo* is an inactivated (non-functional) gene in all and only the non-vitamin C synthesizing mammals, likely explaining this phenotypic loss.

Can we apply forward genomics to other phenotypic differences apart from vitamin C synthesis? Firstly, we demonstrated the power of the method on another repeatedly changed phenotype: The bile of guinea pigs and horses (two independent lineages) contains almost no phospholipids, in contrast to other mammals. Forward genomics detected the loss of the *Abcb4* gene (a transporter that secretes phospholipids into bile) in guinea pigs and horses as the most likely genomic change underlying this phenotypic difference. Interestingly, *Abcb4* mutations in humans lead to the same phenotype as in guinea pigs and horses, but - in contrast to these "healthy" species - this gene loss in human results in a severe disease. This raises the question how two natural species avoid the deleterious consequences of losing *Abcb4* and suggests that guinea pigs

and horses have acquired other compensatory changes. Studying these compensatory mechanisms could lead to new strategies for ameliorating the consequences of *Abcb4* mutations in humans. Secondly, we simulated whole genome evolution of more than 20 species to obtain test cases to further explore the performance of forward genomics. We could show that our approach can detect some genomic regions for the simulated vitamin C and biliary phospholipid phenotypic loss as well as a variety of other phenotypic loss scenarios. These simulations suggest broad applicability to many other independent phenotypic losses and provide a basis for optimizing the underlying algorithms to improve sensitivity and specificity. Thirdly, by analyzing large sets of phenotypic data collected by systematists, we found that phenotypes with changes in independent lineages - the prerequisite for forward genomics to achieve specificity - are quite frequent and comprise about 40% of all measured phenotypes. Therefore, together with near future availability of thousands of new genomes [3, 4], forward genomics can be applied to many more phenotypic differences and will help to explain how nature's great phenotypic diversity is encoded in the DNA.

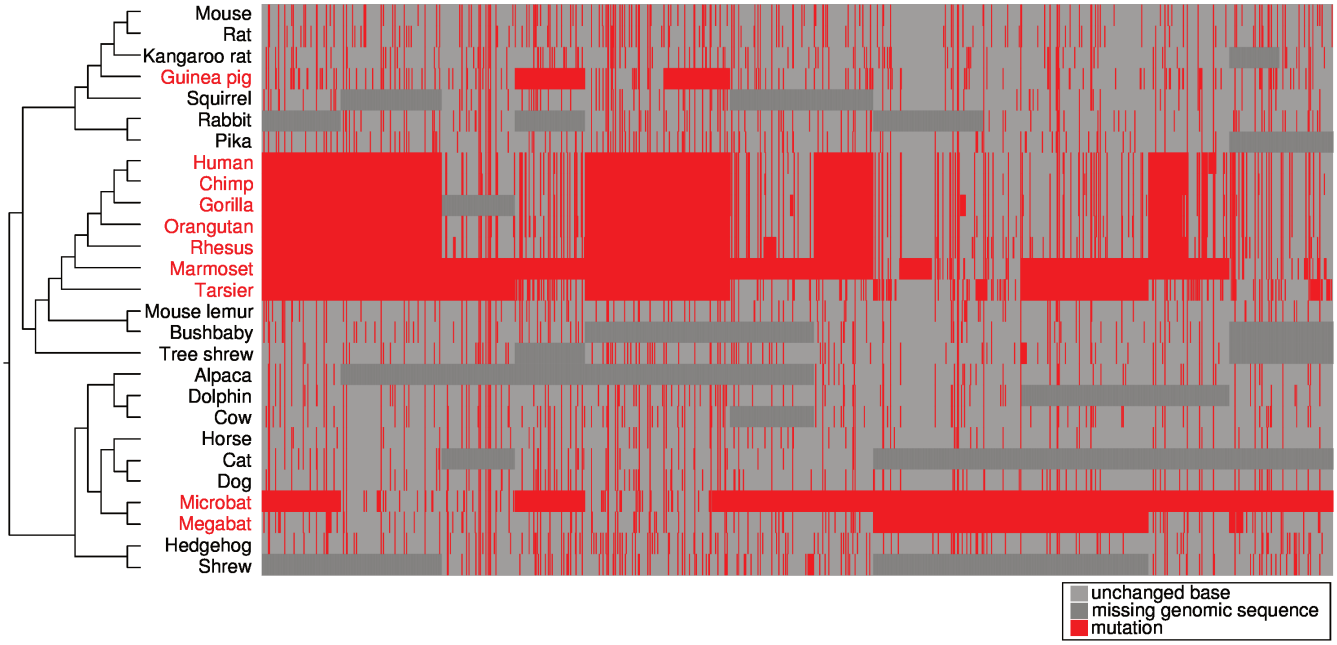

Figure 2: The *Gulo* gene is inactivated in all and only non vitamin C synthesizing mammals. The figure shows the phylogenic tree of mammals (left) and a visualization of a sequence alignment of the entire *Gulo* gene (right). While mutations (red lines or blocks) happened in all species, the non vitamin C synthesizing species (red font) have accumulated many more mutations and some of them inactivate this gene, leading to the loss of this phenotype.

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2.31 Protein aggregate fusion facilitates a transition between symmetric and asymmetric damage segregation

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Asymmetric segregation of damaged proteins at cell division generates a cell that retains damage and a clean cell that supports population survival. In cells that divide asymmetrically, such as *Saccharomyces cerevisiae*, segregation of damaged proteins is achieved by retention and active transport. Yet, the mechanisms underlying damage segregation in symmetrically dividing cells have remained largely elusive. Here we show that protein aggregates in *Schizosaccharomyces pombe* segregate symmetrically or asymmetrically depending on the amount of aggregates, where the transition between these two modes is facilitated by fusion of aggregates. Using the GFP-labeled chaperone Hsp104 to monitor protein aggregates *in vivo* we determined that aggregate dynamics is consistent with a stochastic aggregation model. Upon stress aggregates fuse into a large unit, which segregates asymmetrically at division, generating a daughter cell free of aggregates. Our work shows a new mode of damage segregation, where the transition from symmetric to asymmetric segregation may promote cell survival under non-favorable conditions.

Proteins are labile entities that can unfold and engage in unfavorable interactions that give rise to protein aggregates (Fig. 1). These aggregates represent a type of cellular damage, composed of insoluble and dense protein particles, which instead of being degraded, accumulate in the cell during stress and ageing. The aggregates interfere with cell cycle progression and cell function.

A central question is how a cell deals with protein aggregates during division. In principle, two scenarios can be envisioned. First, the aggregates can be segregated asymmetrically during division, such that they are retained in one of the two cells while the other cell is born clean. Second, aggregates can be segregated symmetrically, resulting in both cells inheriting the same amount of aggregates. Under non-favorable conditions, where damage levels are high, asymmetric segregation may be the only way to ensure survival.

To deal with damaged proteins during cell division, *Escherichia coli* and *Saccharomyces cerevisiae*, as well as stem cells, use asymmetric segregation, where damaged proteins are retained by one cell, generating a clean sister cell [1, 2]. However, the mechanisms of damage segregation in cells that divide symmetrically have remained unclear.

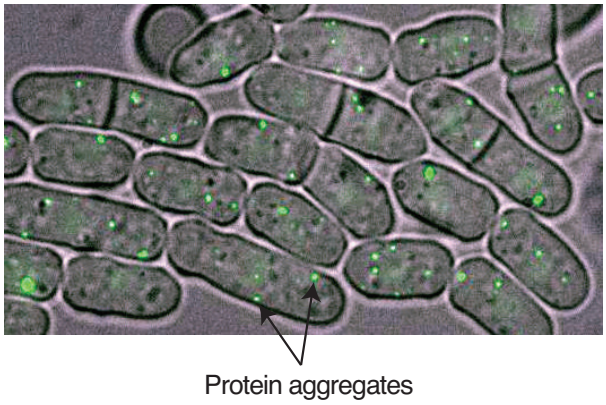

Figure 1: Protein aggregates. Fission yeast cells expressing Hsp104-GFP show protein aggregates as green puncta in the cytoplasm.

To study aggregate dynamics during the cell cycle, we followed Hsp104-associated aggregates with wide-field fluorescence microscopy. We tracked individual aggregates on time scales from miliseconds to minutes and observed them to undergo diffusive motion (see also [3]). Furthermore, the diffusion coefficient decreased with increasing aggregate area, as expected for Stokes diffusion.

Based on our experimental observations, we developed a stochastic aggregation model that allows for the simulation of aggregate size distributions (Fig. 2). Three key processes operate on size distributions of aggregates in each of the two compartments of a cell: (1) generation of the smallest-size aggregates at rate r; (2) fusion of aggregates of sizes i and j at rate $K(i,j)$ to create an aggregate of size $i+j$; and (3) random segregation of aggregates to two new compartments at division. We use the Brownian kernel

$$K(i,j) = k(i^{1/3} + j^{1/3})(i^{-1/3} + j^{-1/3})/4, \qquad (1)$$

where $k = K(1,1)$ is a parameter to be determined. This well-established kernel can be derived from Brownian diffusion of aggregates with a Stokes friction, a fusion rate increasing in proportion to the sum of the aggregate radii, and aggregate packing such that size (volume) is proportional to radius cubed. We introduce a visibility threshold ν below which aggregates cannot be detected by wide-field fluorescence imaging. We define aggregate nucleation as the fusion of two non-detectable aggregates, forming a detectable one. The resulting model was simulated with a stochastic aggregation algorithm, where the parameters of the model were obtained by fitting the experimentally measured

fusion, nucleation and size distribution of aggregates. The model predicts a pattern of aggregate segregation at cell division that is between equal segregation, where the difference in the aggregate number is minimal, and the fully random segregation, which corresponds to the model without compartmentalization. This result from the model is consistent with the experimentally measured segregation pattern.

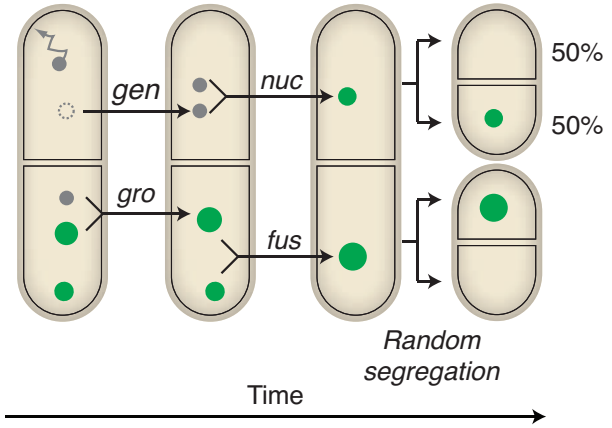

Figure 2: Stochastic aggregation model. Smallest-size aggregates (grey) are generated (*gen*) and fuse, resulting in: nucleation (*nuc*) of an aggregate of size $> \nu$ (green, ν =visibility threshold), fusion events (*fus*) between aggregates of size $> \nu$, and growth (*gro*) of an aggregate of size $> \nu$ due to fusion with an aggregate of size $< \nu$. Aggregates are randomly assigned to one of the two new compartments at division.

While symmetric damage segregation at division may allow viability under favorable conditions where damage is low, survival in severe environments, where damage is high, is more likely to require asymmetric segregation. To test whether stress conditions induce asymmetric aggregate segregation, we used oxidative and heat stress in experiments and simulated stress in the model. Both in the model and in the experiments, there was an increase in the number of aggregates before the first division, which led to an increase in the number of fusion events, which in turn resulted in a shift towards large aggregate sizes, in comparison with the control situation. Remarkably, in the second and third division, further fusion converted the aggregates into a single large one in $\sim$ 15% and 50% of the cells, respectively. This single aggregate was asymmetrically segregated to one of the sister cells at division, while the other sister cell was born without aggregates.

The model predicts that reducing fusion decreases segregation asymmetry (Fig. 3). We tested this prediction in a strain where Hsp16, a chaperone that co-aggregates with aggregated proteins, was deleted. In this strain, aggregate fusion, but not nucleation, was decreased. The decrease in fusion resulted in a decrease in aggregate segregation asymmetry, as predicted by the model. Because fusion facilitates asymmetric segregation, in the model in which aggregates were not allowed to fuse after stress, the fraction of cells born without aggregates was halved. This result from the model is consistent with the data obtained experimentally in cells defective in fusion (Fig. 3). We conclude that fusion facilitates asymmetric damage segregation after stress.

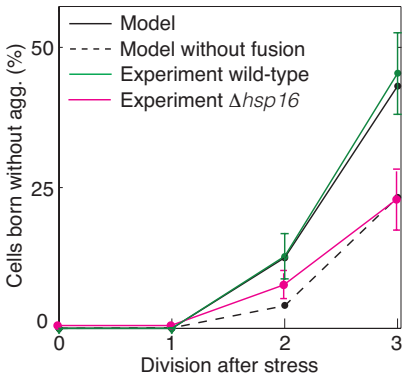

Figure 3: Aggregate fusion facilitates birth of clean cells. Fraction of cells born without aggregates during the first 3 divisions after stress. In the model in which aggregates were not allowed to fuse after stress, the fraction of cells born without aggregates was halved compared to the model with fusion (dashed and solid black line, respectively). A similar reduction in the fraction of clean cells was observed experimentally in mutant cells defective in fusion (green, wild type; magenta, mutant).

In summary, we have shown that the transition from symmetric to asymmetric segregation is facilitated by aggregate fusion: in response to increased aggregate nucleation, the stochastic movement and chaperone-mediated fusion of aggregates contribute to form a single unit of damage, which has to be segregated asymmetrically, resulting in the birth of a damage-free cell. The concepts introduced in this work may extend to other phase-partitioned molecules, such as prions, metabolic enzymes or RNA granules. In general, fusion of cellular factors may represent a universal mechanism to achieve asymmetric segregation at cell division.

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2.32 Artificial gauge fields – shaken, not stirred

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Ultracold atomic quantum gases are realized by tapping and cooling neutral atoms. Their great appeal lies in the combination of quantum optical precision and controllability with many-body physics. These systems are extremely clean, highly tunable and well isolated from (unwanted) coupling to the environment. Optically created lattice potentials allow to realize paradigmatic Hubbard-type lattice models and to reach the interesting regime of strong coupling. Moreover, densities and few-particle correlation functions can be measured both *in situ* (with single-site resolution) and, after time of flight, with respect to momentum. This makes ultracold atoms in optical lattices a unique platform for engineering coherent many-body physics, e.g. for the purpose of quantum simulation.

In order to mimic the physics of charged particles such as electrons in solids, it would be desirable to be able to create not only scalar potentials (as they can be implemented using light-shift potentials), but also to subject the motion of the neutral atoms to artificial gauge potentials mimicking magnetic fields or spin-orbit coupling. This would allow to study phenomena such as the quantum Hall effect and interesting physics in which the discreteness of the lattice becomes relevant. The latter happens for extremely strong uniform magnetic fields when the magnetic length becomes comparable to the lattice constant, leading to the famous fractal Hofstadter butterfly spectrum [1]. Another scenario of interest are Chern or topological insulators, i.e. lattices with gauge fields that vanish when averaged over a lattice cell, but nevertheless lead to a quantized Hall (or spin Hall) conductivity for a completely filled Bloch band [2]. Finally, further motivation lies in the fact that in the presence of gauge fields a systems can become highly susceptible for intriguing interaction-driven phenomena like the formation of fractional-quanutm-Hall-type states with anyonic excitations that are proposed to have applications in robust quantum information processing [3].

There are promising proposals for the realization of artificial gauge fields that take advantage of the internal atomic degrees of freedom; one idea is based on Laser-assisted tunneling in state-dependent optical lattices [4], another approach uses laser and rf-field configurations that directly create a lattice with topologically non-trivial band-structure [5]. Challenges lie in the experimental complexity or in losses due to spontaneous emission for near-resonant radiation. We have proposed an experimentally low-demanding scheme for the creation of artificial gauge fields that does not involve the internal atomic structure (so that these degrees of freedom also remain available) [6–8]. It is based on time-periodic forcing in the kHz regime. In contrast to stirring techniques (with microrotors driving specific staggered fields) [9] our approach is based on lattice shaking. We have developed our scheme in close collaboration with the experimental group of Klaus Sengstock in Hamburg, where already first experiments have been done [7, 10].

Basic scheme Consider the Hubbard Hamiltonian

$$\hat{H}(t) = -\sum_{\langle ij\rangle} J_{ij}\hat{a}_i^\dagger \hat{a}_j + \sum_i [v_i^\omega(t) + \nu_i \hbar\omega]\hat{n}_i + \hat{H}_{\rm os} \quad (1)$$

with (bare) tunneling matrix elements J_{ij} and annihilation and number operators $\hat{a}_i$ and $\hat{n}_i$ for particles (bosons or fermions) at site i of an optical lattice. $\hat{H}_{\rm os}$ collects on-site terms describing interactions or a weak static potential. The system is driven by a rapid periodic drive $v_i^\omega(t) = v_i^\omega(t+T)$ of frequency $\omega = 2\pi/T$ and zero average $\langle v_i^\omega(t)\rangle_T \equiv \frac{1}{T}\int_0^T \mathrm{d}t\, v_i^\omega(t) = 0$ as it can be realized as an inertial force by shaking the lattice in space along a periodic orbit. Additionally, the lattice might comprise strong potential off-sets (like a superlattice modulation or a Wannier-Stark tilt) that are resonant with the forcing and described by the integers ν_i. The gauge transformation $\hat{U} = \exp(i\sum_i \chi_i(t)\hat{n}_i)$, where $\chi_i(t) = \chi_i^\omega(t) - \nu_i\omega t + \gamma_i$ with $\hbar\chi_i^\omega(t) = -\int_0^t \mathrm{d}\tau v_i^\omega(\tau) + \langle\int_0^t \mathrm{d}\tau v_i^\omega(\tau)\rangle_T$ and constants γ_i, leads to the new Hamiltonian $\hat{H}'(t) = \hat{U}^\dagger\hat{H}\hat{U} - i\hbar\hat{U}^\dagger(\mathrm{d}_t\hat{U})$, which for large frequencies $\hbar\omega \gg J_{ij}, U$ (with Hubbard interaction U comprised in $\hat{H}_{\rm os}$) can be approximated by its time average

$$\hat{H}_{\rm eff} \equiv \langle \hat{H}'(t)\rangle_T = -\sum_{\langle ij\rangle} J_{ij}^{\rm eff}\hat{a}_i^\dagger\hat{a}_j + \hat{H}_{\rm os}. \quad (2)$$

with effective tunneling matrix elements

$$J_{ij}^{\rm eff} = |J_{ij}^{\rm eff}|\mathrm{e}^{i\theta_{ij}} = J_{ij}\langle \mathrm{e}^{-i[\chi_i(t)-\chi_j(t)]}\rangle_T. \quad (3)$$

For $\nu_i - \nu_j = 0$ the forcing leads to a modification of the bare tunneling matrix element. In turn, a finite energy off-set $(\nu_i - \nu_j)\hbar\omega \neq 0$ between neighboring sites suppresses tunneling, thus $|J_{ij}^{\rm eff}| = 0$, unless finite driving $v_i^\omega(t) - v_j^\omega(t) \neq 0$ leads to AC-induced coherent tunneling (ACT) with $|J_{ij}^{\rm eff}| \neq 0$.

The aim of our work is to use this control scheme to induce non-trivial Peierls-type phases θ_{ij} that cannot

[5] in collaboration with Lewenstein's group (theory) at ICFO Barcelona (P. Hauke, A. Celi, and M. Lewenstein) and Sengstock's group (experiment) at University of Hamburg (J. Struck, C. Ölschläger, M. Weinberg, J. Simonet, P. Windpassinger, and K. Sengstock)

be eliminated globally by choice of gauge (i.e. by adjusting the constants γ_i). Such non-trivial phases correspond to artificial abelian gauge fields; the gauge-invariant magnetic flux $\phi_P \in (-\pi, \pi]$ piercing a lattice plaquette P is (modulo 2π) obtained by summing the θ_{ij} around P.

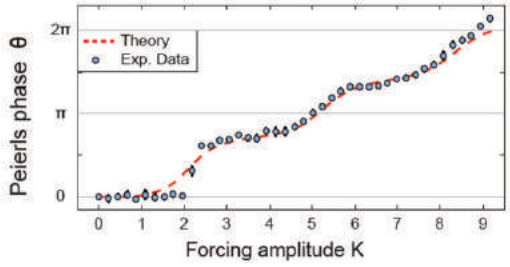

Figure 1: Peierls phase in a 1D lattice, the theoretical prediction is confirmed by the experimental data, taken from Ref. [7] .

Symmetries We find that the *global* reflection symmetry (r) $v_i^\omega(-t-\tau) = v_i^\omega(t-\tau)$ with respect to a global time τ implies trivial phases $\theta_{ij} = 0$ (using the choice $\gamma_i = -\nu_i\omega\tau$). Moreover, if ACT is not involved ($\nu_i - \nu_j = 0$), $\theta_{ij} = 0$ follows already from the *local* reflection symmetry (r') $v_{ij}^\omega(-t-\tau_{ij}) = v_{ij}^\omega(t-\tau_{ij})$ with independent local times τ_{ij} (since $\gamma_{ij} = \nu_{ij}\omega\tau_{ij} = 0$, independent of τ_{ij}), or from the shift antisymmetry (s) $v_i^\omega(t-\frac{T}{2}) = -v_i^\omega(t)$ (choosing $\gamma_i = 0$) [11]. Therefore, ACT significantly reduces the constraints on the driving function $v_i^\omega(t)$ for the creation of artificial magnetic fields. This is nicely exemplified by a recent proposal where already simple sinusoidal forcing [fulfilling (r') and (s)] leads to magnetic fields when combined with ACT – provided the temporal phase of the driving can be made site dependent [thus breaking (r)] [12].

Proof of Principle Our theory was confirmed in an experiment where a tunable artificial gauge potential has been induced in a 1D lattice [7]. The induced Peierls phase was inferred from a shift of the measured momentum distribution (Fig. 1).

Triangular and Kagomé lattice The simplest scenario for inducing a magnetic flux via lattice shaking involves triangular plaquettes, here no energy off-sets are required ($\nu_i = 0$). Using a driving function that breaks both symmetries (r) and (s), like the one depicted in Fig. 2d, one can achieve a finite flux φ_Δ through a plaquette Δ. The inverted plaquette ∇ will be pierced by the opposite flux, $\varphi_\nabla = -\varphi_\Delta$, such that tunable staggered flux configurations can be induced in triangular or Kagomé lattices (Fig. 2a and b) [8]. This allows to smoothly tune the system to the fully frustrated π-flux configuration for which exotic quantum-disordered ground state are expected in a system of hard-core bosons [6] or to bias the system towards one of the time-reversal symmetry broken ground states found for weakly interacting bosons [10].

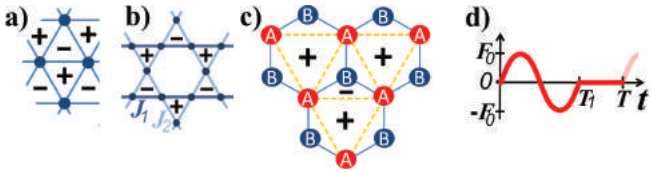

Figure 2: (a,b) Triangular and Kagoḿe lattice with staggered plaquette fluxes $\pm\varphi$ (indicated by $+$ and $-$ signs). (c) Lattice used to create a Chern insulator. (d) Periodic force breaking symmetries (r) and (s).

Chern insulators and non-abelian gauge fields In a hexagonal lattice system (Fig. 2c) with a staggered energy off-set between A and B sites, $\nu_A - \nu_B = \hbar\omega$, we have shown that lattice shaking can lead to a situation where the lowest band of the effective Hamiltonian possesses a quantized Hall conductivity when filled with fermions; the system is a Chern insulator [8]. If the energy off-sets are spin-dependent (a situation that can be realized using the polarization of the laser light creating the lattice), a topological insulator with quantized spin-Hall conductivity can be realized. Note that our scheme is different from recent proposals for Floquet topological insulators in condensed matter [13]. For a configuration with site-dependent Zeeman-fields of varying quantization axes, one can create any non-abelian SU(2)-flux (Wilson loop) for spin-1/2 particles on a square plaquette via lattice shaking [8].

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2.33 Universal Quantum Localizing Transition of a Partial Barrier in a Chaotic Sea

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Introduction In the phase space of generic two-degree-of-freedom (2D) Hamiltonian systems regions of regular and chaotic motion are dynamically separated by impenetrable barriers. Within a chaotic region so-called *partial barriers* are ubiquitous. They divide it into distinct sub-regions, connected by the *turnstile mechanism*, which works like a revolving door between two rooms. The volume in phase space, which is transported across the partial barrier in each direction per time is the flux Φ. Partial barriers can originate [1] from a cantorus or the combination of the stable and unstable manifold of a hyperbolic fixed point. A hierarchy of these partial barriers gives rise to a power-law decay of correlations and of Poincaré recurrence time distributions.

What is the implication of a partial barrier on the corresponding quantum system? In 1984 MacKay, Meiss, and Percival [2] conjectured that the flux Φ, an area in phase space, has to be compared with the size h of a Planck cell to judge the quantum implications. For $h \gg \Phi$ quantum transport is suppressed. A time-evolved wave packet, initially associated with a phase space region on one side of the partial barrier, cannot acquire a substantial weight on the other side of the partial barrier even in the limit of arbitrarily large times; see Fig. 1. This is also reflected in the eigenstates having much stronger projection in either one of the two sides. In contrast, for $h \ll \Phi$ wave packets in the long-time limit as well as eigenstates extend over both regions as if the partial barrier were not present. This corresponds to the classical behavior where in the long-time limit chaotic orbits explore both regions ergodically. The quantum localizing transition between quantum suppression and classical transport has been studied theoretically and experimentally and the most extensive study goes back to Bohigas, Tomsovic, and Ullmo (BTU) [3]. While the quantum localizing transition is partially understood, the full quantitative transition even for an isolated partial barrier so far is not. In particular one is interested in the transition curve, including its universal scaling, center, width, shape, and whether it has quantized steps. Here we review results reported in Ref. [4].

