Contents

Chapter 1

Scientific Work and its Organization at the Institute – an Overview

1.1 History and Development of the Institute

1992-1994 • The Max Planck Institute for the Physics of Complex Systems (mpi**pks**) was founded by the Senate of the Max Planck Society in November 1992. The concept for the Institute provides for three scientific divisions and a large Visitors Program. The mission is to contribute to the research in the field of complex systems in a globally visible way and to promote it as a subject. One of the central goals is to pass on the innovation generated in the field as quickly and efficiently as possible to the young generation of scientists at universities. Dresden was chosen as the location for the institute for its favorable scientific environment and its location near the German-Polish-Czech border triangle. In July 1993, Founding Director *Prof. P. Fulde* launched the scientific activities of the first division *Electronic Correlations* in Stuttgart. Work in Dresden started in January 1994 thanks to the TU Dresden which generously offered 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 mpi**pks** 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 Chemistry* headed by *Dr. M. Dolg* soon after. At the same time, plans for the institute's building and guest houses took shape. The architects Brenner und Partner (Stuttgart) won the competitive bidding, and construction started in September 1995. After less than two years the institute moved into the new main building and took into service the three guest houses. In the meantime, the Seminar and Visitors Program gained momentum with hundreds of scientists visiting the institute.

1999-2001 • In 1999, the *Finite Systems* division was installed under the directon of *Prof. J. M. Rost*. In the same year, *Dr. A. Buchleitner* arrived at the institute to launch the research group *Nonlinear Dynamics in Quantum Systems*. After *Dr. Dolg* accepted an offer for a professorship at the University of Bonn, *Dr. U. Birkenheuer* became his successor in March 2000. Soon afterwards, *Dr. K. Richter* left for a chair of Theoretical Physics at the University of Regensburg. To continue the successful work in mesoscopics, *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 • In 2001, *Prof. F. Jülicher* was appointed as head of the third division *Biological Physics* establishing a bridge between physics and biology. 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. 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* set up the Emmy Noether Group *Electronic Structure of Finite Systems* at the Institute. In the following year, the **mpipks** and the Max Planck Institute for Molecular Cell Biology and Genetics (MPI-CBG) launched the joint research program *Physics of Biological Systems* and established its first two Junior Research Groups: *Dr. K. Kruse*, head of the group *Physics of Cell Division*, working theoretically at the **mpipks**; *Dr. I. M. Tolić-Nørrelykke*, head of the group *Mechanics of Cell Division*, experimentally at the MPI-CBG. 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* moved to a faculty position at Lancaster University. *Dr. M. Hentschel* started the activities of the Emmy Noether group *Many Body Effects in Mesoscopic Systems*. *Dr. S. Grill* completed the joint research program of the **mpipks** and the MPI-CBG by launching the Junior Research Group *Motor Systems*. The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* started operation and the new wing of the institute was completed providing additional office space and a new seminar room. In 2006, *Dr. K. Kruse* and *Dr. R. Everaers* accepted professorships at the University of Saarbrücken and the École Normale Supérieure in Lyon.

2007-2008 • During this period *Prof. P. Fulde* retired from his position as a director of the **mpipks** and head of the division *Electronic Correlations*. *Prof. R. Moessner* was appointed as new director, and started to set up his division *Condensed Matter* in early 2008. *Dr. A. Becker* accepted a fellowship at the Joint Institute for Laboratory Astrophysics together with a faculty position at the University of Colorado, *Dr. A. Buchleitner* took up 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 turn, several new groups were installed. In 2007, *Dr. T. Gross* joined the **mpipks** 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 groups *Complex Dynamics in Cold Gases* and *New States of Quantum Matter* were founded under the direction of *Dr. T. Pohl*, and *Dr. A. Läuchli* respectively.

2009-2010 • In 2009, *Dr. S. Kirchner* joined the **mpipks** as head of the Junior Research Group *Collective Phenomena in Solid State and Materials Physics*, operating jointly with the neighboring Max Planck Institute for Chemical Physics of Solids (MPI-CPfS). Moreover, *Dr. K. Hornberger* arrived at the **mpipks** 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 **mpipks**. 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 renewed for a second six-year period.

2011-2012 • In 2011 and 2012, several Junior Research Group leaders left the **mpipks** 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 new Junior Research Group *Computational Quantum Many-Body Physics* was concluded in August 2012, when the group leader *Dr. E. Gull* accepted a faculty position at the University of Michigan. Several new groups were etablished: *Dr. F. Pollmann* set up the activities of the Junior Research Group *Topology and Correlations 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 head of the group *Quantum Aggregates*, and *Dr. N. Rohringer* 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 built 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* (CSBD).

2013-06.2015 • During the past thirty months, the research at the mpi**pks** has once more acquired new foci due to the conclusion of existing and the installation of new temporary working groups. *Dr. G. Salbreux* took up a group leader position at the Crick Institute in London; *Dr. S. Skupin* moved to a CNRS research position at the Centre Lasers Intenses et Applications in Bordeaux. *Dr. S. Kirchner* and *Dr. S. Grill* accepted professorships at the Zhejiang University and the Technical University Dresden. As planned, the Junior Research Group of *Dr. N. Rohringer* changed its affiliation when the theory division of the MPI for the Structure and Dynamics of Matter in Hamburg was established in spring 2015. Meanwhile, all three divisions recruited new Junior Research Groups: *Dr. J. Bardarson* complements the Condensed Matter division as head of the group *Quantum Matter - Transport and Dynamics*, *Dr. A. Landsman* and her group *Ultrashort laser-matter interaction* add to the Finite Systems division, and *Dr. J. Brugués* and his group *Self-organization of biological structures* to the Biological Physics division and the CSBD. In 2015, the Max Planck Fellowship of *Prof. R. Ketzmerick* (TU Dresden) and his Max Planck Fellow Group *Chaos and Quantum Chaos* were extended to a second five-year period by the Max Planck Society.