Designed map Consider a family of designed area preserving maps F of the two-torus, see Fig. 1(a) for an illustration. The phase space consists of a large chaotic sea between the regular tori. There is a hyperbolic fixed point at the center whose stable and unstable manifold can be used to construct a partial barrier separating the regions 1 and 2 of approximately the same size. The region between the partial barrier and its preimage defines the turnstile areas of size Φ [1]. The map F was designed such that this partial barrier is well isolated with a small tunable flux. Quantum mechanically the system is described by a unitary operator U acting on a Hilbert space of finite size N with effective Planck's constant $h = 1/N$. The time evolution of a wave packet $\psi(t)$ is given by $\psi(t+1) = U\psi(t)$.

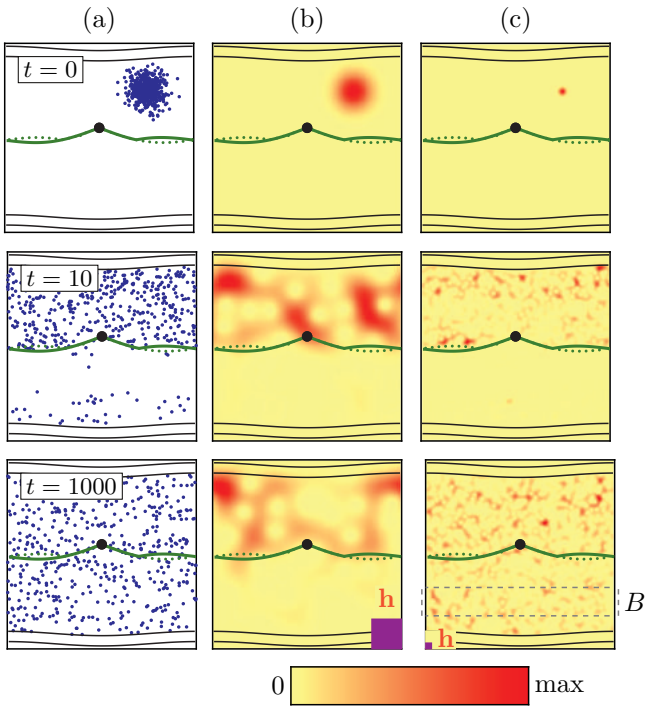

Figure 1: Classical (a) and quantum (b, c) time evolution across the partial barrier (solid green line) with classical flux $\Phi \approx 1/200$, the area between partial barrier and its preimage (dotted line). (a) Time evolution of an ensemble of 100 orbits shown at times $t = 0$, 10, and 1000. (b) Time evolution of a coherent state in Husimi representation for $h = \frac{1}{40}$ (violet square at the bottom) and (c) $h = \frac{1}{1000}$.

Wave packet dynamics In order to quantify the quantum transition of a partial barrier we define the (relative) asymptotic transmitted weight w_∞ of a wave packet ψ started in region 1 as

$$w_\infty[\psi] := \frac{\langle \mu[\psi(t)] \rangle_t}{\mu^{\mathrm{cl}}}. \qquad (1)$$

It is the time-averaged transmitted weight divided by the corresponding classical weight μ^{cl}. As initial state we choose $p_0 = 0.7$ and as a measure μ the probability of $\psi(t)$ within the lower region. The classical weight μ^{cl} is the relative time a long chaotic orbit spends in the lower region. The definition of w_∞ implies that it makes a transition from 0 for $h \gg \Phi$ to 1 for $h \ll \Phi$.

In the latter case this happens because any initial state becomes uniformly distributed at large times as would a classical distribution of trajectories.

Figure 2 shows the resulting transition of w_∞ vs. Φ/h for three different fluxes Φ, averaged over 100 values of the Bloch phase and 100 time steps after time $T = 2^{20}$. All data sets fall on top of each other under this scaling, i.e. Φ/h is the correct scaling parameter as conjectured in Ref. [2]. We expect that the quantum localizing transition for any partial barrier follows the same universal curve as a function of Φ/h. This expectation assumes that the relative volumes of the two regions are of the same order and that the mixing time is much shorter than the dwell time. Figure 2 shows that on a logarithmic scale the transition is symmetric with respect to the point $\Phi/h = 1$, $w_\infty = \frac{1}{2}$. Thus the transition point is reached when flux Φ and Planck's constant h are equal. The transition is found to be smooth with no indications for quantized steps at integer values of Φ/h. By defining the transition region as the interval in Φ/h for which $w_\infty \in [0.1, 0.9]$, the width is found to be quite large, namely two orders of magnitude, indicated by the arrow in Fig. 2. The overall behavior of the transition is well described by the symmetric curve

$$w_\infty = \frac{\Phi/h}{1 + \Phi/h}. \qquad (2)$$

This equation can also be motivated by a phenomenological 2×2 matrix model [4].

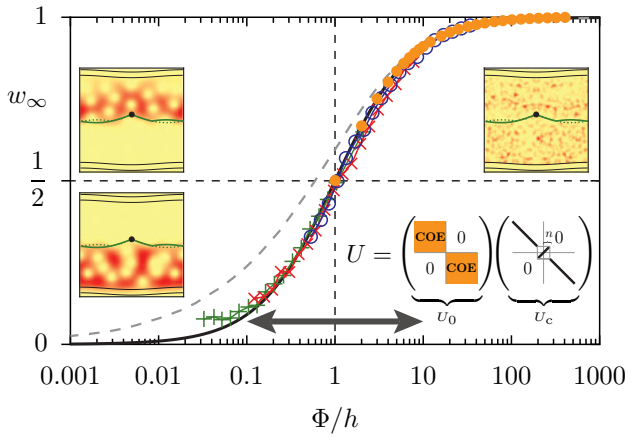

Figure 2: Asymptotic transmitted weight w_∞ vs. Φ/h for $\Phi \approx \frac{1}{3000}$ (pluses), $\frac{1}{800}$ (crosses), $\frac{1}{200}$ (circles), $h = \frac{1}{100}, \ldots, \frac{1}{6400}$ compared to Eq. (2) (solid line), the BTU model (gray dashed line) and the channel coupling model (orange circles) using 1000 realizations with $N = 1000$. Insets: Husimi representation of typical eigenstates for $\Phi \approx \frac{1}{200}$, $h = \frac{1}{40}$ (left) and $h = \frac{1}{1000}$ (top right). Illustration of the matrix structure (bottom right).

Eigenstate properties Complementary to the time evolution of wave packets, one can consider properties of eigenstates of the quantum map. States are dominant in one of the regions in the case of $h \gg \Phi$, while for $h \ll \Phi$ they extend over the whole chaotic region, see insets of Fig. 2. Thus the behaviour is similar to the wave-packet dynamics at large times, see Fig. 1. We define an average eigenstate equipartition measure $\langle w_{12} \rangle$ and observe the same transitional behavior as for w_∞, again well described by Eq. (2).

Matrix Modeling In order to gain insight into the quantum mechanism of a partial barrier we now study appropriately adapted random matrix models. In the BTU model [3] two matrices of the Gaussian orthogonal ensemble, representing two chaotic regions, are globally coupled with a strength determined by Φ/h. Figure 2 shows that for $\Phi/h < 10$ this model overestimates the value of $\langle w_{12} \rangle$ found for the quantum map. We attribute this discrepancy to the global coupling of the BTU model. Instead we propose to model the classical turnstile mechanism by a local coupling via a channel. In a unitary model $U = U_0 \cdot U_c$ we decompose the dynamics into a coupling matrix U_c modeling the turnstile transport multiplied by an uncoupled matrix U_0 modeling the mixing in each of the regions, see Fig. 2 inset. The coupling matrix U_c is an identity matrix, where the central $2n \times 2n$ block has ones on the anti-diagonal. It couples the two regions via n modes for each direction of the channel. This models the directed transport of a turnstile in the classical system. The matrix U_0 is block diagonal consisting of two matrices of the circular orthogonal ensemble (COE) of sizes $N/2 \times N/2$ and the limit of large N is considered. This model has only one parameter, namely the number of modes $n = \Phi/h$. The resulting $\langle w_{12} \rangle$ for this unitary channel coupling model is shown in Fig. 2 and is in very good agreement with the numerical data of the designed map F. It is stressed that this agreement has been obtained without any fitting parameter. We observe that this model with local coupling is better describing the data for the map F for $\Phi/h \leq 10$ compared to the global coupling BTU model. A more detailed model with continuous transmission is investigated in Ref. [5] and gives similarly good agreement and extends even into the regime of $\Phi/h < 1$. These results suggest that the turnstile mechanism of the classical system is quantum mechanically described by a local coupling via a channel.

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2.34 Boltzmann-Ginzburg-Landau approach to simple active matter models

HUGUES CHATÉ

Active matter loosely refers to all situations where some energy is spent locally to produce some directed, persistent motion. In this context, collective motion naturally occupies a central spot. The statistical physics approach has been, not surprisingly, aimed at uncovering generic, universal properties to be exhibited in many different situations. To this aim, simple "microscopic" (particle-, agent-based) models have been studied and continuous theories have been proposed.

Of the particular importance of connecting the micro and macro descriptions in active matter Because the equations constituting these continuous "hydrodynamic" theories typically contain many terms, deriving them from generic, simple, microscopic starting points is very important, since then all transport coefficients of these compressible active fluids are defined in terms of a few microscopic control parameters and one is not faced with the exploration of a huge parameter space containing many "non-physical" regions.

Previous attempts to derive hydrodynamic equations for active matter systems have yielded interesting equations but suffer from the absence of a real control on the balance of the various terms written. We have recently proposed to combine a classic kinetic theory approach with ideas stemming from weakly nonlinear analysis in order to obtain well-controlled, minimal, continuous field equations from simple models for collective motion.

The Boltzmann-Ginzburg-Landau framework Consider a simple self-propelled particle model like the celebrated Vicsek model: point particles move at constant speed v_0, aligning their heading with local neighbors, in the presence of noise. It has only two key parameters, the global density of particles ρ_0, and the noise strength σ. At low enough σ/large enough ρ_0, a fluctuating, orientationnally-ordered collectively moving phase exists, which typically presents spontaneously-segregated nonlinear structures and/or anomalous, long-range correlations.

In the dilute limit, interactions are only binary, and one can write a Boltzmann equation ruling the evolution of the one-particle function $f(r,\theta,t)$ representing the probability of finding a particle of orientation θ at time t and position r. Classically, this equation takes the form:

$$\partial_t f(\mathbf{r},\theta,t) + v_0\,\mathbf{e}(\theta)\cdot\nabla f(\mathbf{r},\theta,t) = I_{\rm dif}[f] + I_{\rm col}[f] \quad (1)$$

where the angular diffusion and collision integrals are defined according to the local dynamical rules.

A usual procedure to derive hydrodynamic equations is to expand the above equation in Fourier series of the angular variable θ, yielding an infinite hierarchy of equations for various fields $\hat{f}_k$. While $\hat{f}_0$ is nothing but the density field, some $\hat{f}_k$ actually represent "hydrodynamic fields" ($\hat{f}_1$ codes for a polarity field, $\hat{f}_2$ a tensorial field, etc.). For a problem where polar order emerges, one tries to write a closed equation for $\hat{f}_1$, whose variations are assumed to be small and slow. Assuming, in this case, that $\hat{f}_2$, $\hat{f}_3$, etc., are faster fields, one can express all these fields in terms of $\hat{f}_1$. This formally yields an infinity of terms, and one then resorts to "counting gradients" to limit them.

If we suppose further that one is in the vicinity of the transition at which order emerges, one can formalize, in the spirit of the Ginzburg-Landau approach to amplitude equations, an explicit scaling ansatz which allows a full control of all terms. In the case of the emergence of polar order in a system of self-propelled polar particles, the correct scaling reads:

$$\rho-\rho_0\sim\epsilon,\ \ \hat{f}_k\sim\epsilon^k,\ \ \nabla\sim\epsilon,\ \ \partial_t\sim\epsilon \quad (2)$$

If one assumes to be at distance ϵ^2 from the threshold, one obtains, at order ϵ^3, a well-behaved equation for $\hat{f}_1$ containing proper nonlinear terms insuring the saturation of linear instabilities.

Results We have applied this approach to the basic universality classes of self-propelled particles systems interacting solely by alignment. A thorough analysis of the obtained equations reveal that they possess nonlinear solutions in excellent qualitative agreement with the behavior of the Vicsek-style models they are derived from. Some of these results are already published [1,2]. This is yet another instance where the extra constraint of being near an instability threshold actually helps to obtain well-behaved sets of equations observed to be valid well beyond this vicinity, as long as no other symmetry-breaking transition occurs.

For instance, in the case of polar point particles aligning nematically (metaphorical "self-propelled rods"), the procedure described above yields, in addition to the continuity equation, the following equations ruling the polar field f_1 and the tensorial field f_2 (here in two space dimensions, dropping the $\hat{}$, and using the complex gradient $\nabla=\partial_x+i\partial_y$, see details in [2]):

$$\partial_t f_1 = -\frac{1}{2}(\nabla\rho+\nabla^* f_2)+\frac{\gamma}{2}f_2^*\nabla f_2-(\alpha-\beta|f_2|^2)f_1+\zeta f_1^* f_2 \quad (3)$$

$$\begin{aligned}\partial_t f_2 \;=\; & -\frac{1}{2}\nabla f_1+\frac{\nu}{4}\nabla\nabla^* f_2-\frac{\kappa}{2}f_1^*\nabla f_2-\frac{\chi}{2}\nabla^*(f_1 f_2)\\ & +(\mu-\xi|f_2|^2)f_2+\omega f_1^2+\tau|f_1|^2 f_2 \end{aligned} \quad (4)$$

where all coefficients depend only on the noise strength σ (via the $\hat{P}_k$ coefficients) and the local density ρ (again, see [2] for details and explicit expressions of the 11 remaining transport coefficients) .

A combination of analytical and numerical analysis of these coupled nonlinear partial differential equations shows that they are faithful, at a semi-quantitative level, to the original Vicsek-style model (see Figure 1 for a pictorial confirmation).

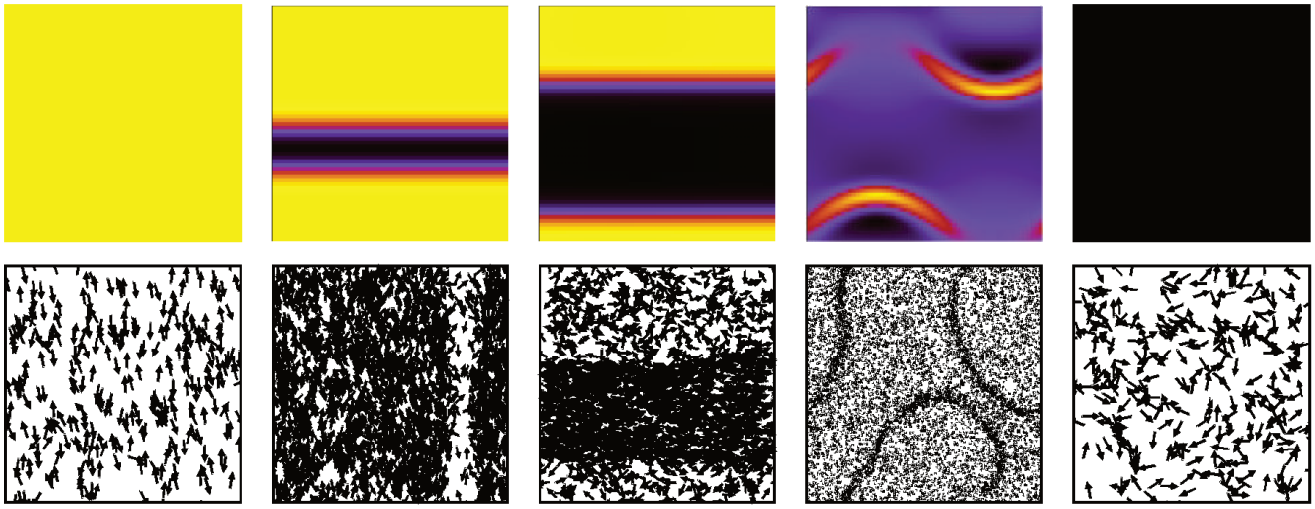

Figure 1: Snapshots of simulations of (i) the Vicsek model with nematic alignment (bottom row); (ii) the field equations derived using the Boltzmann-Ginzburg-Landau approach described here (top row) in two dimensions. For the microscopic model, a fraction of the particles are represented in each panel. For the continuous equations, the amplitude of the nematic field ($|f_2|$) is represented on a color scale going from black ($f_2 = 0$) to yellow (maximum value). In each case, 5 values of the noise strength σ are represented. From left to right, increasing σ: (i) homogeneous nematically-ordered state; (ii-iii) inhomogeneous ordered state with an nematically-ordered dense band; (iv) space-time chaos of nematic bands; (v) homogeneous, microscopically-disordered state. For details, see [2, 3].

Perspectives All basic classes of "dry flocking" problems will soon have been treated using our approach. Some discrepancies between the obtained continuous equations and the original Vicsek-style models do exist in some cases. We suspect that most of them are due to truncation effects: increasing the order at which the truncation/closure is made should resolve them. In some cases, we believe the microscopic models need to be "revisited" as the continuous descriptions hint at overlooked phenomena. We plan to investigate all this in the near future, performing more extensive simulations of the micro models, building more refined hydrodynamic descriptions, and comparing them to direct numerical simulations at the Boltzmann level.

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Chapter 3

Details and Data

3.1 PhD Program

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

Prospective PhD students have several options of contacting scientific advisors at the 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 the 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 the mpi**pks**. In 2011, a total of 85 PhD students were working at the mpi**pks**, including 39 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 2012 were 91 PhD students working at the mpi**pks**, including 42 students from abroad. We counted 6 successful final PhD exams for the year 2011 and 9 exams for the year 2012.

Besides their scientific work at the 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 the mpi**pks**. Many of them participate actively in these events by presenting short talks or posters. All students of the 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 the 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* (IMPRS) was founded in 2005, within the 4th round of approved research schools of the Max Planck society. After a positive evaluation by the Max Planck society in 2008, the research school has successfully completed its first funding period of six years by the end of 2010. Our application for a second funding period for further six years, starting in January 2011, was approved by the Max Planck Society. With the beginning of the new funding period, our IMPRS underwent directional changes regarding its research focus and the affiliated partner institutions. It is currently a collaboration of the followning institutions:

- Technische Universität Dresden — TUD
- Max Planck Institute for Chemical Physics of Solids — MPI-CPfS
- Max Planck Institute for the Physics of Complex Systems — mpi**pks**
- 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)

During the first six years, the IMPRS comprised research groups working both theoretically and experimentally. However, due to current development of the scientific landscape in Dresden and in coordination with our experimental colleagues, we decided to shift the focus of our research school towards "Modelling in the natural sciences - from algorithms to applications" for the second funding period. Our former partner institutions with mainly experimental research focus, namely the Leibniz Institute for Solid State and Materials Research (IFW) and the Helmholtz-Zentrum Dresden-Rossendorf (HZDR), are no longer affiliated with the IMPRS, but envisage the foundation of a separate graduate school. A close collaboration of this school with our IMPRS is anticipated. At the same time, the number of participating research groups from the TU Dresden has increased. The departments of engineering, math and computer science joined the IMPRS, harmonically complementing the research fields in concordance with our new focus.

PhD students Since its foundation, the IMPRS has so far admitted 117 students in total. By the end of 2012, 59 students have obtained their doctoral degree, 9 moved to another location, while 49 are currently enrolled in our PhD program. Approximately half of the present students are Germans, the other students come from all over the world. The distribution by geographical origin is as follows, Europe: 35 (Germany 23, Czech Republic 5, Italy 3, Poland 2, Sweden 1, France 1), Asia: 8 (India 4, Iran 2, Turkey 1, Jordan 1), South and Central America: 5 (Mexico 3, Brazil 1, Colombia 1), Africa: 1 (Ethiopia). The distribution among the affiliated partner institutions is TUD: 19, mpi**pks**: 19, IOCB: 3, ICT: 3, MPI-CPfS: 2, ILTSR: 2, HZDR: 1. The Polish PhD students are enrolled in Wrocław universities, while the Czech PhD students are members of the Czech Academy of Sciences and financially supported by the IMPRS.

Scientific events After the official opening ceremony in September 2005 we started a series of annual IMPRS retreats held in autumn at different locations on the countryside around Dresden (see picture). In these meetings, with a total duration of three days, the PhD students present their work in talks to provoke discussions among all students including those working in different fields. Furthermore, the retreats are an important component to facilitate the initiation of recently enrolled PhD students of the IMPRS and to strengthen their interaction with IMPRS students who are in an advanced stage of their PhD. In 2011, the annual retreat simultaneously served as a kickoff-meeting for the second funding period, to which we also invited senior scientists affiliated with our research school. They introduced themselves and their research topics to the IMPRS students during the first afternoon, and due to the positive reception by the PhD students, we decided to keep this format for future annual retreats as well.

In order to closely integrate our Polish and Czech partner institutions, we organized joint block seminars in Wrocław and Prague. 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. The most recent event was a Winter school in Wrocław in October 2012. The lecture

IMPRS meeting in Käbschütztal in September 2012.

program was devoted to GPU computing and its methods and applications in the natural sciences. All of these events were open to local students as well.

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 our institute. They are open to students from the Technische Universität Dresden; Participation of the IMPRS students in the lectures is monitored by a credit-point system.

Organization and administrative matters The school is operated by the IMPRS board with the following members:

Prof. Jan-Michael Rost (chairman, mpi**pks**)	
Prof. Walter Strunz (TUD)	Prof. Roderich Moessner (mpi**pks**)
Prof. Gotthard Seifert (TUD)	Prof. Pavel Jungwirth (IOCB Prague)
Prof. Juri Grin (MPI-CPfS)	Prof. Jozef Sznajd (ILTSR Wrocław)
Prof. Wolfgang Nagel (TUD)	Prof. Gianaurelio Cuniberti (TUD)
Prof. Axel Voigt (TUD)	Dr. Michael Genkin (coordinator, mpi**pks**)

The board meets approximately once per year. All matters regarding the operation of the IMPRS are discussed and decided in these board meetings. 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. Seifert and Dr. Genkin, meets upon demand. In particular, it pre-screens the numerous applications within each call for applications, which are announced twice per year.

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 by the coordination office at our institute.

Future events and prospectives In May 2013, our institute will host a new kind of scientific IMPRS event. Together with three other International Max Planck Research Schools, with which our scientific focus partly overlaps, we organize a joint workshop. The primary aim is to bring together the PhD students of the four research schools, but also to strengthen the interaction between the involved Max Planck institutes and the affiliated partner institutions.

3.3 Workshop and Visitors Program

The Visitors Program of the 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 Mentoring Program, a Platform for Social Activities 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 the mpi**pks**.

International Workshop "Noise in Non-Equilibrium Systems: From Physics to Biology", April 11 - 14, 2011

During 2011, the mpi**pks** hosted 192 guest scientists with contracts for at least three months, and 193 during 2012 including predocs. We received a large number of senior scientists who used their sabbatical time for long-term research stays at the mpi**pks**. This led to an enhanced 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. From 2011-2012, we enjoyed large scale activities of two Advanced Study Groups, one of which was formed in 2011, one in 2011/2012.

The guest scientists are usually linked to the research groups at the mpi**pks**. In some cases they conduct more independent research, which leads to synergy effects. Synergy effects are further enhanced due to the opportunity to listen to talks and lectures within the Seminar and Workshop Program of the mpi**pks** (see p. 131).

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 the mpi**pks**: *Dr. Achilleas Lazarides* on *Collective phenomena*, in Condensed Matter, *Dr. Benjamin Friedrich* on *Mechanical and chemical regulation in biological systems*, and *Dr. Robert Johne* on *Light-matter interaction at the single photon level* (see reports on p. 125). Two PKS fellows have left the institute: *Dr. Emil Bergholtz (Correlated quantum matter)* moved to a staff position at Freie Universität Berlin, and *Dr. Chiu Fan Lee (Physical properties and pathogenesis of protein aggregation)* took up a faculty position at the Imperial College in London.

To strengthen the transfer of knowledge and experience at the 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 the mpi**pks** and can nominate a young guest scientist for the Visitors Program. The 2011 and 2012 fellows were *Prof. B. Altshuler* and *Prof. T. Nakayama* (see report on p. 121).

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 related to collaborations between the mpi**pks** research groups and other institutes. Their number reached 302 during the year 2011, and 311 during the year 2012.

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.

3.3.1 Institute's Fellows

3.3.1.1 Gutzwiller-Fellows

Clathrate compounds as phonon-glass thermoelectric materials: Why glass-like though crystalline?
(Prof. T. Nakayama)

The high performance of thermoelectricity is achieved for materials possessing the lowest possible phonon thermal conductivity $\kappa(T)$ and the highest possible electric conductivity $\sigma(T)$. These impose the conditions on searching efficient thermoelectric materials which should simultaneously possess glass-like phonon thermal conductivities and crystalline electrical conductivities [1]. This is really a controversial concept from the aspect of materials science. If such materials can be synthesized, this truly becomes one of the most significant innovations in alternative energy technologies.

In this decade, type-I clathrate compounds have attracted a great deal of interest as potential thermoelectric materials satisfying these conditions. These compounds constitute networked cages consisting of nano-scale tetrakaidecahedron with 14 flat faces (14 hedrons) and dodecahedron with 12 flat faces (12 hedrons), in which the group 1 or 2 elements in the periodic table are en-caged as the so-called "rattling" guest atom. It is remarkable, though these compounds take "crystalline" cubic structure, they emerge glass-like phonon-thermal conductivities $\kappa(T)$ when the guest atoms in etrakaidecahedron take the off-center position [2–4]. In particular, these symmetry-broken off-center systems show unusual glass-like thermal and dynamical properties, providing the remarkable broad-peak at 0.5 THz frequencies in specific heats [5] and optical spectroscopies [6, 7] which are almost identical to the so-called Boson peak observed in structural glasses. The efficient thermoelectric effect is realized in clathrate compounds showing these glass-like characteristics.

The point is why these clathrate compounds without topological disorder, different from conventional disorder systems, show almost identical dynamical and thermal properties to those of structural glasses. The aim of my research project is to theoretically investigate the physical origin of glass-like behaviors observed in these clathrate compounds. The research is important not only from the view-point of solid state physics itself, but also from the practical problem exploring efficient thermoelectric materials.

The followings are the subjects I have investigated during the stay 2012/13 in mpi**pks**.
1). The first is on the dynamic properties of type-I clathrate compounds in the THz frequency range. I have investigated the glass-like characteristics observed in this frequency range by highlighting the role of randomly oriented guest ions in network cages. The potential function for guest ions takes the form

of the "sheared" bottom of wine bottle. This type of the potential is expressed by the discrete Ginzburg-Landau-Higgs potential in the local gauge theory. Here I introduce two variables on small fluctuations around the equilibrium position of guest ions expressed by the radial displacement $h_\ell(t)$ and the angular one $\theta_\ell(t)$ in the cage of the site ℓ. These correspond to two different type of low-lying optic modes observed in terms of infrared-spectroscopy [7] and Raman scattering [6]. The hybridization between acoustic phonons and these optic modes yields the flattening of acoustic phonons starting from the middle of Brillouin zone, which leads the disappearance of the Umklapp process and the appearance of the plateau in $\kappa(T)$.
The onset temperatures $T_{\rm p}$ of the plateau temperature region of $\kappa(T)$ depend on the kind of element of encaged guest ions. These characteristics are correlated with the lowest-lying mode expressed by the dynamic variable $\theta_\ell(t)$ attributing to the libration mode of off-center guest ions. The proposed analytic relation between the onset temperature T_p and the eigenfrequency of the lowest optic mode ω_0 can be utilized in finding efficient thermoelectric materials, namely, type-I clathrate compounds possessing the lowest frequency ω_0 of the optic mode relevant to the libration motion.

2). The second is on the theory of quasi-T-linear specific heats observed in symmetry-broken clathrate compounds. The specific heat of type-I clathrate below 1 [K] is in general scaled by the relation $C(T) \simeq \alpha T^{1+\delta} + \gamma T^3$ with $\alpha \simeq 30\ \left[\mathrm{mJ\,mol^{-1}\,K^{-2}}\right]$, $\delta \simeq 0.1$ and $\gamma \simeq 50\ \left[\mathrm{mJ\,mol^{-1}\,K^{-4}}\right]$ [5]. The temperature dependence $T^{1+\delta}$ is not exactly linear to T. This term has no connection with conduction electron specific heat proportional to γT, where γ is much smaller than α in the above expression. At such low temperatures, the experimental data have been analyzed in a line with the two-level tunneling model (TLS) suitable to the cases of structural glasses, which predicts the T-linear dependence of $C(T)$. If each off-center guest-ions would independently contribute to the low temperature specific heats, the estimated specific heat $C(T)$ becomes two orders *larger* than the observed values at 1 K.
The key to understand this contradiction is that the deviation of guest ions from the center of the cage induces electric dipole moments due to the effective charges of the guest ion and the the cage. Electric dipole moments provide long-range interactions among dipoles in cages. These dipoles constitute equilateral-triangle configuration, which generates a frustrated situation necessary to the emergence of glass-like properties. I have pointed out that the exponent δ should appear also in the temperature dependence of phonon thermal conductivity in the form of $\kappa(T) \propto T^{2-\delta}$. I have tried to explain the origin of the finite exponent δ highlighting the long-range interactions among dipoles.

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The Coarse-Graining of Complex Networks
(Prof. Dr. Yannis Kevrekidis)

The subject I focused on, along with students and collaborators, during my several stays at the **mpipks** in Dresden over the period of the Fellowship was the *coarse-graining of complex evolving networks*. This is a subject of joint interest with the group of Dr. Thilo Gross, his students, visitors and collaborators (notably Prof. Bassler from Houston and Dr. del Genio); but also the subject of joint interest with the Center for Dynamics at TU Dresden and many scientists visiting the Institute and participating in its scientific events, culminating with the May 2012 conference on complex networks. Significant advances were made during this period in the equation-free modeling of complex networks and in the discovery of coarse-grained variables capable of describing their evolution via data-mining, and, in particular, via appropriate modifications/extensions of the Diffusion Map approach to the study of graph-type data.

Our fundamental tool is *equation-free computation* [1, 2] – a systematic approach that links detailed, fine scale simulation codes (e.g. molecular dynamics, individual-based simulators) with traditional continuum numerical analysis, and facilitates the extraction of information at the macroscopic, systems level. Designing and exploiting appropriately designed brief bursts of fine scale simulation, we can circumvent the derivation of accurate model closures and the explicit resulting reduced macroscopic models (typically partial differential equations for the evolution of low-order statistics of the relevant molecular

distributions). Evolving networks can also be thought of as complex systems [3,4] in which, however, the interacting entities are not molecules but rather nodes and edges, and the rules of evolution do not come from physics/chemistry but from, say, social interactions. The overarching goal is to link, through judicious computational modeling, established tools of statistical mechanics with the study of large complex network evolution dynamics.

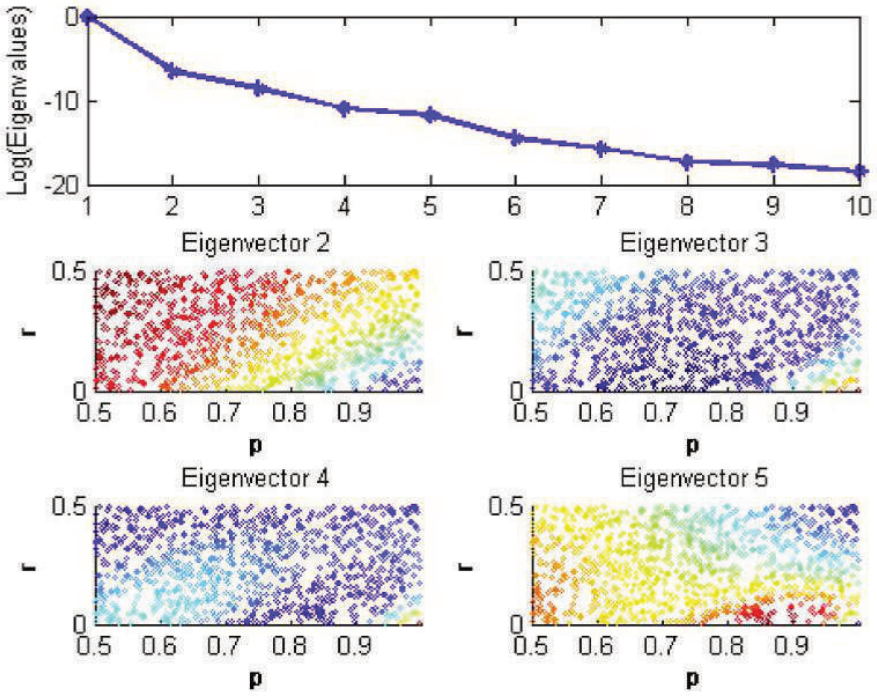

Figure 1: Data-mining ensembles of two-parameter Chung-Lu graphs: The leading eigenvalues of the random walk matrix calculated using the subgraph similarity measure are first plotted. The corresponding first four non-trivial eigenvectors are then illustrated in a way that brings forth their relation to the construction parameters p and r. In these plots, each graph is denoted as a point. The x and y coordinates of the point correspond to the parameters p and r used to construct that particular graph. The graphs are colored based on the magnitude of their components in the eigenvectors of the diffusion mpa random walk matrix A.

To help explore this, we plot eigenvectors 2 and 3 against each other in Fig. 2. The figure clearly suggests (through its obvious two-dimensionality) that these two eigenvectors are independent of each other. Furthermore, when the points in these plots are colored by the two parameters p and r used to construct the graphs, two independent directions - a roughly "left-to-right" for p and a roughly "top-to-bottom" for r- can be discerned on the $v2$-$v3$ plane, Fig. 2. This strongly suggests that the Jacobian of the transformation from (p, r) to ($v2$, $v3$) is nonsingular on our data. Thus, these two eigenvectors, obtained solely through our data-mining approach, can equivalently be used to parameterize the set of graphs constructed using the parameters p and r. The spectral similarity approach yields qualitatively comparable results (with slight quantitative differences).

We have been able to demonstrate such an equation-free approach to network evolution in a sequence of publications (including recent ones, supported in part through the Fellowship [5–7]). The crucial issue, however, that underpins such efforts, is the *a priori* knowledge (through experience, intuition, or firm physical/mathematical justification) of what the right macroscopic observables are – the variables in terms of which we can causally model the coarse-grained network evolution. The most important component of our work was the use of data-mining tools to extract the "right macroscopic observables" – when those are not known *a priori* from massive simulation data. Our method of choice is a nonlinear extension of Principal Component Analysis: Diffusion Maps [8, 9]. In Diffusion maps (DMAPs), one constructs a graph with the data points as vertices, using a pairwise similarity measure between the data points to weigh the corresponding edges. In broad terms, the eigenfunctions of the diffusion process on this graph are used to embed the data. If the data points actually lie in a low dimensional nonlinear subspace, the first few of these eigenfunctions will suffice to embed the data using their intrinsic geometry, and still be able to summarize their salient features. A crucial step in the implementation of DMAPs is the definition of a measure of pairwise similarity between data points. If the data points lie in a Euclidean space, it is straightforward to use the Euclidean distance as a measure of the closeness

between pairs of nearby points. When the data points arise in the form of graphs, however, it is not trivial to define good measures of similarity between them. Thus, for the machinery of non-linear data-mining to be successfully adapted to the case of data in the form of graphs, one has to be able to define a useful scalar measure of similarity (closeness) between pairs of graphs. Although measures of similarity in the context of graphs have been discussed in the literature [10], established classifications are still lacking. One of the simplest options to evaluate similarities between graphs is to directly compare a few chosen, representative features of the network. The chosen features may consist of structural information (degree distribution, for instance) or include spectral measures (eigenvalues and/or eigenvectors of the graph Laplacian matrix). In our work we considered two options for defining similarities between graphs: (i) using subgraph densities and (ii) an approach using spectral information. For a detailed description of our two measures of graph similarity see [11].

Figure 1 summarizes the results of our approach in an illustrative example: a two-parameter family of maps constructed using the Chung-Lu algorithm [12]. In this example the graphs consist of n = 100 vertices, and our model has 2 construction parameters: p and r. If $r = 0$, the resulting graphs are Erdos-Renyi graphs and p controls the edge density. When $p = 1$ and r = 0, the resulting graphs are complete. As r is increased, this procedure creates graphs whose degree distributions are skewed to the left (long tails towards lower degrees). 1000 graphs were created using this model with 100 nodes each. The values of p and r were chosen by uniformly sampling in the intervals (0.5, 1) and (0, 0.5) respectively. The diffusion map algorithm was used on this set of graphs. The results obtained using our two pairwise similarity measures convey essentially the same qualitative information. The first 10 eigenvalues of the random walk matrix calculated by using the subgraph approach for evaluating similarities are shown in the top plot of Fig. 1. The first four non-trivial eigenvectors are plotted below. In these plots, each of the 1000 graphs is represented as a point in the p-r two parameter plane. The colors represent the magnitude of the components of the corresponding graph data on each of the first 4 non-trivial eigenvectors. The gradient of colors in these plots suggest the "direction" of each of these eigenvectors in the p- r plane. However, a more careful inspection of the plots is required to determine independent subsets of these eigenvectors.

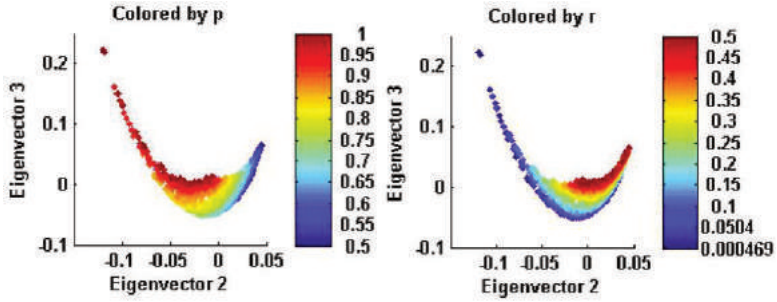

Figure 2: Data-mining the two-parameter family of Chung-Lu graphs using the subgraph similarity metric leads to an apparent two-dimensional embedding. In these plots the x and y coordinates of each point (i.e. of each graph in the dataset) denote the components of that particular graph in the second and third eigenvectors of the random walk matrix respectively. Each point is now colored based on the parameter values of p (left) and r (right) used to construct the particular graph.

Good low-dimensional observables for an ensemble of graph data (like the ones found here through data-mining) can find several uses in a modeling context. One can, for example, try to close effective dynamic equations in terms of these reduced observables, explicitly if possible through appropriate assumptions, or even "on the fly" numerically, in the spirit of multiscale modeling algorithms like those of our equation-free approach (see [1, 2] and for applications to network problems [5–7]).

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3.3.1.2 PKS-Fellows

Chemical and mechanical regulation of cilia and flagella
(Dr. Benjamin Friedrich)

How do single cells swim using flagella and steer their path in response to environmental cues? How do physical forces regulate the flagellar beat to facilitate e.g. synchronization among flagella?

I want to understand how complex biological systems such as flagella work. In my theoretical work, I employ minimal theoretical descriptions that focus on key biological components by using dynamical systems theory, advanced data analysis, and geometric thinking, while enjoying a close collaboration with experimentalists. A long-standing interest of mine concerns the function of *cilia and flagella*:

Eukaryotic flagella are slender cell appendages that can bend actively and thus propel swimming microorganisms and sperm cells. Arrays of short flagella called cilia clear mucus in our airways. Flagella appeared early in evolution and their internal structure, the axoneme, is highly conserved among eukaryotes including amoeba, animal, plant and fungi cells. Flagella are a best-seller of nature. The regular bending waves of flagella are shaped by the stochastic stepping of thousands of nano-scale molecular motors within the axoneme. This complex system has long served as a model of choice to study the emergence of mechano-chemical oscillations and is under active study at the **mpipks** as well at the Max-Planck Institute for Cell Biology and Genetics, also in Dresden. What interests me is how cells regulate the flagellar beat to achieve specific cell functions. To fulfill its purpose of a propeller, steering rod, or mixing blade, the flagellar beat is regulated both chemically and mechanically.

As an example of *chemical regulation*, past work in collaboration with Frank Jülicher dealt with the chemotaxis of sperm cells: In many species, flagellar motility of sperm is directed towards the egg. To achieve this, motility and sensation have to be integrated in a tight control loop [1]. Receptors on the flagellar membrane bind chemoattractant molecules released by the egg or egg-associated cells, which trigger an intraflagellar calcium response through a signaling cascade. Calcium regulates the asymmetry of the flagellar beat, and thereby tunes the turning rate of the swimming cell [2]. Together with Frank Jülicher, we developed a theoretical description of sperm chemotaxis that comprises a generic description of chemotactic signaling and stochastic differential geometry. While swimming along circular paths in a concentration gradient of a chemoattractant, sperm cells sample a temporal concentration stimulus that varies periodically with the frequency of circular swimming. This periodic concentration stimulus triggers a periodic modulation of the asymmetry of the flagellar beat and thus of the curvature of the sperm swimming path. As a consequence, swimming circles deform and drift upwards the chemoattractant gradient. In an ongoing collaboration with the experimental laboratory of UB Kaupp at the CAESAR institute in Bonn, this navigation strategy is confirmed for sperm cells from marine invertebrates with external fertilization [1, 2]. Sperm chemotaxis in us humans, however, is not understood and may hold surprises [3].

The beat of a flagellum is also susceptible to external forces, accounting for *mechanical regulation*. The striking phenomenon of flagellar synchronization of collections of flagella is believed to result from mutual mechanical interactions between flagella, *e.g.* through the surrounding fluid. Flagellar synchrony is observed for example in ciliar arrays, where the beating of numerous cilia is coordinated in metachronal waves to allow for efficient fluid transport. The unicellular green algae *Chlamydomonas* provides a model system for flagellar synchronization. *Chlamydomonas* swims with a pair of flagella, thus resembling a breast swimmer, see figure 1A. Synchronization of its two flagella is a prerequisite to swim along a straight path.

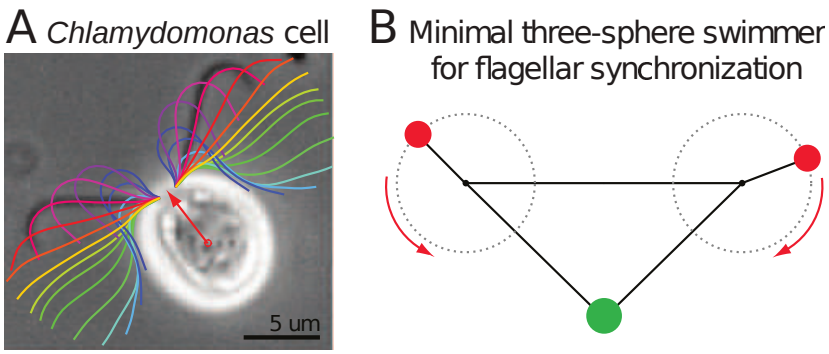

Figure 1: **A.** *Chlamydomonas* cells swim with two flagella that can beat in synchrony. Shown is a micrograph of this cell superposed with the regular flagellar beat pattern tracked from the same experiment. **B.** A minimal model swimmer consisting of three spheres, which retains the basic symmetries of a *Chlamydomonas* cell, allowed us to identify the mechanical basis of flagellar synchronization: Asynchronous beating results in a rocking motion of the swimmer that imparts hydrodynamic forces on the two red "flagellar spheres" and restores in-phase synchrony.

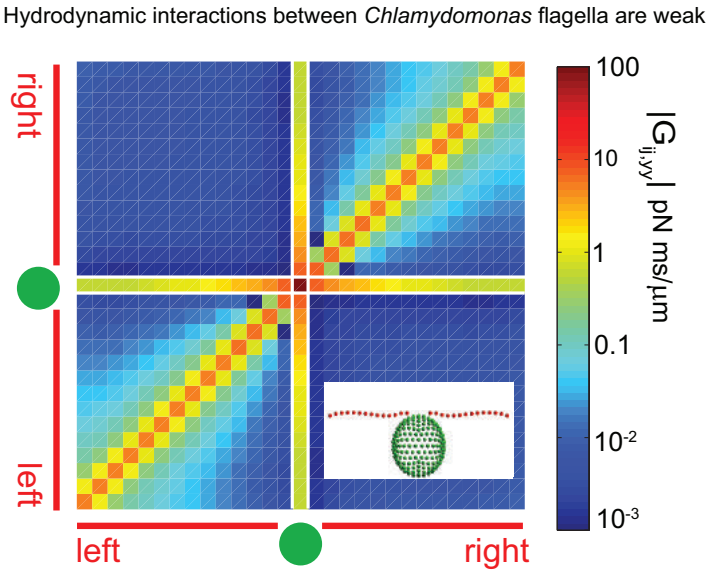

Figure 2: We computed hydrodynamic friction forces and hydrodynamic interactions between different body parts for a swimming *Chlamydomonas* cells using a 300 sphere model (inset). The color coded matrix shows part of the hydrodynamic friction matrix that relates the *velocity* of individual flagellar spheres or the cell body (column index as indicated by cartoon below the matrix) to the *hydrodynamic forces* exerted by the spheres or the cell body (row index). While diagonal entries indicate usual Stokes friction, off-diagonal entries characterize hydrodynamic interactions. For simplicity, only velocity and force components parallel to the long axis of the cell were considered.

We have developed a hydrodynamic theory for flagellar synchronization in these cells and propose that synchronization results from a feedback of their swimming motion on the flagellar beat [4–6]: For asynchronous beating of the two flagella, the cell body will rock as a result of imbalanced torques generated by the two flagella. In our theory, any rotation of the cell body changes the hydrodynamic resistance that opposes the flagellar beat. Assuming a simple relationship between these hydrodynamic forces and the flagellar phase speeds results in a mechanical coupling between the two flagella. If the cell body rocks to one side, one flagellum will slow down, while the other speeds up. This mechanical coupling between the two flagella stabilizes the synchronized state and ensures robust synchronization even in the presence of noise. In a first study, to cut-down on the complexity of this biological system, we had devised a minimal model swimmer of maximal simplicity that retained the basic symmetries of a *Chlamydomonas* cell [4, 5], see figure 1B. In this model swimmer, the regular bending waves of each flagellum were replaced by a single sphere moving along a circular orbit. A third sphere plays the role of the cell body. This model swimmer propels itself a low Reynolds numbers by purely viscous forces, just as a *Chlamydomonas* cell does. Moreover, the two driven spheres robustly lock into a synchronized state. Importantly, this synchronization mechanism relies crucially on the ability of the swimmer to move. This generic synchronization mechanism differs fundamentally from previously studied mechanisms, which relied on direct hydrodynamic interactions between flagella instead of a coupling through motion. Our analysis shows that swimming and synchronization can be inseparably intertwined. In a follow-up study,

we devised a more realistic hydrodynamic computation of a swimming *Chlamydomonas* cell [6], see also figure 2. We can accurately predict the swimming behavior of real cells tracked with high-speed video-microscopy. These experiments were performed by Veikko Geyer in the laboratory of J Howard at the MPI-CBG in Dresden. Combining theory and experiment, we show that the synchronization mechanism exemplified by our three-sphere model swimmer generalizes to the case of a swimming *Chlamydomonas* cell. This novel mechanism for robust synchronization mechanism could in principle apply also in other systems, such as carpets of cilia anchored or man-made nano-swimmers.

In summary, I am aiming at a systems-level regulation of flagellar dynamics, which is pivotal to understand its different physiological functions. I am strongly benefiting from interactions with several groups in Dresden that work on the internal working mechanisms of flagellar beating, both experimentally (Howard laboratory, MPI-CBG) and theoretically (Pablo Satori, André Scholich, Jülicher group).

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Collective phenomena

(Dr. Achilleas Lazarides)

I study various subjects related to collective phenomena in condensed matter physics, currently with an emphasis on non-equilibrium dynamics.

*Work completed and submitted during the last two years at the **mpipks***

While at the **mpipks**, I have so far published on:

- the equilibrium properties of one-dimensional strongly interacting bosons under weak periodic potentials [1, 2] (with Olivier Tieleman and Cristiane Morais Smith from Universiteit Utrecht and Masud Haque from the **mpipks**). In [1] we have found that a supersolid phase is stable close to commensurability, while in [2] we present an exact phase diagram of hard-core bosons in one-dimensional periodic potentials with the potential depth as a parameter (the tight-binding limit of the Bose-Hubbard model is one limit of this).
- A stochastic description of cold bosons [3] during the approach to thermal equilibrium (with P. Navez from the TU Dresden). Here, we developed a Langevin equation (or a quantum kinetic theory) describing the approach to thermal equilibrium of a general nonintegrable system and applied it to a 1-d model.
- The effect of quantum statistics on the escape from the vicinity of a wall with Robin boundary conditions [4] (with A. Goussev, O. Georgiou, G. Gligoric and J. D. Bodyfelt of the **mpipks** and D. F. M. Oliveira of the Friedrich-Alexander Universitat Erlangen). With some of the same authors, we also studied the Goos-Hänchen effect near a normal-superconductor interface [6] (with S. Y. Lee and O. Georgiou of the **mpipks**, A. Goussev of Northumbria University and G. Gligoric of the University of Belgrade). In these two articles we study the dynamics of two different quantum systems near walls, that is, in spatially inhomogeneous situations.
- Fractional quantum Hall (FQHE)-like phases in lattice models with gauge fiels [5] (with T. Duric from the **mpipks**); here, we discuss a projective symmetry group analysis of a tight-binding model with a magnetic field. This approach allows us to relate numerically-observed FQHE-like phases that only exist in lattice systems to the better-understood continuum FQHE phases.
- Static and dynamic properties of hard-core bosons in a disordered system with mobility edges [7] (with O. Ribeiro and M. Haque of the **mpipks**). This is a detailed study of the effect of a mobility edge on the many-body statics and dynamics of the hardcore boson system.

Cooperations

I am collaborating with a number of groups and individuals both inside and outside the mpi**pks**, as mentioned above.

External collaborations which have already resulted in publications include Ref. [1] with O. Tieleman (before moving to the mpi**pks**) and C. Morais Smith of Universiteit Utrecht. Ref. [3] with P. Navez of TU Dresden, [4] and [6] with A. Goussev from Northumbria University and G. Gligoric of the University of Belgrade, Serbia.

Internal collaborations which have resulted in publications include M. Haque and P. Ribeiro (hard-core bosons with quasiperiodic disorder [7]); O. Tieleman (one-dimensional strongly-interacting bosons, currently working on chaos and thermalization [1]); S. Y. Lee and O. Georgiou (quantum dynamics in spatially inhomogeneous situations [4, 6]) and T. Duric (FQHE [5]).

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[6] S.-Y. Lee, A. Goussev, O. Georgiou, G. Gligoric and A. Lazarides, under review (ArXiv:1212.6188).
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Self-organisation and pattern formation in biology
(Dr. Chiu Fan Lee)

My research interest is in the theoretical understanding of self-organisation phenomena and pattern formation in biological systems. Specific examples include protein amyloid self-assembly, cytoplasmic pattern formation, tissue homeostasis, and collective behaviour in living organisms. I employ tools of statistical mechanics, soft condensed matter physics, applied mathematics, and computation methods in my research. My work is typically performed in close collaboration with experimental biologists.

Cooperations

The cell cytoplasm consists of many different levels of organisation. Supported by a cytoskeleton network, the cytoplasm further contains subunits called organelles, such as mitochondria and centrosomes. The dynamical and mechanical properties of the cytoplasm as a structured fluid are currently under intense investigation. A striking example of the dynamic nature of the cytoplasm is the first cell division of the embryo of the nematode *Caenorhabditis elegans* (*C. elegans*). In order to achieve asymmetric cell division different organelles, P granules being a particular example, self-organise spatially to distinct locations in the cell but the mechanism is unclear. P granules are aggregates of RNA and proteins that are important for germline specification. These non-membrane-bound organelles localise to the posterior of the embryo before cell division. The segregation of P granules to the posterior depends on the formation of the cytoplasmic concentration gradient of Mex-5 protein. P granules were also shown to exhibit liquid droplet-like properties. This discovery led to the proposal that P granule localization is based on a phase separation phenomenon that is controlled by the Mex-5 concentration gradient. In close collaboration with experimental biologists Clifford Brangwynne at Princeton University and Anthony Hyman at the MPI-CBG, and Professor Frank Jülicher at the mpi**pks**, I am currently working on a firm theoretical basis of the proposed phase separation in P granules by providing a detailed model for the underlying biophysical mechanisms. Specifically, the state of the art experimental evidence led us to construct a model of phase separation driven by a spatially varying free energy landscape controlled by nonequilibrium processes.

The potential of this research is not confined to the *C. elegans* embryo since spontaneous organelle formation is ubiquitous in many organisms. Two other prominent examples include the formation of stress granules in the cytoplasm when the cell is under stress, and the formation of mitotic spindles during cell division. Therefore, further development of my research in P granule localisation may lead to the understanding of a set of universal mechanisms for spatial organisation in the cytoplasm.

External collaboration Driven by the structural properties of a generic polypeptide chain, proteins have a natural tendency to form fibrillar aggregates. These fibrillar aggregates are called amyloid fibrils, and

are in the order of micrometers in length, in the order of ten nanometers in width, and are stabilised by a network of hydrogen bonds and hydrophobic interactions. Amyloid formation is intimately related to human pathology. Although it is generally accepted that amyloid fibrils are causal agents of many diseases including Alzheimer's, Parkinson's and other prion diseases, how toxicity arises is still an open question. The answer to this question is directly relevant to what interventions are appropriate, and thus intimately related to treatment development.

With members of the Vaux group at the Dunn School of Pathology in Oxford, I have been tackling the problem of amyloid formation with a tightly-coupled-theory-and-experiment approach. Recently, the Vaux group and I have demonstrated that the interface can be critical for amyloid fibril formation. These studies signify the importance of the heterogeneous nature of the environment in the in vivo situation and helped to shift the focus of amyloidogenesis to the protein-membrane interactions, which also holds the key for the understanding of amyloid-related pathogenesis.

Invited external presentations
1. "Spatial organization of the cell cytoplasm: P granule localisation in the C. elegans embryo."
Laboratoire J. A. Dieudonné, Université de Nice-Sophia Antipolis, France [04/2012]
2. "Self-organisation in molecular biology."
School of Mathematics and Statistics, University of Sheffield, UK [01/2012]
3. "Self-organisation in biology: Modelling of cytoplasmic compartmentalisation."
Department of Bioengineering, Imperial College London, UK [12/2011]
4. "Self-organisation in biology: Cytoplasmic organelle formation."
Mathematical Institute, University of Oxford, UK [11/2011]
5. "Self-organised structures in biology: from protein amyloids to cytoplasmic organelle formation."
Laboratoire interdisciplinaire de Physique, Grenoble, France [11/2011]
6. "Self-organised structures in biology: from protein amyloids to cytoplasmic organelle formation."
Laboratoire de Physique Théorique, Toulouse, France [10/2011]
7. "Self-organised structures in biology: from protein amyloids to cytoplasmic organelle formation."
Biological Physics Group, Imperial College London, UK [09/2011]
8. "Self-Organisation in Biology."
Department of Mathematics, University of Sussex, UK [06/2011]
9. "Self-Organisation in Molecular Biology."
Centre for Complexity Sciences, University of Warwick, UK [06/2011]
10. "Protein aggregation phenomena."
Department of Physiology, McGill University, Canada [11/2010]
11. "The physics of protein amyloid formation."
Department of Physics and Astronomy, University of Edinburgh, UK [08/2010]

*Articles completed and written at the mpi**pks***

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[2] C. F. Lee*, S. Bird*, M. Shaw, L. Jean and D. J. Vaux, Journal of Biological Chemistry **287**, 38006-38019 (2012).
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[6] C. F. Lee, Phys. Rev. E **82**, 021103 (arXiv:1005.4116) (2010).
[7] C. F. Lee, Phys. Rev. E **81**, 031125 (arXiv:1001.2684) (2010).

3.3.2 Collaboration with Experimental Groups

A number of joint collaborations with experimental groups in Germany, Europe and the US has been partially supported by the mpi**pks**.

- *Thermal non-equalibrium fluctuations* with J. Mehlis, M. Diestelhorst, Halle University (Germany)
- *Nichtlinearer Transport in Quantentöpfen* with G. Scott , Bell Laboratories/Alcatel-Lucent and D. Natelson, Rice University (Houston, USA)
- *Transcription* with P. Cramer, LMU München (Germany)
- *Myosin II Stepping* with Z. Bryant, Stanford University (USA)
- *Cortical Flow Suppressors* with J. Ahringer, Cambridge University (UK)
- *Genome comparisons in planarians* with J. Rink, MPI-CBG Dresden (Germany)

- *Noncoding RNAs during brain development* with F. Calegari, CTRD Dresden (Germany)
- *Femtosecond filamentation* with G. Steinmeyer, Max Born Institute (Berlin)
- *THz Generation by ultrashort ionizing laser pulses* with E. Cabrera-Granado, Universidad Complutense (Madrid, Spain)
- *Single-Photon Nonlinear Quantum Optics with Interacting Atoms* with V. Vuletic, MIT (Cambridge, USA)
- *Quantum Dynamics of Interacting Rydberg Lattices* with I. Bloch, MPQ Garching (Germany)
- *Ultralong-range Molecules* with T. Pfau, Stuttgart University (Germany)
- *Quantum Interference in Interacting Three-Level Systems* with C. S. Adams, Durham University (UK)
- *Quantum Interference in Interacting Three-Level Systems* with M. Weidemüller, Heidelberg University (Germany)
- *Twitching motility of bacteria* with N. Biais, Columbia University (New York, USA)
- *Studies of fluid channels in B. subtilis biofilms* with D. A. Weitz, Harvard University (USA)
- *Physics of the actin cortex* with E. Paluch, MPI-CBG Dresden (Germany)
- *Mechanics of interkinetic nuclear migration in the zebrafish embryonic retina* with C. Norden, MPI-CBG Dresden (Germany)
- *Cell oscillations in dorsal closure* with J. Solon, Center for Genomic Regulation (Barcelona, Spain)
- *Cyst formation in the Drosophila wing disc* with A. Classen, LMU München (Germany)
- *Mechanics of zebrafish epiboly* with C. P. Heisenberg, Institute of Science and Technology (Vienna, Austria)
- *Mechanics of Drosophila wing disc development* with S. Eaton, MPI-CBG Dresden (Germany)
- *Uniformed Individuals Promote Democratic Consensus in Animal Groups* with I. Couzin and N. Leonard, Princeton University (USA)
- *Measurement of the Goos-Hänchen shift in a microwave cavity* with J. Unterhinninghofen, U. Kuhl, H. J. Stöckmann, Marburg University and J. Wiersig, Magdeburg University (Germany)
- *Resonant Stimulated X-ray Raman Scattering in atomic gases* with J. Rocca, Colorado State University and G. Brown, Lawrence Livermore National Laboratory and J. Bozek, SLAC National Accelerator Laboratory (USA)
- *Stimulated Raman Scattering and X-ray Lasing in Molecular Gas Targets* with A. Foehlisch, P. Wernet, M. Beye, Helmholtz-Zentrum Berlin and D. Rolles, DESY, CFEL Hamburg (Germany) and A. Rudenko, Kansas State University, (Manhattan, USA)
- *NMR on magnetic materials* with M. Takigawa, ISSP Tokyo (Japan)
- *Magnetic Susceptibility in unconventional magnets* with P. Schiffer, Pennsylvania State University (USA)
- *Ultrasound Studies* with J. Wosnitza, Hochmagnetfeldlabor Dresden (Germany)
- *Pnictide Superconductivity* with B. Büchner, IFW Dresden (Germany)
- *Pnictide Superconductivity* with H.-H. Klaus, TU Dresden (Germany)
- *Fermionic quantum dimer and fully-packed loop* with K. Shtengel, University of California (USA), P. Fulde, APCTP (Pohang, Korea)
- *Supersolid phase and magnetization plateaus observed in the anisotropic spin-3/2 Heisenberg model on bipartite lattices* with J. Romhanyi, K. Penc, Research Institute for Solid State Physics and Optics (Hungary)
- *Extended quantum U(991)-liquid phase in a three-dimensional quantum dimer model Quantum Ice: A Quantum Monte Carlo Study* with O. Sikora, N. Shannon, H.H. Wills Physics Laboratory, University of Bristol (UK), K. Penc, Research Institute for Solid State Physics and Optics (Hungary), P. Fulde, APCTP (Pohang, Korea)
- *Matrix-procuct-based project wave functions ansatz for quantum many-body ground states* with Ch.-P. Chou, Brookhaven National Laboratory (New York, USA), T.-K. Lee, Academia Sinica, (Taipei, Taiwan)
- *Unbounded Growth of Entanglement in Models of Many-Body Localization* with J. H. Bardarson, J. E. Moore, University of Carlifornia (Berkeley, USA)
- *Symmetry protection of topological order in one-dimensional quantum spin systems* with E. Berg, Harvard University ((Cambridge, USA), A. M. Turner, University of Amsterdam (The Netherlands), M. Oshikawa, University of Tokyo (Japan)
- *Detection of symmetty-protected topological phases in one dimension* with A. M. Turner, University of Amsterdam (The Netherlands)

- *Linear quantum quench in the Heisenberg XXZ chain: time dependent Luttinger model description of a lattice system* with B. Dora, Budapest University (Hungary)
- *Topological characterization of fractional quantum Hall ground states from microscopic Hamiltonians* with M. P. Zaletel, University of California (Berkeley, USA), R. S. K. Mong, Caltech (USA)
- *Topological Phases of Para-Fermions in One-Dimension* with E. Berg, Harvard University (Cambridge, USA), A. M. Turner, University of Amsterdam (The Netherlands)
- *Coulombic Charge Ice* with A. O Brien, The University of Sydney (Australia)
- *Phase diagram of the isotropic spin-3/2 model on the z-3 Bethe Lattice* with S. Depenbrock, LMU München (Germany)
- *Effective gauge field description for the biliniear-biquadratic spin-one chain* with A. Turner, University of Amsterdam (The Netherlands)
- *Interplay of charge and spin degrees of freedom on the kagome lattice* with K. Penc, Research Institute for Solid State Physics and Optics (Hungary), C. Hotta, Kyoto Sangyo University (Japan)
- *Loschmidt echo and the many-body orthogonality catastrophe of a Luttinger Liquid* with B. Dora, G. Zarand, A. Delon, Budapest University (Hungary)
- *Ground state fidelity approach to the spin-1 Heisenberg chain with single ion anisotropy* with A. Langari, Sharif University of Technology (Teheran, Iran)
- *Periodicity in Spin Chains and Space-Time defects* with A. Turner, University of Amsterdam (The Netherlands), A. Vishwanath, University of California (Berkeley, USA)
- *Dipolar interactions in Quantum-Spin Ice* with O. Sikora, N. Shannon, H.H. Wills Physics Laboratory, University of Bristol (UK), K. Penc, Research Institute for Solid State Physics and Optics (Hungary)
- *Detecting topological order in Tensor-Network, States* with N. Schuch, RWTH Aachen (Germany)
- *Tensor-Product state based variational Approach to 2D Many-Body system* with O. Sikora, Y.-J. Gao, National Taiwan University (Taipei, Taiwan)
- *Matrix-Product state approach to Fractional Chern insulators* with M. P. Zaletel, University of California (Berkeley, USA)
- *Cell division, cellular pattern formation and dynamics* with the groups of Jonathon Howard and Anthony Hyman, MPI-CBG Dresden (Germany)
- *Segmentation of vertebrates through oscillating and spatio-temporal gene expression patterns* with Andy Oates, MPI-CBG Dresden (Germany)
- *Active cell mechanics and cell adhesion* with Ewa Paluch, MPI-CBG Dresden (Germany)
- *Dynamics of endosomal transport and signaling networks in cells* with Marino Zerial, MPI-CBG Dresden (Germany)
- *Collective behaviors of molecular motors* with Stefan Diez, MPI-CBG Dresden (Germany)
- *Spontaneous emissions from the ear* with Benjamin Lindner, Humboldt-Universität zu Berlin (Germany)
- *Microtubule dynamics* with Marileen Dogterom, AMOLF Amsterdam (The Netherlands)
- *Dynamics of morphogens in growing tissues and their role in growth control* with Marcos González-Gaitán, University of Geneva (Switzerland)

3.3.3 Conferences, Workshops and Symposia

1. *Korrelationstage 2011*
   Workshop: February 28 - March 4, 2011 — 172 participants
   Scientific coordinators: M. Eschrig, M. Fiebig, M. Kollar
2. *Mechanics and Growth of Tissues: From Development to Cancer*
   Workshop: March 21 - 25, 2011 — 86 participants
   Scientific coordinators: S. Eaton, J.-F. Joanny, F. Jülicher, J. Prost
3. *Physics of Immunity: Complexity Approach*
   Workshop: April 4 - 8, 2011 — 67 participants
   Scientific coordinators: M. Ivanchenko, C. Molina-Paris, M. Or-Guil
4. *Noise in Nonequilibrium Systems: From Physics to Biology*
   Workshop: April 11 - 14, 2011 — 79 participants
   Scientific coordinators: W. Häusler, G.-L. Ingold, P. Talkner

5. *Development and Prospects in Quantum Impurity Physics*
   Advanced School and Workshop: May 30 - June 10, 2011 — 103 participants
   Scientific coordinators: C. J. Bolech, S. Kirchner, P. Wölfle

6. *Advanced Study Group: Focus week*
   Workshop: June 14 - 18, 2011 — 25 participants
   Scientific coordinators: A. Bäcker, R. Ketzmerick, P. Schlagheck, S. Tomsovic

7. *Quantum Physics with Non-Hermitian Operators*
   Seminar and Workshop: June 15 - 25, 2011 — 97 participants
   Scientific coordinators: A. Fring, I. Rotter, G. Wunner

8. *Large Fluctuations in Non-Equilibrium Systems*
   Seminar: July 4 - 5, 2011 — 67 participants
   Scientific coordinators: M. Henkel, D. Mukamel, M. Pleimling, G. M. Schütz

9. *Weak Chaos, Infinite Ergodic Theory and Anomalous Dynamics*
   Seminar and Workshop: July 25 - August 12, 2011 — 85 participants
   Scientific coordinators: E. Barkai, H. Kantz, R. Klages, R. Zweimüller

10. *Collective Dynamics and Pattern Formation in Active Matter Systems*
    Seminar and Workshop: August 29 - September 23, 2011 — 105 participants
    Scientific coordinators: M. Bär, H. Chate, K. Kruse

11. *Quantum Simulations and Design*
    Focus Workshop: September 27 - 29, 2011 — 52 participants
    Scientific coordinators: H. Ebert, D. Ködderitzsch, M. Ogura

12. *Engineering and Control of Quantum Systems*
    Workshop: October 10 - 14, 2011 — 77 participants
    Scientific coordinators: C. Koch, G. Morigi

13. *Carbon-Based Spintronics*
    Workshop: October 24 - 28, 2011 — 76 participants
    Scientific coordinators: G. Cuniberti, L. Hueso, S. Roche

14. *Rogue Waves*
    Workshop: November 7 - 11, 2011 — 69 participants
    Scientific coordinators: M. Akhmediev, E. Pelinovsky, A. C. Newell

15. *Atomic Physics 2011*
    Workshop: November 21 - 25, 2011 — 74 participants
    Scientific coordinators: J.-M. Rost

16. *Beyond Molecular Dynamics: Long Time Atomic-Scale Simulations*
    Workshop: March 26 - 29, 2012 — 68 participants
    Scientific coordinators: C. Becquart, M. Posselt, R. Smith

17. *Impurities and Textures in Unconventional Magnets*
    Workshop: April 2 -4, 2012 — 51 participants
    Scientific coordinators: R. Moessner, H. Tsunetsugu

18. *Laser-Plasma Interaction at Ultra-High Intensity*
    Workshop: April 16 - 20, 2012 — 65 participants
    Scientific coordinators: M. Bussmann, E. D Humieres, M. Grech, S. Skupin

19. *Finite Systems*
    Workshop: May 4 - 6, 2012 — 42 participants
    Scientific coordinators: J.-M. Rost

20. *Mathematical Physics of Complex Networks From Graph Theory to Biological Physics*
    Workshop: Max 14 - 18, 2012 — 77 participants
    Scientific coordinators: C. D. Genio, K. E. Bassler

21. *Itinerant Spin-Orbital Systems: From Magnetic Frustration to Novel Superconductivity*
    Workshop: May 21 - 25, 2012 — 81 participants
    Scientific coordinators: I. Eremin, N. B. Perkins, H. Takagi

22. *Correlated Multielectron Dynamics in Intense Light Fields*
    PhD school of the INT-network CORINF: June 11 - 15, 2012 — 45 participants
    Scientific coordinators: M. Ivanov, J.-M. Rost

23. *Quantum Matter from the Nano-to the Macroscale*
    Seminar and Workshop: June 18 - July 6, 2012 — 96 participants
    Scientific coordinators: J. S. Meyer, D. Morr, T. Vojta, M. Vojta

24. *Ordered and Non-Ordered Superstructures of Nanosized Objekts: Preparation, Properties Applications and Modeling*
    Workshop: July 9 - 13, 2012 — 98 participants
    Scientific coordinators: A. Eychmüller, A. Govorov, D. Talapin

25. *The Emerging Dynamic View of Proteins: Protein Plasticity in Allostery Evolution and Self Assembly*
    Workshop: July 16 - 20, 2012 — 60 participants
    Scientific coordinators: U. Bastolla, M. Porto, H. E. Roman

26. *Multi-Scale Physics of Lymphocyte Development*
    Seminar: August 6 - 31, 2012 — 52 participants
    Scientific coordinators: M. Ivanchenko, C. Molina-Paris, M. Or-Guil

27. *Entanglement Based Approaches in Quantum Chemistry*
    Focus Workshop: September 4 - 6, 2012 — 41 participants
    Scientific coordinators: O. Legaza, B. Paulus, M. Reiher, R. Schneider

28. *Statistical Inference Models in Physics and Learning*
    Seminar: September 10 - 28, 2012 — 44 participants
    Scientific coordinators: M. Biehl, M. Opper, T. Villmann

29. *Quantum Noise and Measurement in Engineered Electronic Systems*
    Workshop: October 8 - 12, 2012 — 74 participants
    Scientific coordinators: W. Belzig, M. Devorent, Y. V. Nazarov

30. *Wave Chaos from the Micro- to the Macroscale*
    Workshop: October 22 - 26, 2012 — 61 participants
    Scientific coordinators: M. Hentschel, S. Shinohara, S. Tomsovic, J. Wiersig

31. *Multiscale Complex Fluid Flows and Interfacial Phenomena*
    Focus Workshop: October 29 - November 1, 2012 — 71 participants
    Scientific coordinators: D. Lohse, S. Kalliadasin, H. A. Stone, U. Thiele

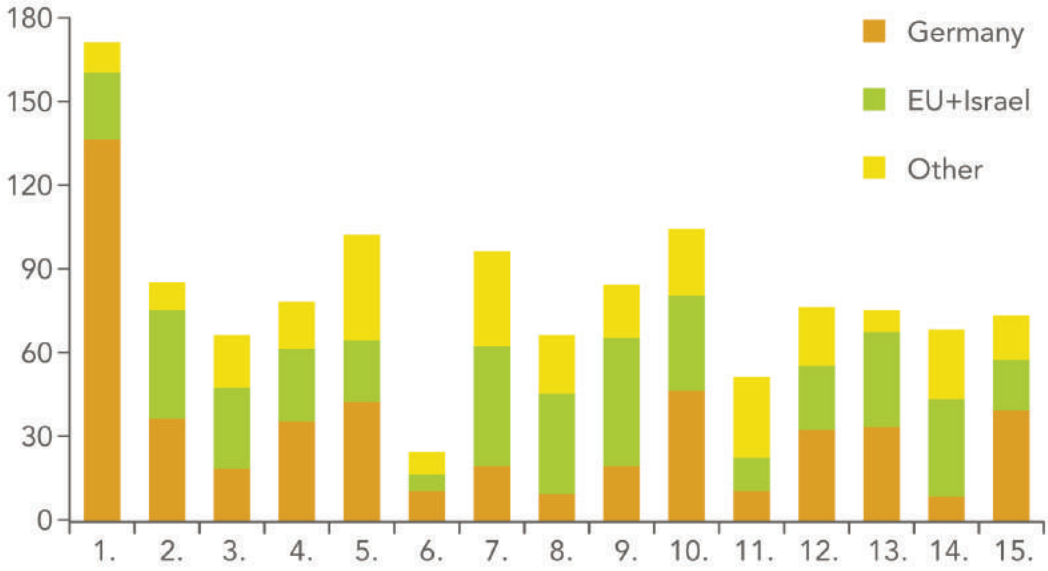
32. *Scales and Patterns in the Earth System*
    Workshop: November 5 -9, 2012 — 43 participants
    Scientific coordinators: J. Lelieveld

33. *Entanglement Spectra in Complex Quantum Wavefunctions*
    Workshop: November 12 - 16, 2012 — 67 participants
    Scientific coordinators: A. B. Bernevig, M. Haque, A. Läuchli

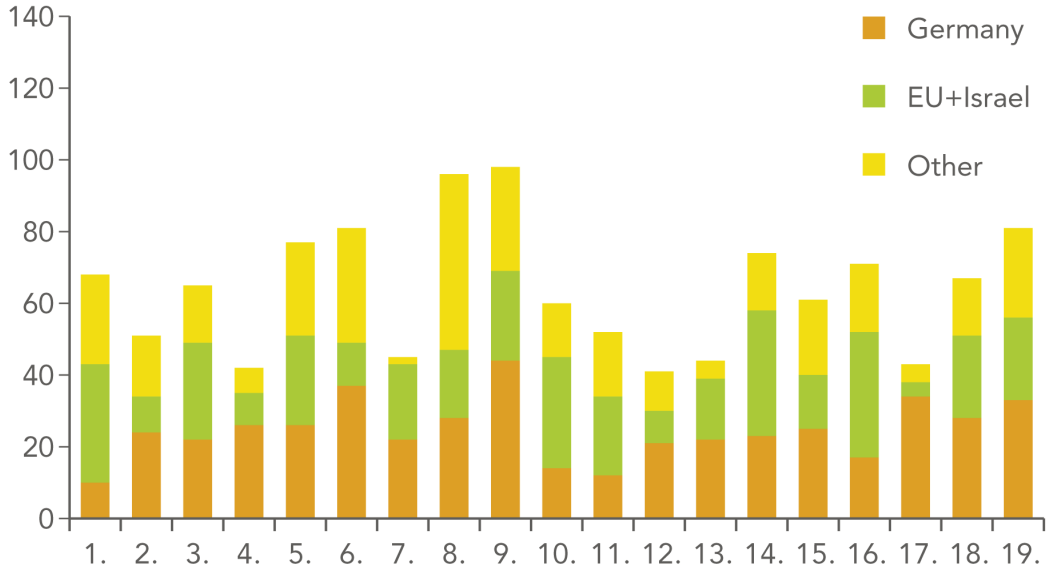
34. *Atomic Physics 2012*
    Workshop: November 26 - 30, 2012 — 81 participants
    Scientific coordinators: J.-M. Rost

3.3.4 Workshop Participation and Dissemination of Results

Statistics of Workshop participation



Number of Workshop/Seminar participants in the year 2011.



Number of Workshop/Seminar participants in the year 2012.

Dissemination of Workshop Results

As the topics of Workshops and Seminars at the 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:
  Quantum Physics with Non-Hermitian Operators, June 2011
  C. M. Bender, A. Fring, U. Guenther, H. F. Jones Journal of Physics A 45 (Special Issue 44)

- Workshop:
  The Emerging Dynamic View of Proteins: Protein Plasticity in Allostery, Evolution and Self Assembly, July 2012
  U. Bastolla, M. Porto, H. E. Roman: *The emerging dynamics view of proteins.*, Biochimica et Biophysica Acta Proteins and Proteomes (Special Issue 2013) (in preparation)

- Workshop:
  Quantum Noise and Measurement in Engineered Electronic Systems, October 2012
  M. Vanevic, W. Belzig: *Control of electron-hole pair generation by biharmonic voltage drive of a quantum point contact*, Physical Review B 86, 241306 (2012)
  A. Bednorz, C. Bruder, B. Reulet, W. Belzig: *Nonsymmetrized Correlations in Quantum Noninvasive Measurement*, arxiv: 1211.6056

- Workshop:
  Multi-Scale Physics of Lymphocyte Development, July 2012
  M. Ivanchenko, C. Molina-Paris, M. Or-Guil
  Frontiers of Immunology (in preparation)

3.3.5 Workshop Reports

Korrelationstage 2011 Workshop
Scientific coordinators: M. Eschrig, M. Fiebig, M. Kollar

The "Korrelationstage" ("Correlation Days") are a meeting on strongly correlated electron physics, the style and topics of which have continuously been adapted to novel developments in the field and to the group of participating physicists. The Korrelationstage started as an event attended by about 20 theoretical physicists in the late 1980's at the University of Dortmund and have developed over the years into a five-day conference. The Korrelationstage 2011 at the mpi**pks** Dresden had 168 participants (including local participants from the research institutions in Dresden), of which approximately 20 percent were experimentalists. In total 65 talks were presented from 28 February to 4 March. This was complemented by 102 posters during two poster sessions on Monday and Tuesday. One of the important goals of the Korrelationstage is to highlight current trends and topics in condensed-matter physics with particular attention to emerging subjects of interest. At the Korrelationstage 2011 a variety of particularly timely topics played a major role. One of them was the study of topological insulators and entanglement, which was emphasized by inviting Ali Yazdani from Princeton University for the colloquium talk on Monday; he gave a very well-received experimental talk on Helical metals on the surfaces of topological insulators, for which the lecture hall was packed to the last seat. This was complemented by several theoretical talks on entanglement in correlated systems and its use in analytical and numerical methods for many-body systems. Another focus was on new experimental and theoretical results on correlated materials and models, such as spin liquid phases, orbital physics, cuprates, and pnictides. Furthermore, several sessions were devoted to various aspects of nonequilibrium physics, including a session on cold atomic gases; in addition, an evening session was held on Thursday for the presentation of recent remarkable results obtained by pump-probe spectroscopy on correlated materials. This session was well attended and characterized by engaged discussions despite the late hour. The program of Korrelationstage 2011 was very much appreciated by the participants. The atmosphere of the meeting was informal but professional, with many lively discussions both during and outside the sessions, in particular during the coffee breaks.

In general the participants expressed a preference for this type of dense program with many speakers and a broad scope of different topics, rather than reducing the number of presentations. On the other hand, the general sentiment was that the Korrelationstage should not grow any further. The poster sessions were considered to be particularly valuable. With their informal atmosphere and the provided amenities the discussion of the posters lasted until late in the evening. It is the express aim of the Korrelationstage to give young scientists the opportunity to report on their work. About 30 talks were presented by younger speakers, several of them advanced PhD students. They blended very well into the sessions with more experienced speakers without reservation. The scientific level of these talks was high and most of them were quite skillful. In conclusion, the Korrelationstage represent a unique meeting for physicists working in the field of strongly correlated electrons, especially for the German community as well as international guests. It fosters the exchange of new ideas and is in particular a forum for young physicists who submitted applications in great numbers and contributed with some highly original work in the form of both posters and talks.

Mechanics and Growth of Tissues: From Development to Cancer, Workshop
Scientific coordinators: S. Eaton, J.-F. Joanny, F. Jülicher, J. Prost

The workshop focused on the dynamics of tissues and in particular the role of cell division in tissue organization. Cell division is a key process which shapes developing tissues that form complex structures and morphologies from a small number of initial cells. In order for tissue shape, size and morphology to correctly emerge, the integration of tissue mechanics with cellular communication by signaling systems is essential. Tissue growth control implies a tight interplay of active mechanical processes with chemical pattern formation. These subjects and in particular the regulation of cell division and the resulting active tissue mechanics are also of fundamental importance to tumor formation in cancer. The workshop brought together physicists and biologists with a common interest in multicellular dynamics and active mechanics in tissues. Furthermore, theorist and experimentalists presented their work in mixed sessions which led to stimulating discussions and a broad perspective on the subjects covered in the meeting. The invited speakers were almost exclusively international leaders in the field. Different communities met for the first time such as theorists working on multicellular dynamics (e.g. David Nelson and Michael Brenner, Harvard University) and developmental biologists (e.g. Olivier Pourquie, Strasbourg and Dan Kiehart, Duke University). A very stimulating colloquium talk was given by Ben Simons of Cambridge University who introduced novel ideas from statistical physics that provide a very different perspective on tissue homeostasis and may well lead to a rewriting of textbooks on this very fundamental field. There were also several talks of outstanding young scientists (e.g. Guillaume Salbreux and Barry Thompson). The meeting was well attended by many young scientists with a strong interest for this emerging field. There were two very lively poster sessions where scientific newcomers could present their work. The workshop brought together different communities in a very stimulating format. During the workshop it became increasingly clear that the combination of physics and biology will in the future be of particular importance for our understanding of tissue dynamics. An enthusiasm about recent progress and future perspectives created a special atmosphere, reminiscent of that which prevailed at the beginning of the "soft matter physics-chemistry adventure" and the “cell biology- biophysics adventure". We hope that this workshop will play a key role to trigger similar event in the coming years and to act as a catalyst to foster interdisciplinary exchanges.

Physics of Immunity: Complexity Approach, Workshop
Scientific coordinators: M. Ivanchenko, C. Molina-Paris, M. Or-Guil

The Workshop proved to be a vibrant forum for reporting the recent successes and discussing new perspectives and open problems in mathematical, physical and computational approaches to immunological processes. The cohort of scientists in Theoretical and Experimental Immunology at the Workshop addressed the following topics: (i) lymphocyte population dynamics and T cell receptor diversity, (ii) model selection, experimentally-based and multi-scale modelling in Immunology, (iii) immune responses against viruses, (iv) humoral immune response and affinity maturation, (v) T cell receptor signalling and T cell activation and (vi) clinical and medical Immunology. Talks spurred hot discussions, manifesting keen interest from the participants. A unique feature of this Workshop was that, despite it being centred on mathematical, physical and computational methodologies, it counted with the participation of world-renowned experimental immunologists, who themselves make use of mathematical approaches. One of

them, Andreas Radbruch, director of the German Arthritis Research Centre in Berlin, held the Colloquium lecture. He could not better convey the spirit of the Workshop having focussed in his Colloquium talk on bringing together the modelling and experimentation approaches towards understanding principles of immunity. The following key participants and their respective presentations deserve special note: Antonio Freitas – Role of quorum-sensing mechanisms in lymphocyte homeostasis. Robin Callard – T cell homeostasis in health and disease. Phil Hodgkin – An evolutionary theory to bind together our molecular, cellular and systems based understanding of the immune response. Rob de Boer – How to properly estimate cellular turnover rates from in vivo labelling data? Grégoire Altan-Bonnet – Differential suppression of effector T cells by regulatory T cells derives from a highly- dynamic IL-2 tug-of-war. Ken Duffy – How many distinct heritable factors are required to explain correlation structures in proliferating lymphocytes Ruy Ribeiro – How fast are virions cleared from the body? Steven Kleinstein – Unravelling antiviral regulatory networks using systems biology. Deborah Dunn-Walters – B cell repertoire changes in ageing. Arup Chakraborty – How T cells see antigen: from statistical mechanics to human disease. Benedita Rocha – The complexity of gene expression during CD8 activation in immune responses. Ria Baumgraß – Quantitative single cell analysis of transcription factor expression and activation to discover limiting factors for Th cell activation. Dagmar Iber – Activation by trans auto-activation allows binding discrimination at high receptor occupancy. Scientific newcomers had the opportunity to present a poster in a poster session held on Monday. Additionally, several young PIs and newcomers to the field were invited to present a talk. A special presentation on career advice was offered to students, post-docs, and young PIs.

With over 70 participants from all over the world, this Workshop was a huge success. Out of 23 participants who filled in a feedback form, 13 marked the Workshop as "excellent", 9 as "very good" and 1 as "good". 11 responders expressed an interest in a 1-3 month Seminar as a follow-up to the Workshop. The Workshop will certainly boost the visibility of the field of Theoretical Immunology within the immunology (both experimental and theoretical) community, both because of the seminal immunological questions which were discussed and the influencial immunologists who took part. During the discussions, several topics were identified as the most daunting for future research: • One of the greatest challenges in Immunology is to understand immunological processes at the single cell level, as pointed out by Dr. Altan-Bonnet in his talk during the Workshop. In order to do that, there is a need to bring together theoretical and experimental immunology approaches that can provide single cell resolution and move away from population approaches. • A second challenge is to measure the diversity of the T and B cell receptor for antigen, as discussed by Dr. Venturi and Dr. Dunn-Walters in their respective talks. In order to do that, there is a need to bring together mathematical and statistical approaches that, combined with the sequencing data, provide accurate measurements of both human and mice T cell and B cell receptor diversity. This work has implications on the development of vaccines and adoptive cell immune therapies. 1 • A third challenge is to understand the specific mechanisms that regulate gene expression during immune responses and cellular differentiation, as discussed by a number of speakers during the Workshop (Dr. Rocha, Dr. Hoefer and Dr. Carneiro). There is a need to develop new mathematical and physical models that can truly integrate processes at the different levels of complexity (population, cellular, molecular and genetic). We conclude by saying that the atmosphere of the Max Planck Institute helped to trigger new research collaborations between the participants. This meeting has been a booster to the field of theoretical immunology and definitely has set the standard of how research should be done in this relatively novel field of research.

Noise in Nonequilibrium Systems: From Physics to Biology, Workshop
Scientific coordinators: W. Häusler, G.-L. Ingold, P. Talkner

This workshop displayed a broad panorama of the state of the art of Non-Equilibrium Statistical Physics. The topics presented ranged from the foundations of thermodynamics of small systems and the impact of quantum mechanics on various transport phenomena over different features and variants of Brownian motion to specific aspects of biophysical problems. A unifying theme of the workshop has been the ubiquity of noise in small systems and its impact on transport properties. The breadth of this field manifested itself in the wide variety of topics of the talks a selection of which is given in the following. Fundamental Problems: Wolfgang Schleich (Ulm) discussed in his presentation non-classical aspects of the marginal position distribution of a free quantum particle. Different ways to control coherent electron dynamics were presented and analyzed by Gloria Platero (Madrid). An analysis of single realizations of Langevin-type dynamics describing for example the random motion of single colloidal particles in terms of

thermodynamic notions was proposed by Udo Seifert (Stuttgart) and an analysis of the efficiency of nano-engines was introduced by Christian van den Broeck (Hasselt). Transport in physical systems: The talks by Miguel Rubí (Barcelona) and Thomas Franosch (Erlangen) dealt with different aspects of diffusional transport in confined geometries. José Mateos (Mexico City) analyzed an optical ratchet as a means of selectively transporting dielectric particles of different size in water. The influence of internal degrees of freedom of a ratchet was analyzed by Thomas Dittrich (Bogotá) in view of applications to molecular motors in cells. Steps to an experimental realization of an artificial molecular motor were discussed by Heiner Linke (Lund). Further aspects of driven Brownian motion in nonlinear potentials were discussed in the talks by Jerzy Luczka (Katowice) and Manuel Morillo-Buzón (Sevilla). Igor Sokolov (Berlin) and Igor Goychuk (Augsburg) reported on anomalous transport and its modeling. Problems related to the transport of heat in nanoscopic systems were the subject of the talks by Baowen Li (Singapore), Giuliano Benenti (Como), Abraham Nitzan (Tel Aviv) and Keiji Saito (Tokyo). Transport in biological systems: The dynamics of biological networks was the topic of the talk by Sophia Yaliraki (London) and gave the motivation for the investigation of energy harvesting presented by Thomas Wellens (Freiburg). The transport of neurofilaments in nerve axons as a regulating mechanism of the axon morphology was the topic of the colloquium presented by Peter Jung (Athens). Hans Frauenfelder (Los Alamos) reported on the glass-like dynamics of the proteins. In two long evening poster sessions mainly young scientists presented their results to an highly interested audience. Discussions were lively not only during these poster sessions but also after, and sometimes during, the talks, the coffee, lunch and dinner breaks. It was this intense interaction of scientists from different fields with the common background of Statistical Mechanics that made this workshop a vivid market of scientific exchange and a true source of inspiration.

Quantum Physics with Non-Hermitian Operators, Seminar and Workshop
Scientific coordinators: A. Fring, I. Rotter, G. Wunner

The original plan of the International Seminar and Workshop was to organize a seminar with about 30 participants and a following workshop with about 80 participants. The purpose of the seminar was to discuss, in detail, unexpected (mostly counterintuitive) results obtained experimentally in different fields of quantum physics. The main focus of the workshop was twofold: firstly an exact mathematical description of model systems and secondly the discussion of physical results that can not be explained in the framework of the standard Hermitian quantum physics, but can be explained by considering non-Hermitian operators. It turned out that the original plan could not be carried out since (i) most applications were for participation during the whole time 15 - 25 June and (ii) the number of applications was much larger than expected. As a compromise, we had a 10-day conference with 65 talks of 45 minutes each and, additionally, the PHHQPX11 Colloquium on Monday, 20 June, and an evening lecture on Friday, 24 June. The slides of almost all the talks are made available on the conference web site. It was impossible to include all the applications for a talk into the program, and some of them were moved to the poster sessions. The number of posters was 31, each could be represented at all four poster sessions. Furthermore, we had to restrict the length of time of participation to 9 days at most (including arrival and departure). The number of registered participants was 134. According to our original aim, the scope of the conference was highly interdisciplinary. This allowed very many fruitful discussions between the participants. In particular, the exchange of experiences in using non-Hermitian operators for the description of physical phenomena in different fields of physics was very valuable. In many cases, the counterintuitive results obtained experimentally can be understood by considering the corresponding non-Hermitian Hamilton operator. Many participants underlined that they have learned a lot during the conference. After many fruitful discussions during the International Seminar and Workshop on *Quantum Physics with Non-Hermitian Operators*, Dresden, June 15 - 25, 2011, the two scientific journals Journal of Physics A and Fortschritte der Physik - Progress of Physics plan to publish a Special Issue related to the topic of the conference. The Special Issues are not Conference Proceedings but are open to all who are interested in sending an original contribution. All contributions to both Special Issues will be peer-reviewed.

Large Fluctuations in Non-Equilibrium Systems, Seminar
Scientific coordinators: M. Henkel, D. Mukamel, M. Pleiming, G. M. Schütz

The main aim of this seminar was to bring together people working on several aspects of systems out of thermal equilibrium, particularly fluctuation relations, large deviations, front propagations, and applications to biological systems. Nonequilibrium statistical physics is at the forefront of theoretical

research. The choice of the topic of the seminar seems timely, reflecting recent reports of the American NSF and the DoE.

The announcement of the seminar drew considerable response and interest in the community. We had twenty-three invited speakers and we received sixty-three applications of which forty-one were approved. The participants came from Europe, Asia, Africa, Australia, and North and South America. In spite of very generous aid from the mpi**pks**, we could only accept about two thirds of the total number of applicants. Among the participants there was a large number of PhD students and young researchers at the beginning of their career.

Twenty-three longer lectures were held by the invited speakers in addition to twenty-two shorter talks and two poster sessions. This gave especially younger colleagues the opportunity to present their work. The talks generated lively and long lasting discussions in which many different people took an active part. The fact that the seminar lasted for two weeks gave us the possibility to include longer breaks for discussions of existing projects and for starting new collaborations.

All in all, we have been very happy and satisfied with the scientific success of the seminar and the perfect support provided by the mpi**pks** for which we are extremely grateful.

Weak Chaos, Infinite Ergodic Theory and Anomalous Dynamics, Seminar and Workshop
Scientific coordinators: E. Barkai, H. Kantz, R. Klages, R. Zweimüller

The scientific focus of this three-week conference was on systems exhibiting dynamical randomness in form of weak chaos characterized by zero Lyapunov exponents, where the separation of nearby trajectories is weaker than exponential. Rigorous mathematical results about such systems were recently obtained by infinite ergodic theory, which is an extension of ordinary ergodic theory to dynamical systems with non-normalizable measures. These concepts predict novel nonequilibrium physical properties in form of anomalous dynamics, which can be tested in experiments.

The main purpose of this conference was to initiate cross-disciplinary collaborations between physicists working on both the deterministic and the stochastic aspects of weakly chaotic systems and anomalous dynamics, and mathematicians being active in the relevant branches of dynamical systems and ergodic theory. The workshop week brought together key players in both fields for surveying the state of the art in a quick, compact way. The two seminar weeks served as a forum for in-depth and informal discussions by also comprising a series of advanced lectures to provide review and training for young scientists.

It was a big pleasure to have Prof. Joseph Klafter delivering the Colloquium's talk of the conference on "How strange is strange kinetics". Prof. Klafter, currently president of Tel Aviv University, is one of the pioneers of the stochastic theory of anomalous dynamics. He was joined at this conference by an amazing number of world-class leading scientists working on ergodic theory, dynamical systems theory and the stochastic theory of anomalous dynamics.

Apart from such established experts, we welcomed a large number of highly promising young scientists, ranging from masters students and PhD students to postdocs and young group leaders. Many of these young scientists were already among our invited speakers. All of them had the opportunity to present themselves at the workshop by either giving contributed talks, or by presenting posters during two very lively poster sessions. These sessions were preceded by a special session where all poster presenters advertised their works in form of four minute mini talks. We furthermore awarded prizes for the best three poster presentations, selected by a commision consisting of Profs. Bunimovich, Keller, Sokolov and Vulpiani. During the two weeks of seminar, many young scientists presented contributed talks.

A key to the success of this conference was whether a sound communication between mathematicians and physicists working on quite different aspects in this highly interdisciplinary field of research could be established. As expected, the seminar weeks were much more appreciated in this respect than the workshop. This is exemplified by two special talks given by mathematicians in order to elaborate on specific questions raised in previous talks. Two round table sessions at the end of both workshop weeks were very useful for summarizing interesting open problems. The last one significantly exceeded the allocated period of time because of the lively discussions and contributions by all participants.

Naturally, there was less time for such in-depth discussions during the workshop. However, this week was very useful for making a large international audience of about 90 participants from 17 different countries aware of the most recent, important developments in this new field of research. Feedback from many

participants received during and after the conference showed that this combination of in-depth seminars and compact workshop week was very successful for establishing cross-links between these different scientific communities by providing much motivation and inspiration for future research.

We wish to acknowledge the excellent conference organization provided by Katrin Lantsch, which included a very dedicated social programme. Her efforts helped significantly to make this three-week conference a great success.

Collective Dynamics and Pattern Formation in Active Matter Systems Seminar and Workshop
Scientific coordinators: M. Bär, H. Chate, K. Kruse

The main focus of the seminar and workshop was to discuss current developments in the field of active matter systems. The four-week event started with an embedded three-day focus workshop on "Dynamic Organization and Motility of Single Cells" organized by Carsten Beta, Martin Falcke, and Marcus Hauser. This workshop had a stronger focus on biology than the rest of the event. It featured notably a talk by Vic Small, Vienna, Austria, who presented the latest news on cell locomotion. Another highlight was the presentation of Ewa Paluch, Dresden, Germany, on the mechanics of the cell cortex during migration and division. The second week was mostly reserved for lecture series delivered by Igor Aronson, Argonne, USA and Jean-François Joanny, Paris, France. They gave courses on "Pattern formation in model active systems" (Aronson) as well as on the "Hydrodynamics of active polar gels" (Joanny). Both lecture series were very well received and lead to many discussions. Notably the younger participants profited enormously from these highly didactic introductions. The week ended with a presentation by Erwin Frey, Munich on patterns in bacterial populations.

The third week of the event was devoted to a five-days workshop. It started with an inspiring and comprehensive overview of active matter systems by Jacques Prost, Paris, France, covering classical as well as quantum mechanical systems. The remainder of the workshop continued to be on a very high level covering collective effects in systems in flocking systems by widely recognized pioneers in the field (e.g. talks by Vicsek, Toner) as well as by many younger scientists, during tissue development (e.g. Hufnagel, Peyriéras, Jülicher), and other active systems (e.g. Bausch on patterns in collective actin filament dynamics or Tsimring on dynamics of bacterial colonies). It was a balanced mixture of experimental and theoretical talks and covered also some formal aspects of theoretical approaches to understanding these systems. Outstanding presentations were given by G. Théraulaz, Toulouse, France, on the construction of ant nests (including virtual walks through nests in 3D) and by I. Aronson on active magnetic colloids. The latter was at the same time a PKS colloquium talk. A small number of contributed talks by young scientists had been selected: Thomas Guérin, Paris, France, talked about collective effects in assemblies of molecular motors, Alexander Morozov, Edinburgh, UK, discussed his results on the hydrodynamics of rotating bacteria, Pawel Romanczuk, Dresden, Germany, offered his view on collective motion of Brownian particles, and Shashi Thutupalli, Göttingen, Germany, presented his observations of squirming droplets. All these presentations were well received. On Monday evening a poster session was organized that gave all participants a possibility to present their work. It generated lots of discussions and provided notably a forum for young participants to get into contact with senior researchers. The fourth week was mostly reserved for discussions among the participants, although one presentation was given each day, mostly delivered by young scientists. The final talk was given by Cristián Huepe, Dresden, Germany, who presented intriguing observations on collective animal motion. The event has shown that research on active matter systems is a rapidly developing field with many facets. The seminar and workshop revealed important lines of research. They include on large scales the dynamics of groups of animals, on smaller scales the dynamics of developing tissues, and on even smaller scales the dynamics of active molecules. A strong part of the field as demonstrated by many of the presentations given during these four weeks is the tight connection between experiments and theory. It showed nicely how complex experimental situations can be analyzed using comparatively simple models, which in turn motivate simplified experiments. The event furthermore confirmed that physical concepts from non-equilibrium statistical mechanics and non-linear dynamics are most valuable tools to understand biological as well as artificial active matter.

Quantum Simulations and Design, Focus Workshop
Scientific coordinators: H. Ebert, D. Ködderitzsch, M. Ogura

The International Focus Workshop on Quantum Simulations and Design (QSD11) was held at the Max-Plank Institute for the Physics of Complex Systems in Dresden (mpi**pks**), Germany, from 27 to 29

September 2011. This conference was organized under the auspices of the **mpipks** and the Grant-in-Aid for Scientific Research on Innovative Areas "Materials Design through Computics: Complex Correlation and Nano-Equilibrium Dynamics", MEXT, Japan. The conference focused on the development of methods for first principles electronic structure calculations and their applications. The aim was to provide an opportunity for discussion on the progress in computational materials design and, in particular, the development of quantum simulations and quantum design. A second goal was to strengthen the exchange and cooperation between European researchers with Japanese partners.
Computational materials design is a computational approach for the development of new materials. The essential ingredient is the use of quantum simulations to design a material that meets a given specification of properties and functionality. For this to be successful, the simulation has to be very reliable and be applicable to systems of realistic size. During the conference, new approaches were discussed including methods beyond the local density approximation of density functional theory, order-N methods, methods dealing with excitations, reactions and finite temperatures, and the application of these methods to the design of novel materials, devices and systems.
The conference provided an international forum for experimental and theoretical researchers to exchange ideas. A total of 50 delegates from ten countries participated in the conference. There were 14 invited talks and 18 contributed oral presentations. Young researchers were given a platform to present their work in front of the experts, allowing invited (3) as well as contributed talks (7) for them. Ample time for discussion was given in two poster sessions with 18 contributions presented. Important highlights of the workshop were the talks of the invited speakers: Prof. Igor Abrikosov (Linköping University, Sweden) Prof. Hisazumi Akai (Osaka University, Japan) Prof. Gerrit Bauer (Delft University of Technology, Netherlands) Dr. Markus Eisenbach (Oak Ridge National Laboratory, USA) Prof. Olle Eriksson (Uppsala University, Sweden) Dr. Martin Gradhand (University of Bristol, UK) Prof. Koichiro Inomata (National Institute for Materials Science, Tskukuba) (E) Prof. Takao Kotani (Tottori University, Japan) Dr. Jan Minar (Ludwig-Maximilians-University, München, Germany) Prof. A. Oshiyama (University of Tokyo, Japan) Dr. Mark Stiles (NIST, USA) Prof. Shinji Tsuneyuki (University of Tokyo, Japan) Prof. Wulf Wulfhekel (Universität Karlsruhe (TH), Germany) (E) The talks, mostly of colleagues active in the field of theory were complemented by contributions of two colleagues from experiment (E) who presented the state of the art in GMR- and TMR devices and spin-resolved STM. Altogether the stimulating atmosphere of the workshop venue led to very lively and fruitful discussions. Following to the great and positive resonance among the participants it was agreed to organize a similar workshop in 2013.

Engineering and Control of Quantum Systems, Workshop
Scientific coordinators: C. Koch, G. Morigi

A prerequisite for quantum technologies is the creation of robust quantum mechanical coherence and entanglement. A major challenge that any implementation of quantum technologies has to face is that coupling to the environment leads to loss of coherence: This problem represents a serious obstacle for realizing scalable protocols. Therefore the search for strategies to combat the detrimental effects of dissipation and decoherence is at the center stage of current theoretical and experimental research and requires the development of novel concepts.
The workshop ECOQAS was devoted to the discussion of the challenges and perspectives for scaling control strategies up to the mesoscopic regime. For this purpose, we brought together world-leading scientists from the fields of physical chemistry, atomic, molecular and optical physics, and quantum information science. Most of the speakers addressed the characterization and control of specific physical systems providing the common ground. The subjects ranged from applications of control to atomic and molecular systems, cavity quantum electrodynamics, optomechanics, and NMR systems, to novel concepts and ideas in quantum thermodynamics, quantum communications, and quantum effects in biology. In order to provide a flavour of the conference, we highlight a few presentations: The theoretical underpinnings of quantum control were discussed in detail in the lectures by Tommaso Calarco (Ulm) and Rosario Fazio (Pisa), and in the colloquium by Herschel Rabitz (Princeton), setting the stage for the new challenges, namely, optimal control of quantum many-body systems. Newly developed concepts such as quantum reservoir engineering and noise-assisted transport were introduced by Barbara Kraus (Innsbruck), Birgitta Whaley (Berkeley), Thomas Wellens (Freiburg), and Susana Huelga (Ulm). Ideas and techniques for quantum state estimation and tomography were discussed in the talks by Antonio Acin (Barcelona) and Juan Pablo Paz (Buenos Aires). On the experimental side, in his the femtosecond laser pulse control experiments Kenji Ohmori (Okazaki) applied basic concepts in physical chemistry to quan-

tum information science. Serge Haroche (Paris) presented the first successful demonstration of quantum measurements combined with feedback control in cavity quantum electrodynamics. Ennio Arimondo (Pisa) discussed the experimental application of optimal control protocols to ultracold atomic gases forming Bose-Einstein condensates. Tobias Kippenberg (Basel) presented a review of control achieved in state-of-the-art experiments in optomechanics. A major breakthrough was reported by Immanuel Bloch (Garching), who showed the realization of in-situ measurements of atoms in optical lattices, revealing the microscopic details of these many-body systems. The variety of physical systems provided in first place a diversity of approaches. Moreover, it also contributed to delivering a more complete picture of the limitations and challenges which the issue of scaling up quantum control carries with itself. In passing, we would like to point out that 7 out of 41 talks were presented by women scientists and a number of talks beyond the joint colloquium with the institute were attended by institute members.
Most important participants Due to the diversity of the attendants' background, it is difficult to single out a few major protagonists: Indeed, the conference was characterised by excellent talks and intense discussions, which involved most participants. Discussions took place after the talks, during the various breaks, and at the poster sessions. It is noteworthy that these discussions involved both senior and junior scientists from different fields who exchanged knowledge and identified common questions.
How did scientific newcomers present themselves Young scientists took actively part in the conference program, they were involved in several discussions and, as far as we can say, established new connections. Two young postdocs (Cecilia Cormick and Giulia Gualdi) were session leaders. Young postdocs were also selected for some of the contributed talks, to mention some: C. Cormick, A. Gorschov, M. Khasin. All student participants presented their own work in the poster sessions that were attended by most attendees. Discussions in front of the posters continued even outside the assigned slots of the program.
Scientific results of the conference in a broader sense The objective of the conference was to highlight new theoretical ideas and experimental methods tackling the current challenges and to identify limitations to and future perspectives for scalable control at the quantum level. Considering the excellent talks and the extensive discussions, which saw the active participations of most attendees, the conference has successfully met this objective. We furthermore believe that the conference has also served as an opportunity 2 for scientific networking where collaborations have been both refreshed and newly established and future joint proposals have been discussed. The ECOQAS11 conference has thus significantly contributed to the ongoing effort of identifying perspectives to scalable control of quantum systems.

Carbon-Based Spintronics, Workshop
Scientific coordinators: G. Cuniberti, L. Hueso, S. Roche

CSPIN11 has been focused on recent developments on spintronics in carbon-based materials. Although carbon spintronics is still a nascent field, this workshop has gathered its leading scientific actors. The workshop has covered a broad material portfolio including molecules, molecular magnets, carbon nanotubes and graphene, together with a diversity of quantum spin transport phenomena occurring in coherent and incoherent regimes. Theoretical as well as experimental issues have been addressed such as magnetoresistance phenomena, atomic scale spin engineering, spin injection and spin manipulation, memories and logic device functionalities and spin qubits. Most important participants CSPIN11 has gathered the main contributors of the current progress in carbon-based spintronics. Concerning graphene spintronics, a keynote presentation will be given by Professor Albert Fert, Nobel laureate 2007. Additionally, the key actors were also present including Bart J. van Wees (The Netherlands) and Barbaros Özyilmaz (Singapore). Molecular spintronics was covered by leading scientists such as Herre van der Zant (The Netherlands) and Stefano Sanvito (Ireland); and similarly for organic spintronics with Valentin Alek Dediu (Italy), Bert Koopmans (The Netherlands) and Peter A. Bobbert (The Netherlands). One also notes that a Friday evening lecture was given by Professor Heinrich Kurz (AMO Germany) on "Graphene: Das neue Silizium des einundzwanzigsten Jahrhunderts?". How did scientific newcomers present themselves? The workshop included on the first day a Poster Jam session to allow all participants to present in 1-slide their poster. Two poster sessions (2 hours each) were organized and have allowed many exchanges among participants. The workshop booklet included the whole list of participants together with the details about their presentation and contact address. One also notes that about one third of the young participants could get an oral contribution. Scientific results of the workshop in the broader sense First the scientific content of CSPIN11 has not only been of very high quality, but has also triggered enthusiastic discussions among participants who have been invited to identify the key issues of this field and the possible cross-fertilization among different communities. To that end, on Wednesday, October 26,

a long brainstorming session (16h30-19h) was successfully organized, gathering many viewpoints from participants about key challenges and directions of work for the future. After splitting the audience into four subgroups (Molecular/Organic Theory and Experiments, Carbon Theory/Experiment) for 1h discussion, a general discussion took place, supervised by Stefan Blügel and gathering the initial coordinators of subgroup discussions. The level of participation has been very satisfactory, while some assistants have drafted up the main conclusions of the debate. One notes that this workshop has been a real success, as evidenced by the very active participation of all participants during the talks, question time, brainstorming session, and poster sessions. We finally mention that one important result is the interest in preparing a collective contribution for a scientific journal (under definition), which will let a fingerprint of the philosophy of CSPIN11 and its contours for a broader community.

Rogue Waves, Workshop
Scientific coordinators: N. Akhmediev, E. Pelinovsky, A. C. Newell

The scientific workshop "Rogue waves" took place at the Max Planck Institute for the Physics of Complex Systems in Dresden, Germany from 7–11 Nov 2011. The novel scientific term "Rogue waves" was born in nautical mythology. This term describes waves that appear seemingly from nowhere and may reach the heights of 30 meters. Such gigantic waves often lead to unexpected disasters, involving even the biggest ocean liners. On average, 20 large ships disappear every year meeting these monsters of the deep. No wonder, that other common names for them are "killer waves" or "freak waves". These terms are gradually moved into other scientific fields such as optics, matter waves, superfluidity and even financial world. Common features and analogies help scientists to study the phenomenon of rogue waves in laboratories.
The notion of rogue waves has dramatic impact in many fields in the physical sciences and consequently, the subject is now under intense international research. The lecturers and participants of the workshop (around 70) were all leading experts in the field. Among the lecturers we can mention: Profs. Alan Newell, Yves Pomeau and Vladimir Zakharov from Arizona, Prof. Alfred Osborne from Italy, Prof. Peter Clarkson from the UK, Prof. Bahram Jalali from California, Prof. Helmut Brand from Bayreuth, Prof. Norbert Hoffman from Hamburg and many others. These are just a few names that made significant contributions to the field. Scientists from 18 countries participated in this workshop with the subject at the leading edge of modern science.
Most of the participants are well established experts in the field. The workshop has been a remarkable scientific event for everyone. Prof. Miguel Onorato from Torino, Italy said “I have been to many rogue wave conferences during the last 10 years, and I must say that this last one you have organized has been, by far, the most impressive one.” Professor McClintock from Lancaster, UK said: “I wanted to thank you for an excellent workshop - I hugely enjoyed it and learned a lot.” Exchange of ideas from various fields was one of the main features of the present workshop. Lively discussions over the coffee time, poster sessions and specially designed discussion times also demonstrated success of the workshop.
The Colloquium on Monday “Rogue waves and holes in the sea”, presented by Prof. Alfred Osborne from Torino, attracted wider audience including many scientists from the Max Planck Institute. The author of a recently published book on rogue waves, he presented the subject at the highest scientific level. Evening lecture on Friday presented by Prof. Norbert Hoffmann from Hamburg attracted general public from Dresden. The auditorium was completely full. The high level of interest for the topic has also been seen in the number of questions Prof. Hoffmann had to answer. He had to stay for nearly two hours after the lecture to be able to answer all questions.
Generally, rogue waves can be considered as particular case of extreme events that occur in nature or in the human society. Surprisingly, these events happen more often than people would normally expect. The participants of the workshop agreed that presently, there are many questions to answer. No doubts, the discussions at this workshop generated new ideas and enriched our understanding of extreme events. Ultimately, the discussions at the workshop have influenced the way we will deal with the cataclysms in the future.

Beyond Molecular Dynamics: Long Time Atomic-Scale Simulations, Workshop
Scientific coordinators: C. Becquart, M. Posselt, R. Smith

The BEMOD12 International Workshop was held from 26-29 March 2012 with around 70 participants from 16 different countries. In total we had 54 contributions (1 Colloquium, 28 Invited, 10 contributed and 15 Posters. The theme of the meeting was the subject of how to perform dynamical simulations in atomic

systems over time scales that are longer than those computationally accessible by Molecular Dynamics (MD). At the meeting were a mixture of disciplines and talks and posters varied from descriptions of new algorithms and theoretical underpinning of the techniques, to exciting new applications in materials science, chemistry, biology and physics. Problems considered included the growth of thin films, the long term evolution of radiation damage and the unfolding of protein molecules.

Many techniques were discussed including milestoning, metadynamics and on and off-lattice kinetic Monte-Carlo (KMC) methods even using advanced graphics processors for enhanced speed. However possibly the most exciting new developments were concerning the on-the-fly KMC methods.

For these methods an important theme was the investigation of the transition pathways surrounding local minima on n-dimensional surfaces, especially the best way to determine them when there is no pre-knowledge of where they are located. So far there was no consensus on this point. A second related issue involved the ability to deal with low transition barriers, which can seriously hinder the computational enhancement of many schemes and the best way to initialise searches so as to maximise the number of determined saddles. Other unanswered questions include relationship between minimum energy paths and maximum flux paths and whether it is computationally feasible to map out the transition surface surrounding a local minimum. We look forward to progress on these questions by the time of the next workshop on the subject is organised.

The organisers received a number of very positive comments from the workshop participants most of whom have uploaded their presentations to the workshop web site. However, the success of the meeting was not just because of the quality of the scientific programme but also in a large part due to the MPI for the wonderful facilities offered and to Sabine Strecker for her perfect administrative input.

Laser-Plasma Interaction at Ultra-High Intensity, Workshop
Scientific coordinators: M. Bussmann, E. D Humieres, M. Grech, S. Skupin

Laser-Plasma Interaction (LPI) at Ultra-high Intensities (UHI) is one of today's hot topics in plasma physics. Around the globe, new laser facilities are being built opening new paths towards a wide range of applications: laser-based particle acceleration, novel radiation sources, fast ignition for inertial fusion, hadron-therapy, etc. To trigger and sustain such developments, a deep understanding of LPI is necessary. This understanding relies on theoretical/analytical models as well as on intensive realistic numerical simulations.
This workshop aimed at stimulating and discussing recent progress in this field. To do so, the conference has been organized around 4 main topics, all of them introduced by a 1h30 overview talk. The first day of the conference was dedicated to laser-based electron acceleration and waves in plasmas. This first topic was introduced by an overview talk by Prof. Alexander Pukhov (Düsseldorf) who introduced the basics of theory and simulation of laser-based electron acceleration and presented recent progress toward TeV electron generation. The second day was devoted to laser-based ion acceleration. This topic was introduced by Prof. Vladimir Tikhonchuk (Bordeaux) who gave an overview of the theory and simulation of ion acceleration with lasers, presenting various acceleration mechanisms and addressing some of the newest studies in this field. The third topic of the conference was devoted to fundamental high-field physics, with a particular focus on quantum electrodynamics (QED) processes, which will arise on the forthcoming multi-petawatt lasers. This topic was introduced by Dr. Antonino Di Piazza (Heidelberg), who made a bridge between classical electrodynamics and QED. In particular, he addressed the so-called problem of radiation back-reaction which will give us the opportunity to test both theories on the next generation of lasers. The fourth main topic was addressed on the last day of the conference and concerned the most recent developments in the numerical simulation of LPI. This topic was introduced by Prof. Paul Gibbon (Jülich), who presented the latest advances and emerging trends in this field. In addition to this 4 central topics, Prof. W. Sandner (Berlin) presented the latest European projects of multi-petawatt lasers, and Prof. T. Cowan (Dresden) presented various applications – such as hadron-therapy – of the new particle and radiation sources available using high-power lasers. A visit of the Helmholtz Zentrum Dresden Rossendorf (HZDR) was also organized on the third day of the conference. Finally, the Institute Colloquium was given by Prof. L. Silva (Lisbon) who presented large scale numerical simulations discussing both fundamental applications of LPI, such as the possibility to mimic in the laboratory relativistic astrophysical shocks, and more applied developments in connection with plasma-based particle accelerators. In addition to these seven overview talks, 21 contributed talks were selected by the scientific coordinators of the ENLITE 2012 workshop. PhD students, postdocs and senior scientists had

25 minutes to present their latest results, and 5 additional minutes were attributed to questions and/or discussions. Also, two poster sessions were organized. A total of 38 posters were presented. Among the poster presented by PhD students, four outstanding contributions were selected and awarded prizes provided by two of the conference sponsors, namely NVIDIA (which offered 3 graphic cards designed for scientific computation) and Circular (which offered a mobile workstation as the first prize).
This workshop was organized within the ENLITE (Dresden Exchange oN Laser-plasma Interaction ThEory 09) framework in collaboration with HZDR and CELIA (University of Bordeaux). It was intended as a follow-up of the ENLITE 2009 conference hosted at HZDR three years ago. With more than 60 participants, we believe the conference to be a success. In particular, the overview speakers have given outstanding, pedagogical, presentations which allowed to trigger lively discussions. Contributed talks and posters also allowed to present the latest advances in the field of LPI at ultra-high intensity.
The format of the workshop – combining long overview talks, 30 minutes contributed talks, and posters, thus granting time for extensive discussions – was met with great enthusiasm by the participants. These participants came from all continents, and we obtained an interesting balance between junior (Master and PhD students) and more experienced (postdocs and senior) researchers. Convinced of the success of this workshop, we already plan to organize, within the next three years and in the context of the ENLITE framework, a follow up for this workshop. Finally, we would like to thank the Max Planck Society for providing us with the means to organize this event, as well as the conference sponsors: NVIDIA, Transtec and Circular. The scientific coordinators are particularly grateful to the **mpipks** visitors program for its support and efficiency.

Mathematical Physics of Complex Networks: From Graph Theory to Biological Physics, Workshop
Scientific coordinators: Ch. Del Genio, K. E. Bassler

The workshop, which was held May 14 – 18, 2012, was intended to bring together an interdisciplinary mix of many of the world's leading researchers in the field of complex networks. Its principal aim was to promote the development of analytic results and computational methods and to connect those results to important real world applications. To achieve this goal, a diverse collection of speakers were invited, including researchers whose interests focus on more fundamental issues and methods, as well as researchers investigating applications.
The event brought together top scientists from different backgrounds, creating a stimulating environment for fruitful exchange of ideas and starting collaborations. The workshop exposed the participants to different methods and points of view in the broad topic of complex networks, thereby providing them with approaches they were potentially unfamiliar with and that they might use to the benefit of their research. In attendance were 76 scientists from 28 countries and 5 continents. These attendees included senior researchers, postdocs, as well as doctoral students. The program included a keynote lecture by Prof. A.-L. Barabási from Norteastern University, USA, 25 invited talks, 2 poster sessions mit 35 presenters, 2 social programs, and an official conference dinner.
Among the renowned participants, together with the aforementioned Prof. Barabási were Prof. A. Arenas from the "Rovira i Virgili" University, Spain, Prof. G. Bianconi from Northeastern University, USA, Prof. M. Boguñá from the University of Barcelona, Spain, Prof. B. Drossel from TU Darmstadt, Germany, Prof. S. Dorogovtsev from the University of Aveiro, Portugal, Prof. P. Erdős from the Alfred Rényi Institute for Mathematics, Hungary, Prof. C. Greenhill from the University of New South Wales, Australia, Prof. B. Kahng from Seoul National University, Korea, Prof. G. Korniss from Rensselaer Polytechnic Institute, USA, Prof. S. Redner from Boston University, USA, and Prof. Z. Toroczkai from the University of Notre Dame, USA.
Overall, we believe the conference was highly successful and met all its intended goals. A number of very interesting topics were discussed, including graph sampling, explosive percolation, spectral analysis of graphs, and adaptive network behaviour involving the interplay of topology and dynamical processes. Additionally, many applied topics were also discussed, including neural networks, gene regulatory networks, opinion dynamics, and language development. Of particular note was the presence of many young researchers, who actively participated by presenting their results and by contributing to lively discussions. Indeed, the stimulating environment provided by the institute produced many discussions that will undoubtedly result in new fruitful collaborations. We would like to thank the Institute for making this event possible. We are especially grateful for the exceptional effort that Frau Sabine Strecker gave to every aspect of coordinating it.

Itinerant Spin-Orbital Systems: From Magnetic Frustration to Novel Superconductivity, Workshop
Scientific coordinators: I. Eremin, N. B. Perkins, H. Takagi

The workshop took place at the **mpipks** in Dresden on May 21 – May 25, 2012, and focused on a number of important open problems in the field of complex multi-orbital electronic systems with a strong interplay between charge, spin and orbital degrees of freedom, and geometric frustration. The workshop covered a range of topics, including the unexpected normal state and superconducting properties in cobaltites and ferropnictides; unusual metal-insulator transitions, magnetism and topological properties of strong spin-orbit systems, such as 5d iridium oxides; and peculiar electronic transport appearing when an electron moves in the background of various magnetic textures characteristic to frustrated systems. During the workshop a number of phenomenological and microscopic theories of these systems have been discussed in informal but serious manner. In addition this workshop promoted scientific exchange and interaction between researchers working in these and related areas.
Over 81 participants from Europe, USA, Canada, and Japan took part in the meeting. The program included 48 oral presentations, both invited and contributed, as well as two poster sessions. The interchange of points of view between participants with distinct scientific interests gave rise to a highly stimulating atmosphere. During the workshop, a number of new and exciting results have been presented by, e.g., Claudio Chamon on "Fractional topological insulators", Yong-Baek Kim on "Topological phases of correlated materials with magnetic frustration and spin-orbit coupling", Andy Mackenzie "Electronic nematic physics in Sr3Ru2O7", Ashvin Vishwanath on "Novel phases from correlations and spin orbit", Rafael Fernandes on "Nematic order and itinerant magnetism in the iron pnictides", Yuji Matsuda on "Algebraic spin liquid phase in two-dimensional organic Mott insulator with triangular lattice". Many other, especially young, participants presented talks of high quality and showed new and interesting results. The talks, discussions, and posters at ISOS12 demonstrated that the field of correlated electrons on itinerant frustrated lattices with spin-orbit coupling is developing rapidly and has great prospects.
Two main results of the Workshop are (i) a focused exchange of ideas on the recent experimental and theoretical developments in the field of itinerant spin-orbital systems (like 5d iridate systems where the role of spin-orbit coupling in the formation of the insulating state still has to be understood), and (ii) an involvement of young scientists in the discussion which has stimulated new research collaborations. We would like to thank the **mpipks** for its hospitality and excellent infrastructure provided to the participants of the workshop. We also would like to thank the team of secretaries and, in particular, Claudia Pönisch for their kind assistance and support of this meeting.

Quantum Matter from the Nano-to the Macroscale, Seminar and Workshop
Scientific coordinators: J. S. Meyer, D. Morr, T. Vojta, M. Vojta

The seminar and workshop, which took place at the **mpipks** between June 18 and July 6, 2012, were a forum to bring together leading theorists and experimentalists to discuss recent progress in understanding the unconventional and puzzling properties exhibited by many strongly correlated electron materials and, in particular, the evolution of strong-correlation effects from the nano- to the macroscale. The 52 invited and contributed talks, as well the 36 poster contributions covered a wide variety of topics currently at the center of an intense scientific debate, ranging from Kondo physics in nanostructures and heavy-fermion materials to unconventional superconducting hybrid structures, non-equilibrium transport in quantum-dot arrays, and novel exotic phases in graphene and optical lattices. By bringing together key experts from different subfields, the seminar and workshop led to many fruitful discussions among the 96 participants from Europe, North and South America, Japan, China, and India and initiated a series of new collaborations. While invited talks were presented by a number of leading experts in the field who covered major recent achievement in both theory and experiment, younger participants presented their results in the form of contributed talks and posters.

At the end of this seminar, a roundtable discussion took place that summarized some of the major developments that were reported during the seminar, and discussed some of the most pressing challenges that we face in this field.

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 in order to discuss the recent advances in the area of correlated quantum matter, 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 **mpipks** 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, Mandy Lochar, for their kind assistance and always friendly support in organizing the meeting.

Ordered and Non-Ordered Superstructures of Nanosized Objects: Preparation, Properties, Applications and Modeling, Workshop
Scientific coordinators: A. Eychmüller, A. Govarov, D. Talapin

The ONSNO12 workshop brought together about 100 leading scientists, postdoctoral researchers, and students from Europe, US, Canada, India, China, Australia and other countries working in the field of nanoscale assemblies, colloidal nanoparticles and metallic nanostructures, and their optical and physical properties. In the very productive scientific environment of the **mpipks** young researchers and established senior scientists enjoyed exciting discussions and productive exchange of ideas. All five days of the workshop have been very productive and the participants could listen to lectures given by highly recognized speakers from the various fields including synthesis and fabrication of colloidal nanocrystals, physical chemistry, optical spectroscopy, and theoretical and solid-state physics.
The central themes of the Workshop were the physical and chemical properties of nanoscale assemblies. This is nowadays an extremely "hot" field of research, due to both new fundamental physics and applications. The specific topics covered by the workshop included methods of fabrication of ordered and non-ordered assemblies of nanocrystals and quantum dots; new and optical, transport, and thermal phenomena of assembled nanocrystals, potential and current applications including solar cells, sensors, and thermoelectric devices. The topics of the talks at the Workshop also included fundamental physical aspects of the optical generation of excitons and multi-excitons in colloidal quantum dots and the problems of band-transport in nanocrystal solids. During the Workshop, young scientists were presenting their results in short talks and posters. For some of the young participants, this was the first chance to meet with many well-established scientists from the field. In this way, the Workshop promoted and motivated young active scientists.
The Workshop was open to the public and, therefore, nonregistered 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, and also to listen to the open-access Colloquium talk on the topic of the Workshop. Going back to their home institutions, all of us brought home new ideas, excitement to advance our research further, and knowledge about the cutting-edge developments in the field of nanoscale assemblies and related physical phenomena and applications. The workshop has received many good responses from the participants.
Using this opportunity, we would like to thank the local organizers, Claudia Pönisch and Dr. Sergei Flach, for their excellent and thoughtful organisation and support which was crucial for the success of the workshop.

The Emerging Dynamic View of Proteins: Protein Plasticity in Allostery, Evolution and Self Assembly, Workshop
Scientific coordinators: U. Bastolla, M. Porto, H. E. Roman

Background The reason that motivated us to organize this workshop is that we feel that the study of proteins is experiencing an important change of focus, and we wanted to gather together some of the proposer of this shift of paradigm in areas as different as allostery, structural disorder, evolution and self-assembly. Proteins are involved in essentially all of the biochemical reactions that take place in living organisms, including those required for the control of gene expression, metabolism, transport, and enzymatic catalysis. Their name was inspired by the name of Proteus, the Greek god of versatility and mutability, who could change shape at its will. Nevertheless, the discovery that the native structure of a protein is to a large extent encoded in its amino acid structure, beautifully demonstrated by Anfinsen experiments 40 years ago, has strongly influenced a static view of proteins based on the one-sequence — one-structure — one-function paradigm and on the concept that the fold is conserved during evolution. Recently, in contrast, a more dynamic view of proteins is again drawing the attention of researchers. This appealing change in the point of view has been, in our opinion, mainly influenced by the following factors: (i) the appraisal that a large fraction of the proteins of complex organisms are unfolded (unstructured, disordered) in their native state, and that this structural disorder, far from being a bizarre property, is

crucial for their regulatory function, (ii) the reappraisal of allostery, i.e. the ability of proteins to propagate conformation changes from a control site to an active site, as an intrinsic property of proteins dynamics that is deeply related with enzymatic catalysis, (iii) the increasing number of experimental and theoretical studies on phosphorylation and other post-translational modifications, which are used to achieve allosteric control of proteins structure and function, and (iv) the discovery that changes in the fold during evolution are more common than previously thought and that the interplay between intrinsic protein dynamics and structure change can favor protein evolvability. Moreover, (v) artificial proteins have been engineered to have alternative folded states, a property shared by some natural proteins as well, most notably the prions. The workshop was inspired by the idea that interdisciplinary interaction among scientists from these different fields can greatly help in shaping an integrated and coherent view on protein plasticity.

Themes treated in the workshop and speakers With this background in mind, we decided to organize a workshop for letting leading experts from diverse research areas related with protein plasticity to come together and exchange their opinions. The result was a workshop with a distinctly interdisciplinary character, which was organized in eight topical sessions, namely: (1) 'Allostery', dedicated to the experimental and computational study of protein allosteric regulation and ligand binding, with the invited talks by Dorothee Kern, Igor Berezovsky, Thomas Weikl, Amnon Horovitz and Ruth Nussinov, which we selected as the colloquium talk for the mpi**pks**; (2) 'Self-assembly', with the invited talks by Simon Alberti, Petra Schwille and Joseph Marsh; (3) 'Aggregation', with the invited talk by Fabrizion Chiti and the contributed talk by Francesco Bemporad; (4) 'Protein disorder', with the contributed talks by Vladimir Uversky, Vincent Hilser, Marija Buljan and Monika Fuxreiter; (5) 'Computational methods', with the invited talks by Modesto Orozco, Martin Zacharias, Dave Thirumalai and Garegin Papoyan; (6) 'Evolution of structure-function relationship', with the invited talks by Michael Lässig and Christine Orengo; (7) 'Evolution of protein structures and dynamics', with the invited talks by Nick Grishin and Erich Bornberg-Bauer and the contributed talks by Arne Elofsson, Inmaculada Yruela, Rachel Kolodny, Tobias Sikosek, Jessica Stiltberg-Liberles and Edvin Fugleback; (8) 'Folding', with the invited talks by Gunnar Schröder and Anna Tramontano and the contributed talks by Oxana Galzitskaya and Antonija Kuzmanic.

Discussion sections Moreover, we organized four discussion sections in which the organizers introduced a question related to protein plasticity, and two participants triggered the discussion, exposing their different points of view. Afterwards, all participants took part in the discussions. Discussions were recorded, and we plan to publish a summary of them in a paper that will report the main themes treated at the workshop. The four discussions were related to the main topic sections of the workshop, namely: (I) Is it desirable to move from the single sequence-structure-function view of proteins towards dynamic ensembles, and which computational and experimental methods should be improved to this aim? (II) How is structural disorder related to protein complexity? (III) Do the new developments on the evolution of protein structures require a new view of protein structure space? (IV) Are allostery and structural disorder two sides of the same coin? Many participants, including young ones, took active part in the discussions, taking advantage of the relaxed and informal atmosphere.

Overall balance Besides the contributions of the invited speakers, the workshop has also benefited of 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 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.

Special issue The journal "Biochimica et Biophysica Acta: Proteins and Proteomes", which is a member of the prestigious BBA series, published by Elsevier, will publish a special issue dedicated to the workshop, which we hope will make these different points of view about protein plasticity more visible to the broad protein research community. Seventeen participants already agreed to contribute to the special issue. As organizers, we will write an editorial paper reporting the main subjetcs treated at the workshop and the discussion sections.

Conclusions The organizers wish to express their sincere gratitude to the mpi**pks** for hosting and financing this workshop and for the very generous support, and to Sabine Strecker for her very professional and efficient work with all logistic issues.

Multi-Scale Physics of Lymphocyte Development, Seminar
Scientific coordinators: M. Ivanchenko, C. Molina-Paris, M. Or-Guil

Background The international seminar LymDev12 on Multi-Scale Physics of Lymphocyte Development took place from August 6-31, 2012 at the Max Planck Institute for the Physics of Complex Sytems (mpi**pks**) in Dresden, Germany. It was jointly organized by Mikhail Ivanchenko (University of Nizhniy Novgorod, Russia), Carmen Molina-Paris (University of Leeds, UK), and Michal Or-Guil (Humboldt University Berlin, Germany). The Seminar greatly benefited from the unique Visitors Program of the mpi**pks** which offered on-campus accomodation and boarding for all participants. Local organization before and during the event was done by Katrin Lantsch who is a staff member of the mpi**pks** visitors program. In addition to the official mpi**pks** website, the Workshop is accompanied by the LymDev12 blog (www.lymdev12.eu). The objective of the Seminar was to further a multi-scale description of immune processes by bringing together leading experts in the relevant scientific fields, such as non-linear dynamics, complex networks, stochastic processes and molecular and cellular immunology. In particular, participants were provided with the framework to collaboratively develop and advance physical, mathematical and computational approaches as well as (experimental) methods.
Participants A total of fifty-two researchers from the following countries participated in the Seminar: Australia, Cuba, France, Germany, India, Ireland, Israel, Italy, Portugal, Russia, Spain, Switzerland, United Kingdom, Uni-ted States of America. Among the participants were professors (14), postdoctoral researchers (27) and PhD students (11).
Structure and course of the Seminar The 4-weeks Seminar included three research themes which relate to the major spatio-temporal scales of immune processes : 1. sub-cellular events, 2. single-cell events, 3. ensembles of immune cells and receptors. While the first week focused scientific presentations and afternoon discussions thereof, the second and third week were dedicated to research in small working groups and formation of collaborative initiatives – some of which continued into week four. In additon, week four saw scientific presentations during the morning sessions.
Week 1 The Seminar started with a warm welcome by the Managing Director of the mpi**pks**, Frank Jülicher, and the scientific coordinators (Carmen Molina-Paris, Michal Or-Guil and Mikhail Ivanchenko). Martin Meier-Schellersheim (NIH, Bethesda) kicked off the scientific program giving the first talk in the regulatory networks and signaling session. Further speakers included Jorge Carneiro (IGC, Oeiras) and Ulrich Behn (Universität Leipzig). The session continued on Tuesday with Alexey Zaikin (University College London), Oleg Kanakov (University of Nizhniy Novgorod), Bastian Angermann (NIH, Bethesda) and Kalet Leon (Center of Molecularbiology, Habana). Covered topics ranged from spatially resolved computational modeling to regulatory T cell differentiation, idiotypic networks, cellular decision making, synthetic gene curcuits and cancer therapy. The sessions fueled vivid discussion on the complexity of computational models and the language gap between biology and maths. Wednesday's TCR repertoire, epitopes and signaling session had presentations by Dmitriy Chudakov (Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry, Moscow), Rajat Varma (NIH, Bethesda), Veronika Zarnitsyna (Georgia Institute of Technology, Atlanta) and Alexey Zaikin (University College London). The talks centered on antigen recognition and the proteasome. On Wednesday evening, the work-shop held a poster session featuring 7 posters on a variety of projects. Deborah Dunn-Walters (King's College London) started off Thursday's session on TCR and BCR repertoire analysis and generation mechanisms. She was followed by presentations from Dmitriy Bolotin (Shemya-kin-Ovchinnikov Institute of Bioorganic Chemistry, RAS, Russia), Nicole Wittenbrink (Humboldt University Berlin) and Tom Weber (Humboldt University, Berlin, and IGC, Portugal. The session's focus was on repertoire profiling using next generation sequencing approaches; further subjects were affinity matura-tion and cell cycle variability. Friday opened with Michael Davies (Unilever, Bedford) giving the first talk in the Spatiotemporal analysis and modeling session. Grant Lythe (The University of Leeds), Robin Callard (University College London) and Mark Day (The University of Leeds) completed Friday's session. Thematically, the presentations were set to cover the initiation and dynamics of T cell responses.
Weeks 2 - 3 Working group themes: Theme 1: First few seconds of TCR recognition of antigen. Theme 2: Cellular fate and decision making. Theme 3: Relating CDR3 sequences to antigen recognition and B cell epitopes. Theme 4: Experimental design to measure/assess TCR and BCR cross-reactivity. Theme 5: Technical issues of NGS (next generation sequencing), TCR and BCR diversity. Theme 6: Proteasome and its role in immunology – repertoire of presented epitopes. Theme 7: T cell competition: homeostasis, APC load, fluctuations and bipartite diagrams. Theme 8: Dynamics of CD4 T cell populations. Theme 9: Education – bridging language differences in biology and mathematics. Theme 10:

How can a modeler profit from epitope data bases? Theme 11: Viral dynamics and the immune system. Theme 12: Hypothesis driven modeling of naive CD8 T-cell differentiation in response to activation. In addition, week 2 saw presentations from Edgar Delgado-Eckert (University of Basel), Yanay Ofran (Bar-Ilan University, Ramat Gan), David Olivieri (Universidade de Vigo, Vigo), Phil Hodgkin (The Walter and Eliza Hall Institute of Medical Research, Parkville), Pittu Sandhya Rani (University of Hyderabad), Lars Kaderali (Technische Universität Dresden) and Sebastian Gerdes (Technische Universität Dresden). Monday evening concluded with the colloquium lecture by Ken Duffy (National University of Ireland, Maynooth) and Phil Hodgkin: Reverse engineering the immune system. On Tuesday forenoon, Martin Meier-Schellersheim and Bastian Angermann hosted the Workshop Simmune. Simmune is the name of a suite of software tools that guides the user through the multiple hierarchical scales of cellular behavior, facilitating the generation of comprehensive models. Ruy Ribeiro (Los Alamos National Laboratory), Bjoern Peters (La Jolla Institute for Allergy and Immunology), Hannah Meyer (German Cancer Research Center, Heidelberg), Edward Palmer (University of Basel) and Jose Faro (Universidade de Vigo, Vigo) were the speakers of week 3. During the week, Bjoern Peters and Edward Palmer also moderated special discussions on "Drug induced alterations of MHC-ligand repertoire" and "Why does math work at all?", respectively. Week 4 The last week of the Seminar opened with two presentations on quorum-sensing in the immune system by Antonio Freitas (Institut Pasteur, Paris) and Joseph Reynolds (University of Leeds). They were followed by Benedita Rocha (Inserm, Paris) who talked about thymocyte renewal. Tuesday's presentations centered on profiling of T-cell and B-cell receptor diversity/repertoires. The list of speakers included Aleksandra Walczak (École Normale Supérieure and CNRS, Paris), Vanessa Venturi (University of New South Wales, Sydney), Nina Babel (University Hospital Charité, Berlin), Avidan Neumann (University Hospital Charité, Berlin), Dmitriy Chudakov (Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry, Moscow) and Thierry Mora (École Normale Supérieure and CNRS, Paris). In the evening, Lars Kaderali (Technische Universität Dresden) gave a public lecture titled: Mit Mathematik und Computern gegen Hepatitis-C (Fighting hepatitis C with maths and computers). During the week there were several working groups on TCR sequence analysis, affinity maturation and viral dynamics. Deliveries of the Seminar: The results of the Workshop will be presented/published in a special issue of Frontiers in Immunology.

Entanglement Based Approaches in Quantum Chemistry, Focus Workshop
Scientific coordinators: Ö. Legaza, B. Paulus, M. Reiher, R. Schneider

The focus workshop, which took place at the mpi**pks** between September 3 and 6, 2012, provided a forum to bring together quantum chemists with their expertise on molecular properties, orbital sets, and current quantum chemical methods based on low-rank tensor factorizations on the one hand and condensed matter physicists and mathematicians that are developing more general tensor network methods based on quantum information insights, on the other hand. This currently extremely hot field has already shed light on some of the big outstanding questions in condensed matter physics and has potential to provide a powerful computational approach in quantum chemistry as well. All three days of the workshop were very productive. The workshop stimulated cross fertilization between the different sub-branches of the field which all share the same goal of finding novel theoretical and computational approaches to treat strong correlations in quantum systems.
The participation of top researchers from all these communities has guaranteed that all participants have had the opportunity to obtain a complete picture about the state of the art of the field and the prospects for the future. The focus workshop brought together 42 leading scientists, postdoctoral researchers, and students from all over Europe, from the U.S., and from China working in the field of wavefunction-based electron correlation approaches and in entanglement-based low-rank tensor factorization methods. Since a main goal was to promote the development of new unconventional computational methods in quantum chemistry, experts from different backgrounds focusing on fundamental issues and methods as well as researchers investigating applications were invited. A number of very interesting topics on recent developments from the various communities were considered, including the density-matrix renormalization group and matrix product state methods, the cluster-in-solid approach, density matrix embedding, the semidefinite relaxation method, the methods of increments, various tensor network state approaches, and the graphically contracted electronic structure method. Numerical treatment of tensors, the convergence theory of alternating optimization in multilinear tensor formats, and entanglement in continuous systems were also discussed. Talks on various applied topics such as unconventional approaches to challenges in transition metal chemistry, treatment of strong electron correlations in photochemistry, entanglement-

based analysis of molecular structures, and tunnelling in enzymes, reflected the current state of the art and indicated future perspectives in the application of low-rank tensor factorizations in quantum chemistry.
For many of the outstanding well-established experts, this was the first opportunity to meet with scientists from the other communities working in the same area. The workshop also provided excellent conditions for young researchers who had the opportunity to discuss with leading scientists and to present their results in the form of short talks and posters. In addition to the eleven overview talks, 12 contributed talks were selected and a total of 16 posters were presented. The lively discussions between experts of different communities was a clear indication that our goal was achieved. We have also received many positive comments from the participants including that it would be timely to organize a longer workshop and summer school in the near future. In this sense, we believe that the workshop provided an excellent environment to continue this entirely new field of research to stimulate further developments. A collaboration between these communities will undoubtly open new avenues of research on the problem of strong electron correlation and low-rank tensor factorization, especially theoretical and computational aspects.
Finally, we would like to thank the **mpipks** for giving us the possibility of organizing the EBAQC workshop by providing the funding and a really professional organization and logistics for the event. We would especially like to thank Mandy Lochar and Dr. Sergei Flach for their excellent and thoughtful organization and support which was crucial for the success of the focus workshop.

Statistical Inference: Models in Physics and Learning, Seminar
Scientific coordinators: M. Biehl, M. Opper, T. Villmann

Main focus of the seminar Physics, inference and modeling are related in many ways. Naturally, modeling frameworks require the choice of free parameters which are guided by the aim of explaining observations or available data. On the other hand, statistical physics contributes successfully to the theory and practice of inference itself. Moreover, it continues to inspire novel methods and concepts in other areas such as Machine Learning, Neuroinformatics, or Bioinformatics. The three main themes of the semiinar were:

- Inference in stochastic dynamical systems
- Learning structures from observations
- Statistical Physics of learning

Most important speakers and contributions by junior scientists About 35 presentations covering a variety of topics stimulated intense discussions and provided inspiration for new ideas and research projects. As a particularly positive aspect of our seminar we would like to emphasize the close interaction between senior and junior scientists throughout the event. Almost all younger participants, including PhD students, presented their ongoing work or perspective projects in a short talk. This gave them the chance to discuss their work with some of the leading figures in the field and to put their research into perspective. In our opinion, it seems inappropriate to name the most important speakers. The following should be understood as a subjective selection of just a few highly interesting contributions which exemplify the diversity of topics covered during the seminar:

Ido Kanter (Bar Ilan, Israel) and Ron Meir (Technion, Israel) both reported exciting new possibilities to study the activity and interaction of alive neurons in controlled environments. Fabrice Rossi (Univ. Paris I) summarized and discussed recent developments in the context of deterministic annealing, which is a superb example for the important role statistical physics plays in the area of statistical inference.Guido Sanguinetti (Univ. Edinburgh) presented basic ideas and recent developments in the context of stochastic models and inference problems for systems biology.

Results of the seminar in the broader sense The main aim of the seminar was to provide a platform for extensive discussions, exchange of results and ideas, and active research. The seminar brought together a number of successful senior and young scientists in order to establish new collaborations or intensify existing ones. In this seminar we have presented and discussed most recent developments in the interaction of physics, statistical inference, and modelling. Mainly from the physics perspective, we have discussed on-going projects, presented recent results, and identified new directions of research. The diversity of topics discussed during the seminar provided an excellent basis for establishing cross-disciplinary contacts. A number of novel ideas were developed which combine, for instance, concepts from machine learning

with classical statistical inference. New collaborations will emerge which exploit the analogies of modeling techniques and, e.g., stochastic optimization. As confirmed by many participants, the seminar was considered very fruitful, and a number of promising joint projects is expected to emerge.

Quantum Noise and Measurement in Engineered Electronic Systems, Workshop
Scientific coordinators: W. Belzig, M. Devoret, Y. V. Nazarov

The aim to manipulate, control, and measure nanoelectronic devices deep in the quantum regime has shaped the last decade in mesoscopic physics. Much of the fundamental interest in nanoscopic and microelectronic quantum circuits stems from the fact that environmental effects and the measurement procedure itself have to be considered quantum mechanically, which poses a challenge to experimentalists as well as theorists. Understanding the interplay between quantum fluctuations and amplifcation at the quantum limit requires a more detailed understanding of complex quantum electronic circuits. A similar fundamental motivation comes from the enterprise to experimentally and theoretically investigate higher-order correlations functions or, more generally, the full counting statistics of electrons passing in a nanodevice.

The workshop QNM gathered 70 scientists from 22 countries to discuss the current state of the fields of quantum manipulation and electronic quantum shot noise in experiment and theory. In the field of quantum electronic shot noise the focus was on new aspects of time-resolved correlations in electronic currents (Büttiker, Levitov, Glattli, Reulet) and the detection of unusual statistical many-body properties manifesting themselves in scattered current correlations (von Ruitenbeek, Heiblum, Schönenberger, Martin, Deblock, König, Pothier). The quantum manipulation of superconducting transmon qubits has progressed tremendously, leading extremely long coherence time and long-distance entanglement, paving the way to realistically explore the possibilities of quantum feedback (Schoelkopf, Wallraff, DiCarlo, Siddiqi, Brandes). The fundamentals of quantum thermodynamics can nowadays be detected with single-event resolution allowing to test uctuations relations in a novel regime (Schön, Pekkola, Hänggi). The intimate connection of quantum measurement processes with quantum bits, quantum noise and nano mechanics is underscoring a common theme of the whole workshop (Mølmer, Gefen, Clerk). Manipulating mechanical systems in the quantum regime using optical fields or forces has recently became a major topic in nanomechanics (Kippenberg, von Oppen, Marquardt). A rather new development is the cross coupling of circuit quantum electrodynamics with quantum dots (Ensslin, Kontos). These talks by the invited speakers were complemented by 8 shorter contributions. Note that about a third of the talks were given by younger researchers and caused a wind of change to the field of quantum noise and manipulation. During the two poster session lively discussion continued until late at night and many participants used the whole week to explain their posters to other experts in the field. Finally, the broader scope of quantum measurement with an emphasis on electronic circuits was presented by S. Girvin (Yale) to the public in the framework of the weekly colloquium.

As a result of the workshop different aspects of quantum noise in electronic circuits have brought together the communities of circuit QED, quantum shot noise, full counting statistics and nanomechnics. In future we expect a fruitful interaction to achieve challenging goals like quantum feedback, high-frequency quantum standards and investigations of the full statistics of complex electron-phonon-photon systems deep in the quantum regime.

Wave Chaos from the Micro- to the Macroscale, Workshop
Scientific coordinators: M. Hentschel, S. Shinohara, S. Tomsovic, J. Wiersig

The focus of this international workshop has been on wave and quantum chaos and complex wave phenomena in general in various classical and quantum systems. The workshop brought together theoreticians and experimentalists from all over the world in particular from the fields of optical, acoustic, electronic, atmospheric, and microwave systems ranging in size from few microns (graphene electronics) to thousands of kilometers (ocean acoustics, dynamics of the atmosphere). The aims were: (i) to share the insights gained in mesoscopic systems with researchers from other fields, for example those from the acoustic and optical wave communities, (ii) to learn from their experience and the results they have obtained, (iii) to give an introduction to various aspects of the field to younger scientists.
The main scientific results of the workshop were on the areas of • Optical and microwave systems – Directional coupling of chaotic microcavity emission to waveguides (H. Cao) – Landau-level lasing in strained photonic honeycomb lattices (H. Schomerus) – Wave chaos in rotating optical microcavities

(T. Harayama) – Microwave analogue of graphene (A. Richter, F. Mortessagne) • Electronic systems: – Graphene billiards (K. Richter) – Semiclassical theory of speckle correlations (P. Brouwer) • Acoustic and other waves: – Controlling waves at subwavelength scales (M. Fink) – Coupled phase space flow and wave methods in vibroacoustics (G. Tanner) • Theory: – Complex paths for regular-to-chaotic tunneling rates (R. Ketzmerick) – Random matrix approach to fading statistics in communications (S.M. Anlange) – Effects of anharmonicity on dynamics of trapped cold atoms (S. Fishman) – Application of random matrix theory to the light meson spectrum (L. Munoz)
Discussion among the different communities as well as younger and more senior scientists were facilitated through long coffee breaks (that were very well received) and two poster sessions. The poster sessions 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. 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 workshop was characterized by a very open, harmonic, and cooperative atmosphere and intensive scientific exchange. 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 Sabine Strecker for the absolutely smooth local organisation, also in the name of the participants who praised the atmosphere and organisation many times. We also thank the DFG Research Unit FOR 760 for partial financial support.

Multiscale Complex Fluid Flows and Interfacial Phenomena, Focus Workshop
Scientific coordinators: D. Lohse, S. Kalliadasis, H. A. Stone, U. Thiele

In October 2012 the workshop "Multiscale Complex Fluid Flows and Interfacial Phenomena (MUFLOW12)" took place at the Max-Planck-Institut für Physik komplexer Systeme in Dresden (mpi**pks**) coordinated by D. Lohse (Twente), S. Kalliadasis (London), H. A. Stone (Princeton), and U. Thiele (Loughborough). The workshop was part of the regular workshop programme at the mpi**pks** and furthermore co-financed by the EU ITN MULTIFLOW that ends in December 2012. About one third of the about 70 participants from 25 countries of Europe, Asia and the Americas were present or former members of the EU ITN MULTIFLOW which presented their results to the wider community that was rather well represented. Indeed most speakers and poster presenters, were scientists not related to the ITN what allowed for a lively exchange of ideas across several disciplines and areas of research related to interfacial phenomena in complex fluids or soft matter in general.

Flows of such materials are of central importance in numerous industrial, biomedical, geophysical and domestic applications and display a rich and widely varied range of behaviours, including dewetting, rupture and finite-time blow up, symmetry breaking bifurcations and spontaneous pattern formation. As well as being of great interest in their own right, interfacial flows provide a "test bed" for research into a huge range of challenging nonlinear problems in physics, chemistry and mathematics. As a consequence research is performed by physicists, engineers, chemists, mathematicians and others, using a wide variety of analytical, numerical and experimental techniques. Research on many different aspects of interfacial flows has grown dramatically in recent years as novel applications have continued to appear and increasingly sophisticated theoretical and experimental techniques have been developed. The focus workshop allowed us to exchange information on recent results, to discuss novel approaches and to start new collaborations.

The specific focus of the meeting was the behaviour of free interfaces on a wide range of length scales – the spectrum contains studies of microscopic dynamic processes occurring during phase transitions in colloidal suspensions, as well as macroscopic erosion processes that result from the interaction of fluid flows with their soft substrate (as, e.g., a riverbed). The colloquium talk related to our workshop was given by T. Bohr (Copenhagen) who presented an enlightening overview of spontaneous symmetry breaking phenomena involving fluid surfaces. For illustration, we mention some further speakers and the themes they presented: J. Lister (Cambridge) discussed the spreading of viscous currents under an elastic lid, a problem derived from geo-physical lava flows that lead to the bending of layers of rock; R. Seemann (Saarbrücken) spoke about the manipulation of liquid on elastic grooved substrates, a problem related to emerging microfluidics on elastic supports; P. Colinet (Brussels) presented a detailed mathematical analysis of an approach that alleviates the singularity at a moving three-phase contact line by phase change processes; C. Clanet (Paris) spoke about experiments and theory for the dynamics of cavity collaps; and

E. Knobloch (Berkeley) related various processes of pinning, depinning and self-pinning through their mathematical analysis. Beside these senior scientist, about 20 young scientists presented their results as invited (M. Köpf, Haifa; H. Lopez, Loughborough; A. Galuschko, Göttingen/Dresden) or contributed talks. The programme also contained a very well received evening poster session featuring about twenty posters).

After hearing in August 2012 the sad news that Rudolf Friedrich (Münster) had passed away we decided to dedicate two sessions to him as an important member of the nonlinear science community with a strong interest in the theory of complex systems, in particular, in relation to structure formation. These two dedicated sessions where respectively focused on deposition patterns created at moving contact lines and effects related to concentration gradients at free surfaces or inside thin films.

As expected, the Max-Planck-Institut für Physik komplexer Systeme was an ideal location for the workshop and provided a very stimulating environment. The workshop discussed advances in the particular subjects and also fostered the discussion of underlying conceptional challenges and cross-links between different topics. We expect that it also initiated future collaborations throughout Europe and the world. The feedback we received from participants about the choice of subjects and location was excellent. We are very grateful for the possibility to hold the workshop there and as well for the efficient and smooth organisational support through the members of the Guest Programme Administration.

Scales and Patterns in the Earth System, Workshop
Scientific coordinators: J. Lelieveld

The workshop, which focused on complex earth interactions across disciplines, relevant to global change research, took place at the Max Planck Institute for the Physics of Complex Systems in Dresden (Germany) from 5th to 9th November 2012. The complex non-linear physical, chemical, and biological interactions among the components of the earth system are becoming an increasingly important focus in global change research (R.A. Pielke Sr., H.J. Schellnhuber and D. Sahagian). Therefore, the workshop covered several related topics like the circulations of the earth's atmosphere and ocean as well as biogeochemical processes with modeling and experimental approaches.

Over 40 participants, from different disciplines like chemistry, physics, biology and geosciences took part in this workshop. The program included 14 lectures given by invited experts (Scripps Institution of Oceanography (SIO) and the Max Planck Institutes for Chemistry, for Biogeochemistry, for Meteorology and for Dynamics and Self-Organization) who presented their own work as well as an overview of the field. The audience of mainly young scientists learned, for instance, about recent developments in research of the climate system and climate models, statistical data assimilation, aerosol-cloud interactions, the global carbon cycle and biogeochemistry. Some prominent examples: Prof. Henry Abarbanel (SIO) focused on data assimilation and predictions for shallow water flow; Prof. Meinrat Andreae (MPG) discussed aerosol-cloud-precipitation interactions in the climate system; Prof. Eberhard Bodenschatz (MPG) offered a presentation about Rayleigh-Benard convection in flows; Prof. Martin Heimann (MPG) addressed the role of the global carbon cycle in the climate system; Prof. Ulrich Pöschl (MPG) discussed multiphase processes in the atmosphere-climate system; Prof. Lynn Russell (SIO) focused on the complexity of aerosol-cloud interactions; Prof. Richard Somerville (SIO) presented a climate model concept with super-parameterized clouds. In a poster session all young academics presented new and interesting results of high quality. Fruitful discussions during this poster session but also over coffee/lunch breaks and affiliating the lectures supported the scientific exchange. In particular for the young scientists it was an excellent opportunity to meet renowned scientists and develop new ideas and motivation for their PhD work in the discussions. We are very grateful of the mpi**pks** for the opportunity to use their great facilities and especially Claudia Pönisch for her excellent organization and her kind help. Everything was prepared exceptionally well and we could fully concentrate on the scientific part of the workshop. We received a lot of enthusiastic responses from the participants (and requests to repeat this type of workshops).

Entanglement Spectra in Complex Quantum Wavefunctions, Workshop
Scientific coordinators: A. B. Bernevig, M. Haque, A. Läuchli

Overview. The Focus Workshop was designed to explore emerging results on the entanglement spectrum in quantum many-particle systems. The entanglement spectrum has surprised a rapidly growing community through ongoing discoveries of a remarkable amount of information contained in its structure. The quantity provides a novel opportunity for wavefunction tomography, the mapping out of the

anatomy of complex many-particle wavefunctions. It also contains information about topological order in several ways. The time was appropriate for a critical evaluation of results on the entanglement spectrum that have appeared in the past few years. Since the topic is growing rapidly but still at an early stage of development, a high-intensity one-week workshop was envisaged to help consolidate the community emerging around this topic. The Focus Workshop was very successful in fulfilling this goal. We believe the event has inspired new directions and new questions through communication between researchers who have studied entanglement spectra in diverse models.

Format. There were 30 talks, a colloquium, and two after-dinner poster sessions during the FocusWorkshop. The talks were not organized by subtopic; instead different subtopics were mixed into each session. This seemed to work well as participants at each session got exposure to a variety of emerging themes. F. Duncan M. Haldane was the speaker for the Workshop Colloquium, which was a major highlight of the week. The colloquium was delivered to a packed auditorium and heavily attended, not only by the Workshop attendees and the mpi**pks** members, but also by many people from neighboring Dresden institutes.

Scientific highlights. A prominent theme at the workshop was entanglement spectra in topological states of matter, including fractional quantum Hall states and fractional Chern insulators. This was the setting in which entanglement spectra first gained widespread attention, and the more recent advances were presented and discussed in thorough detail during the Workshop. In addition, entanglement spectra were discussed by speakers and poster presenters in various non-topological states (Bose-Hubbard system, Kugel- Khomskii model, higher-dimensional AKLT models, etc) where it has more recently been explored in some detail, or where its study has led to yet unexplained results. Another recurrent theme involved matrix product and tensor network representations of many-body states and entanglement spectra in such representations.

Talk slides online. The organizers placed slides of all talks online. This provides a snapshot of this emerging field at this point of time, and should be a useful reference for many researchers working in or entering this field.

3.4 Externally Funded Research and Relations to Industry

3.4.1 DFG Projects

Individual Projects

- *Directed Transport within Hamiltonian Dynamics: From Theory to Cold Atoms Experiments*, Dr. S. Flach
- *Kontrolle der epithelialen Zellschichtausbreitung im Zebrafish*, Dr. S. Grill, Dr. G. Salbreux
- *Molecule Interferometry and Metrology*, Dr. K. Hornberger
- *Emmy Noether Group*, Dr. M. Hentschel
- *Graduiertenkolleg "Itineranter Magnetismus und Supraleitung in intermetallischen Verbindungen"*, Prof. Dr. R. Moessner

3.4.2 EU Funding

- EU-FP7 *Systems Biology of Mitosis*, Prof. F. Jülicher
- EU-FP7 *Topological effects in matter with strong spin-orbit coupling*, Prof. R. Moessner
- EU *COST Action CM0702: Chemistry with Ultrashort Pulses and Free-Electron Lasers: Looking for Control Strategies Through Exact Computations*, Dr. U. Saalmann
- EU *Marie Curie Actions - Networks for Initial Training: COHERENCE Cooperativity in Highly Excited Rydberg Ensembles - Control and Entanglement*, Prof. J.-M. Rost, Dr. T. Pohl
- EU *Marie Curie Actions - Networks for Initial Training: CORINF Correlated Multielectron Dynamics in Intense Light Fields*, Prof. J.-M. Rost
- EU *Quantum Integral Light Matter Interface*, Prof. J.-M. Rost, Dr. T. Pohl
- ERC *ACTMECH - Emergent Active Mechanical Behavior of the Actomyosin Cell Cortex*, Dr. Stephan Grill

3.4.3 Additional External Funding

- DAAD, *Transport phenomena at the nano-scale*, Dr. S. Kirchner
- DAAD, *Tailored THz radiation from multicoloar ionizing femtosecond laser*, Dr. S. Skupin
- HFSP Fellowship, *Physical Characterization of cortical dynamics in establishment of polarity in the C. elegans zygote*, Prof. F. Jülicher, Dr. J. Bois
- The Royal Society *Newton Fellow: Singularimetry in light-matter interaction*, Dr. J. Goette
- VW-Stiftung *Towards molecular engines: cooperative coupling of molecular motors in engineered environments*, Prof. F. Jülicher
- VW-Stiftung *Recurrent extreme events in spatially extended excitable systems: Mechanism of their generation and termination*, Prof. H. Kantz
- Helmholtz Gemeinschaft *Helmholtz Virtuelles Institut "New states of matter and their excitations"*, Prof. Dr. R. Moessner
- *Platform for Magnetism and Superconductivity*, Prof. Dr. R. Moessner
- BMBF Grant *Collective organization of cells and tissues: Systems biology of tissue size and shape*, Prof. Dr. F. Jülicher
- European Research Network *European Network in Systems Biology*, Prof. Dr. F. Jülicher

3.4.4 Scholarships

- Dikande, Alain Moise, AvH
- Jorge, Laitao, Erasmus Stiftung
- Langari, Abdolla, AvH
- Dua, Arpid, DAAD
- Fedotora, Olga, DAAD
- Ma, Rui, VW Stiftung
- Knolle, Johannes, German National Scholarship Foundation
- Kaiser, Vojtech, ESN d. Lyon
- Wang, Jing Rong, Chinesische Akademie der Wissenschaften
- Vivek, Lohani, DAAD

3.4.5 Cooperations with Industry

- *Participation in BASF Advanced Research Initiative at Harvard*, Dr. Vasily Zaburdaev
- *Master Thesis: Yixing Chen, Scattered Light of nano particles*, Carl-Zeiss AG 2011, Dr. Stefan Skupin

3.4.6 External Cofunding of Workshops and Seminars

2011

- International Workshop (20% of budget)
  Noise in Nonequilibrium Systems: From Physics to Biology
- Advanced School and Workshop (33% of budget)
  Developments and Prospects in Quantum Impurity Physics
- International Seminar and Workshop (6% of budget)
  Weak Chaos, Infinite Ergodic Theory and Anomalous Dynamics
- International Seminar and Workshop (7% of budget)
  Collective Dynamics and Pattern Formation in Active Matter Systems

2012

- International Workshop (11% of budget)
  Laser-Plasma Interaction at Ultra-High Intensity

- International Workshop (34% of budget)
  Ordered and Non-Ordered Superstructures of Nanosized Objects: Preparation, Properties, Applications and Modeling
- International Seminar (7% of budget)
  Multi-Scale Physics of Lymphocyte Development
- International Focus Workshop (48% of budget)
  Multiscale Complex Fluid Flows and Interfacial Phenomena

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 10/11

Fundamentals of Modern Optics Dr. S. Skupin, FSU Jena

Sommersemester 11

Biophysik III, Theoretical Biophysics Prof. Dr. F. Jülicher, Dr. S. Grill, TU Dresden
Fundamentals of Modern Optics Dr. S. Skupin, FSU Jena

Wintersemester 11/12

Stochastische Prozesse Prof. Dr. H. Kantz, Dr. E. Altmann, TU Dresden
Fundamentals of Modern Optics Dr. S. Skupin, FSU Jena
Engineering Mathematics Dr. T. Gross, University Bristol
Mathematical and Data Modelling II Dr. T. Gross, University Bristol

Sommersemester 12

Biophysik III Theoretical Biophysics Prof. Dr. F. Jülicher, Dr. S. Grill, TU Dresden
Topics in Advanced Many Body Physics Dr. S. Kirchner, TU Dresden
Fundamentals of Modern Optics Dr. S. Skupin, FSU Jena
Nonlinear Optics Dr. S. Skupin, FSU Jena
Nachhaltigkeit, Studium generale Prof. Dr. J.M. Rost, TU Dresden

Wintersemester 12/13

Biological Hydrodynamics Dr. S. Grill, Dr. G. Salbreux, TU Dresden
Nonlinear Dynamics Prof. Dr. H. Kantz, Dr. E. Altmann, TU Dresden
Structure of Matter Dr. S. Skupin, FSU Jena
Nonlinear Quantum Optics Dr. T. Pohl, TU Dresden
Perspektiven auf die Zeit, Studium generale Prof. Dr. J.M. Rost, TU Dresden

3.5.2 Degrees

Dissertations

- *Do, L.: Self-organization in continuous adaptive networks.* Oldenburg, 2011
- *Mikaberidze, A.: Atomic and molecular clusters in intense laser pulses.* Dresden, 2011
- *Mumcu, P.: Self-organized Growth in Developing Epithelia.* Dresden, 2011
- *Roden, J.: Lichtabsorption und Energietransfer in molekularen Aggregaten.* Dresden, 2011
- *Roeder, G.: Orthogonalitätskatastrophe und Fermi-Kanten-Singularitäten in der Photoabsorption ballistischer Quantenpunkte.* Dresden, 2011
- *Zumsande, M.: Extension of Generalized Modeling and Application to Problems from Cell Biology.* Dresden, 2011
- *Dawson, J.: Dynamics of endosomal trafficking.* Dresden, 2012
- *Fuerthauer, S.: Active Chiral Processes in Soft Biological Matter.* Dresden, 2012
- *Höfener,J.: Networks of delay-coupled delay oscillators.* Dresden, 2012
- *Köhler,C.: Ultrashort Light Sources from High Intensity Laser-Matter Interaction.* Dresden, 2012
- *Ranft, J.: Mechanics of Growing Tissues: A Continuum Description Approach.* Paris, Dresden, 2012
- *Staple, D.: Understanding Mechanics and Polarity in Two-Dimensional Tissues.* Dresden, 2012
- *Siegert, S.: Rank statistics of forecast ensembles.* Dresden, 2012
- *Wetzel, L.: Effects of Distributed Delays in Systems of Coupled Phase Oscillators.* Dresden, 2012
- *Zschaler, G.: Adaptive-network models of collective dynamics.* Dresden, 2012

Master

- *Chen, Y.: Scattered light of nano particles.* Jena, 2011
- *Sharafi, N.: Synchrony Codes in Populations of Neurons.* Leipzig, 2011

Diploma

- *Bauermeister, C.: The Effect of Stochastic Oscillations on Neural Firing.* Dresden, 2011
- *Gerlach, M.: Hamiltonians dominanter Wechselwirkung.* Dresden, 2011
- *Kruscha, A.: Destruction of invariant tori under symplectic.* Dresden, 2011
- *Strempel, M.: Dünne Filme aktiver chiraler Flüssigkeiten.* Dresden, 2011
- *Scholich, A.: Collective behavior of molecular motors and elastic filaments.* Dresden, 2012
- *Tschischik, W.: Non-equilibrium dynamics in Bose-Hubbard dimers and ladders.* Dresden, 2012

Bachelor

- *Geisler, L.: Dynamik der Wirbeltiersegmentierung.* Dresden, 2012

3.5.3 Appointments and Awards

Appointments

- *Prof. J. Broecker* accepted the offer for faculty position at the University of Reading
- *Prof. S. Flach* accepted the offer for a Professorship at the Massey University
- *Prof. T. Gross* accepted the offer for a Professorship at the University Bristol
- *Prof. E. Gull* accepted the offer for a Professorship at the University of Michigan
- *Prof. K. Hornberger* accepted the offer for a Professorship at the University Duisburg
- *Prof. M. Hentschel* accepted the offer for a Professorship at the University Ilmenau
- *Prof. A. Läuchli* accepted the offer for a Professorship at the University Innsbruck
- *Prof. C. F. Lee* accepted the offer for a faculty position at the Imperial College London
- *Prof. B. Lindner* accepted the offer for a Professorship at the Humboldt University Berlin

Awards

- *Grill, S.:* Binder-Innovationspreis 2013
- *Hiller, M.:* German Life Science Award 2013
- *Moessner, R.:* Gottfried Wilhelm Leibniz-Preis (DFG) 2013
- *Moessner, R.:* European Physical Society Condensed Matter Division Europhysics Prize 2012
- *Skupin, S.:* Prix Bull-Joseph Fourier 2012
- *Fulde, P.:* Marian-Smoluchowski-Emil-Warburg-Preis (DPG) 2011
- *Grill, S.:* Paul Ehrlich- und Ludwig Darmstaedter-Nachwuchspreis 2011
- *Grill, S.:* ERC Starting Grant 2011
- *Hentschel, M.:* Hertha-Sponer-Preis (DPG) 2011

3.6 Public Relations

3.6.1 Long Night of Sciences

On July 1, 2011 and July 6, 2012 the institute participated in the *Long Night of Sciences* jointly with the Technische Universität Dresden and many other research institutes in Dresden. We opened the doors for everyone interested in visiting our institute from 6pm to 12pm. The members of our institute conveyed the importance and fascination of their research to a broad audience with various talks, a physics show, a physics quiz, a science cinema, poster presentations and a lot of different presentations of their work. The resonance was very good with about 3500 visitors counted at each event.

Long Night of Science, July 6, 2012 - approx. 3500 visitors

3.6.2 Science in the City Hall

Public lecture by Prof. Karl Leo (TU Dresden), approx. 180 visitors

The **mpipks**, the Technische Universität Dresden and the City of Dresden are running a series of public lectures called *Wissenschaft im Rathaus*. The following lectures were delivered during the period 2011-2012:

- 6. April 2011, Prof. Dr. T. Henning, *Von Staubscheiben zu extrasolaren Planeten - Die Entstehung von Planetensystemen*, about 320 participants
- 21. September 2011, Prof. Dr. Martin Melles, *Die Klimageschichte der Arktis - globale Bedeutung und aktuelle Fortschritte*, about 320 participants
- 12. Apri1 2012, Prof. Dr. H. Hatt, *Die Macht der Düfte: Alles über das Riechen und wie es unser Leben bestimmt*, about 320 participants
- 5. September, Prof. Dr. K. Leo, *Organik: Schlechte Halbleiter für wunderbare Bauelemente*, about 180 participants
- 4. Dezember 2012, Prof. Dr. G. Gigerenzer, *Bauchentscheidungen: Die Intelligenz des Unbewussten*, about 360 participants

3.6.3 mpipks School Contact Program

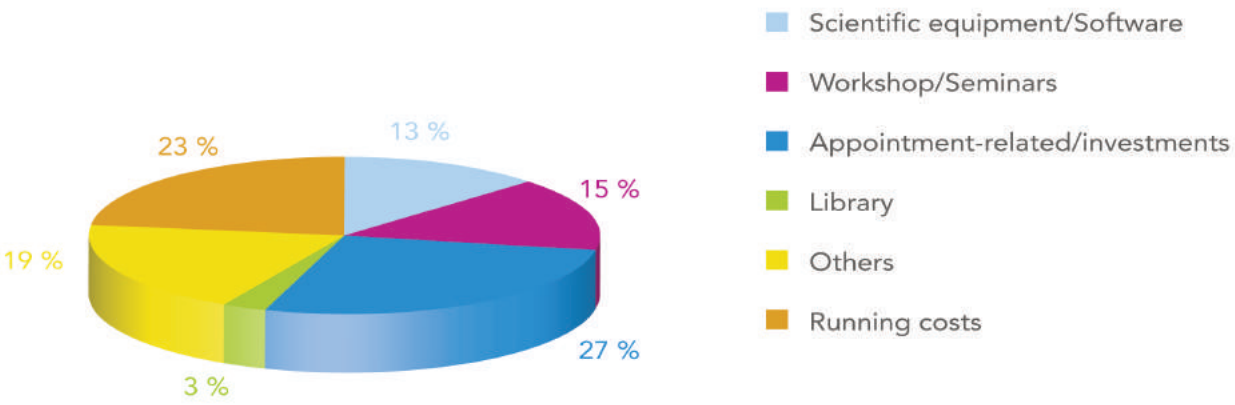
Public lecture for Junior Doctors

mpi**pks** offers lecturing at high schools on a permanent basis. High school teachers receive updated lists of available lecture topics offered. About fifteen lectures are given annually.

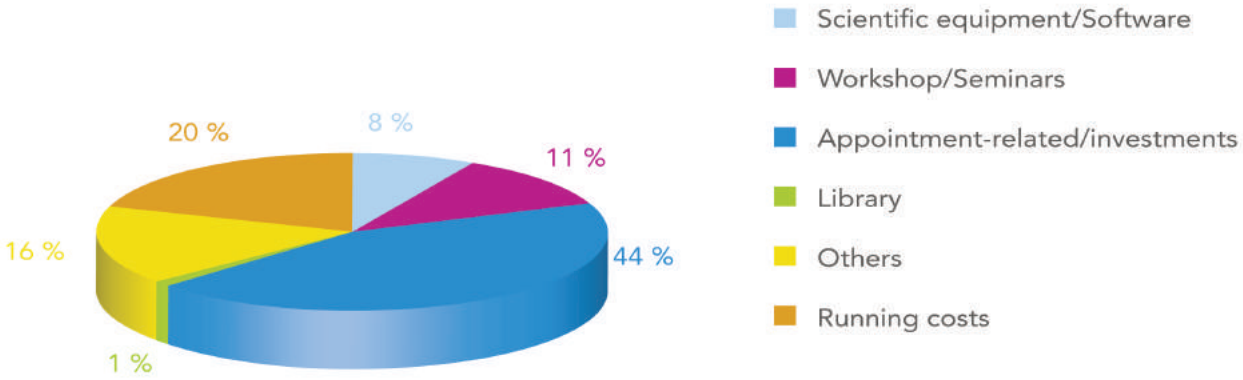
Our Institute participates in the program Junior Doctor with numerous events for students from 3rd class onwards. We provide each school year about 6 lectures for pupils in this context. The program Junior Doctor is a part of the joint project Netzwerk "Dresden - Stadt der Wissenschaft" of the scientific community of Dresden.

3.7 Budget of the Institute

Research Budget 2011

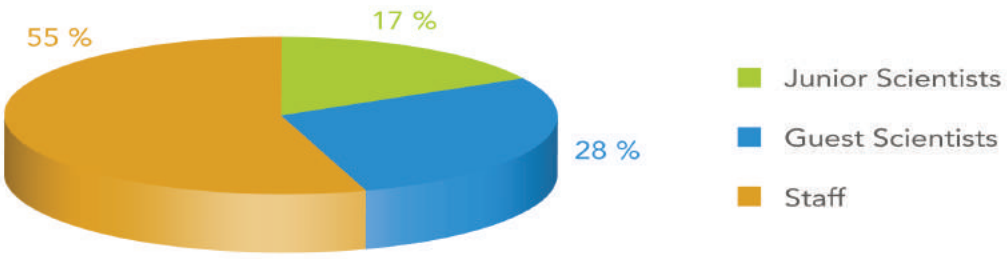


Research Budget 2012

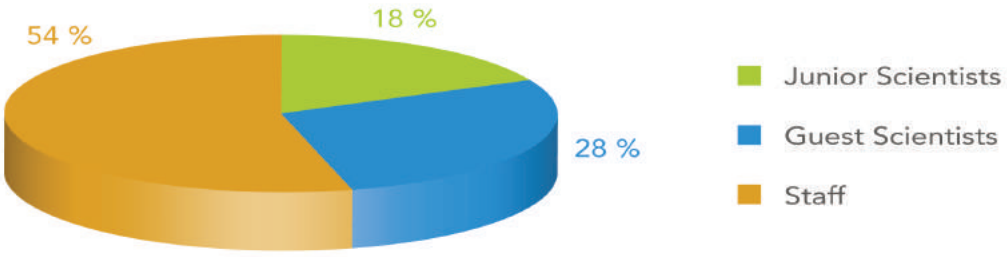


Research budget during the past two years

Personnel Budget 2011



Personnel Budget 2012



Budget for personnel

3.8 Equipment and Premises

3.8.1 Computer Facilities

Computing facilities

Since our scientists are doing their research based on various physical models, many of them even starting from first principles, extensive numerical calculations have played an important role in our institute ever since it was founded in 1993. This is why the main focus of our computer equipment is on the computational throughput, whereas the request for high-end graphics is typically rather moderate. About half of our offices are equipped with X-Terminals (Thin Clients) while the other half of our scientists use workstations. Presently the institute hosts approximately 370 servers with a total of 6000 CPU cores on site and, since 2010, a compute cluster located in Garching with an additional 1500 CPU cores.

Our computers offer from one to 128 CPU cores and a maximum of 3 Terabytes of main memory and a maximum of seventy Terabytes of local disk space. We run 10 Gigabit, 1 Gigabit and Fast Ethernet as a local area network interconnect. By the end of 2012 about 98 % of the computing power available was based on Linux systems and 2 % 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 70 laptops for our scientists in order to provide them the possibility to continue their work while they are abroad. Furthermore, we run 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 few years we noticed a tendency towards integrated software environments while fewer people are writing their own programs using programming languages like C or Fortran.

For our short-term guests who participate in seminars and workshops we run a separate small cluster. We offer those guests the possibility to connect their own laptops to our network or to use X-Terminals to access the aforementioned cluster. The separation was introduced for both greater convenience and higher security.

We are connected to the Internet using a bandwidth of 100 MBit/s. Redundancy is achieved by automatic failover to the neighboring institute's internet connection (and vice versa for their connection) in case of problems with our primary Internet connection.

The computer department is run by five employees with their respective main tasks being unix and networks, web and Windows, hardware and general user support. In addition to those five people we employ two trainees and one student of the Berufsakademie Dresden. Small to medium sized programming tasks are done by our staff and three students who are working part-time in the computer department. The development of large software applications, like a new database system for our visitors program, usually have to be implemented by external companies.

Future

Linux will continue to be the main operating system for our number crunchers in the near future, presently running mainly on Intel Xeon based hardware. Other operating systems like HP UX will only play a minor role for some specialized applications. The near future will see graphics processing units (GPU) and similar hardware being used by our scientists to some extent, since they allow for considerable speedups for some of the codes used at our institute. Due to the fact that the number of cores per CPU is steadily increasing we expect that the total number of systems at our institute will only change moderately in the near future.

History

In 1996 the institute occupied three buildings in Dresden and an outpost in Stuttgart. Before we moved to our new building, a further 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 early 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 delivered several times the CPU performance of that server. The new extension building which was finished in 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 with computers based on Intel's IA64 (Itanium) architecture in order to support some applications that perform particularly well on this platform. In 2010 a large parallel cluster was bought which is installed at the RZG in Garching and is run by the staff there. The following table shows the development of the computer resources on site at our institute in Dresden over time. The numbers do not include our parallel cluster located in Garching.

year	computers	main memory (GB)	disk space (TB)
1996	33	13	0.5
1998	66	60	2.0
2000	95	310	8
2002	162	590	22
2004	327	2600	90
2006	345	5500	190
2008	360	15000	510
2010	400	22000	560
2012	370	75000	770

3.8.2 Library

The library of the mpi**pks** has several tasks. Most evidently, it provides a large stock of scientific books and journals for the use of all members of the mpi**pks**. It is accessible 24 hours per day and provides scientists with media and scientific information in many forms. Scientists from outside the institute can also use the library resources during regular office hours.

Currently, our library stock consists of about 4,900 monographs, about 16,500 bound journal volumes and 52 scientific journal subscriptions in print and online, which can be found in the online catalogue.

The automatic check out system permits institute employees to borrow books at any time. A modern Bookeye machine and Xerox machine allows printing, scanning and copying.

Via the library homepage, our users have access to about 30,000 online journals and 40,000 e-books, as well as numerous literature and factual databases, online encyclopedias, dictionaries, the Virtual Max Planck library, the e-Doc Server, international catalogues etc.

As an additional service, the librarian has access to online document delivery systems. Books or references which are not available in the library or online can be obtained quickly, usually within 24-48 hours, through a simple web-based order form and manual processing by the librarian.

Finally, the library is also responsible for reporting the publication activities of the mpi**pks**, e.g., for the yearbook of the Max Planck Society or the scientific report. Also the demands of Open Access are related to this activities: The old MPG database e-Doc and the new database PubMan which are institutional repositories with a wide variety of services are fed with the mpi**pks** publications' meta data by the librarian.

A library steering committee of scientists representing the departments and research groups of the mpi**pks** makes sure that the needs of scientists are optimally served by the library. In quarterly meetings decisions such as new journal subscriptions are made.

Our library consists of two separate sections: The reading room is located on the second floor of the main building. Here, international newspapers, and copies of the most important books and journals for each group are available for easy access. The main library used to be on the ground floor of the main

building. In autumn 2012, it was relocated into the newly built guesthouse. In the new facilities, books and journals can be found on the four floors of an open-plan room flooded with light.

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 the **mpipks** members through Open Access and an institutional repository. 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 the **mpipks** 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 four guest houses with different apartment types for up to 100 guests in total.

Panorama of the Guest Houses

Guest house 1 has 20 single and 5 double rooms (with two separate bedrooms). All of them have a bathroom, a terrace or a balcony, and are equipped with telephones. Our guests use two fully equipped shared kitchens and one meeting room, with a small library and a TV set.

Guest house 2 offers 10 one-bedroom apartments with kitchen, for up to two persons, and three two-bedroom apartments with a living room, bathroom and kitchen for up to three persons (e.g. families). One of these apartments is suited for handicapped persons. All apartments have a balcony or a terrace, and are equipped with TV connection ports and telephones. In the basement of guest house 2, five washing machines and two tumble dryers are available. They are accessible from guest houses 1, 2 and 3.

Guest house 3 allows to accommodate guests in 5 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 apartments have been converted into offices and are used by short term guest scientists.

Since November 2012, the newly built guest house 4 offers 14 additional single and 8 additional double rooms (with two separate bedrooms). All rooms are equipped with TV connection ports and telephones. Further, the building has a multi-purpose room with kitchen appliances, a large terrace and a light garden for the common use and enjoyment. Moreover, it houses the library and the offices of the visitors program.

The guest house rooms and apartments are cleaned and towels and bed linen are exchanged regularly. Cots can be rented free of charge. WLAN is available in all rooms and apartments.

Additionally, the institute provides a special apartment for scientists with children. It can be used by institute members and workshop participants upon consultation with the visitors program. Moreover, child daycare can be arranged for workshop participants.

3.9 Committees

3.9.1 Scientific Advisory Board

According to the rules of the Max Planck Society the **mpipks** has a Scientific Advisory Board. The members of the Board advise the board of directors concerning the research at the institute. The Board assesses the research direction of the institute, the scientific relevance and chances for success of the research projects, as well as the collaborations among members of the institute, with universities, other research institutions and with industry. The Scientific Advisory Board evaluates the results of the research work presented by the board of directors in the biennial research report and prepares, usually every two years, a report for the President of the Max Planck Society on the research of the institute.
Currently the Scientific Advisory Board has the following members:

Gugliandolo, L.
Professor Dr.

Laboratoire de Physique Théorique
et Hautes Energies
Université Pierre et Marie Curie - Paris VI
Toue 24, 5éme etage
4, Place Jussieu
75252 Paris cedex 05
Frankreich

Frey, E.
Professor Dr.

Ludwig-Maximilians-Universität
Theresienstraße 37
80333 München

Ivanov, M.
Professor Dr.

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Grossbritannien

Kurths, J.
Professor Dr.

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Mahadevan, L.
Professor Dr.

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01069 Dresden

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USA

Starace, A.
Professor Dr.

Department of Physics and Astronomy
University of Nebraska
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855 North 16th Street
Lincoln, NE 68588-0299
USA

Sznajd, J.
Professor Dr.

Institute of Low Temperature and
Structure Research
Polish Academy of Sciences
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50-422 Wroclaw
Polen

Valenti, M.-R.
Professor Dr.

Institut für Theoretische Physik
Universität Frankfurt
Max-von-Laue-Str. 1
60438 Frankfurt/Main

3.9.2 Board of Trustees

In accord with the rules of the Max Planck Society the **mpipks** 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, 2018):

Birgel, D.	Chefredakteur Dresdner Neueste Nachrichten Hauptstraße 21 01097 Dresden
Eschelbacher, H. C. Dr.-Ing.	Ministerialdirigent a. D. Hauptstraße 124 53604 Bad Honnef
Gessner, T. Prof. Dr.	Fraunhofer-Institut für Elektronische Nanosysteme Technologie-Campus 3 09126 Chemnitz
Kaschke, M. Prof. Dr.	Vorsitzender des Vorstandes Carl Zeiss AG 73446 Oberkochen
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3.10 Members of the mpipks

(as of December 2012)

1. mpi**pks positions** — **49**
   - Scientific personnel — 17
     - *Scientific members* — *3*
     - *Research staff (including four junior research groups)* — *14*
   - Technical staff — 9
   - Administration and infrastructure staff — 23

2. **Externally funded research staff** — **10**

3. **PhD students** — **69**
   - PhD students with internal supervision — 53
     - *German PhD students* — *30*
     - *Foreign PhD students* — *23*
   - PhD students with external supervision[a] — 16
     - *PhD students with external funding* — *6*
     - *IMPRS PhD students with external supervision* — *10*

4. **Guest scientists** — **62**
   - German guest scientists — 13
   - Foreign guest scientists — 49

[a] Including 14 IMPRS members

The research positions are generally limited in time. Only *Prof. U. Saalmann* and *Prof. H. Kantz*, head of the group "Time Series Analysis" are employed on permanent positions. Furthermore, *Dr. L. Do*, head of the Visitors and Workshop Program, is a permanent staff member of the scientific service.

Chapter 4

Publications

4.1 Light-Matter Interaction

2011

Babushkin, I., S. Skupin, A. Husakou, C. Köhler, E. Cabrera-Granado, L. Bergé and J. Herrmann: Tailoring terahertz radiation by controlling tunnel photoionization events in gases. New Journal of Physics **13**, 123029 (2011).

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4.2 Ultracold Matter

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4.3 Semiclassics and Chaos in Quantum Systems

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