1.2 Research Areas and Structure of the Institute

The institute investigates collective phenomena in classical and quantum physics. Its three divisions focus their research acitivities on the following main areas:

- 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.

In addition, director emeritus *Prof. P. Fulde* works on electronic structure calculations in the framework of wavefunction based methods as opposed to density functional schemes and on the role of spin-orbit interactions in the theory of superconductivity.

The divisions are supplemented by research and Junior Research Groups, which thematically expand, fortify and bridge the research acitivities:

- The research group *Nonlinear Time Series Analysis* headed by *Prof. H. Kantz* is the only permanent research group and analyzes temporal and spatial fluctuations in different kinds of deterministic and stochastic systems, with particular emphasis on climate dynamics.
- The Otto Hahn Group *Dynamical Systems and Social Dynamics* is headed by *Dr. E. G. Altmann* and applies complexity theory to data of human activities.
- The Junior Research Group *Computational Biology and Evolutionary Genomics* headed by *Dr. M. Hiller* uses computational approaches to link phenotypic differences between species to differences in their genomes, which is key to understand how nature's phenotypic diversity evolved.
- The Junior Research Group *Self-Organization of Biological Structures* headed by *Dr. J. Brugués* is focused on understanding how the large-scale patterns and behaviors of biological structures emerge from the collective behaviors of molecules.
- The research group *Collective Dynamics of Cells* headed by *Dr. V. Zaburdaev* develops and applies methods of statistical physics helping to understand complex biological phenomena.
- The Junior Research Group *Physics of the Cytoskeleton* is headed by *Dr. G. Salbreux* and focuses on understanding physical processes driving cellular and tissue morphogenesis, in close collaboration with experimental biology groups.
- The research group *Topology and Correlations in Condensed Matter* is headed by *Dr. F. Pollmann* and focuses on the study of topological phases of matter, the dynamics in disordered systems, and the applications of quantum information concepts to quantum many-body systems.

- The research group *Quantum Matter — Transport and Dynamics* is headed by *Dr. J. H. Bardarson* and studies quantum matter, condensed matter which properties are dominated by quantum effect, with focus ranging from fundamental theory to direct comparison and collaboration with experimental groups, in particular in Dresden.
- The research group *X-Ray Quantum Optics* is headed by *Dr. N. Rohringer* and studies nonlinear and quantum optical processes with femtosecond high-brilliance x-ray sources both in theory and experiment.
- The research group *Quantum Aggregates* headed by *Dr. A. Eisfeld* investigates the emergence of collective effects in assemblies of atoms or molecules, with a particular focus on the coupling between electronic and nuclear degrees of freedom.
- The research group *Complex Dynamics in Cold Gases* led by *Dr. T. Pohl* explores the interaction of light with cold gases, with special emphasis on emerging quantum many-body and nonlinear optics phenomena.
- The Max Planck Fellow Group *Quantum Chaos and Quantum Dynamics* is headed by *Prof. R. Ketzmerick* and focuses on quantum signatures of regular and chaotic dynamics to ultracold atomic quantum gases.

1.3 Workshop and Visitors Program

Its large program for visiting scientists makes the **mpipks** an almost unique institute within the Max Planck Society comparable perhaps only to the MPI for Mathematics in Bonn. The visitors program administers individual scholarships for guest scientists at the institute (p. 124), but also international workshops and seminars (p. 135). For these we offer both logistical and technical support as well as access to facilities (seminar rooms, offices, guesthouses).

The scholarships are open to scientists at all levels of their career, from students all the way to sabbatical support for professors. The duration of the scholarships varies between a few weeks to a maximum of two years. Scholarships, as well as funding for workshops, are awarded by two separate selection committees that include external experts as members.

Every year, around 1,500 scientists visit the institute, some as part of special programs within the visitors program: The **mpipks** hosts up to two *Advanced Study Groups* per year to foster the exchange between outstanding scientists and young researchers in residence (p. 43). Each group consists of several long-staying senior scientists and focuses on a current and important topic in the field of Complex Systems. The activities are reinforced by short-term visitors who join the group for seminars, lectures, discussions, and other meetings.
Since 2000, the **mpipks** annually awards the *Martin Gutzwiller Fellowship* to an internationally recognized and experienced scientist (p. 125), who spends up to one academic year at the institute.
Moreover, the **mpipks** annually offers one *Distinguished PKS Postdoctoral Fellowship* to an excellent young postdoc (p. 127).

1.4 Teaching and Training

In addition to our core activities, we engage in teaching and training.

Training • The **mpipks** runs the IMPRS *Dynamical Processes in Atoms, Molecules and Solids*, which offers a well-structured PhD training (p. 121). It also participates in the IMPRS *Molecular Cell Biology and Bioengineering*, which provides a similarly broad spectrum of lectures and courses. In addition, it is part of various third party funded structured graduate programs (p. 169).

Our PhD students and postdocs are admitted to the lecture courses of the TU Dresden as well as the events of the Workshop and Seminar Program (p. 139). In addition, the institute organizes soft skill training events such as German courses or a presentation series on professional skills and career coaching (p. 172). These are open to all junior scientists.

Teaching • Experienced postdocs and group leaders conduct lecture series at the TU Dresden and at other universities (p. 171). The benefit is mutual: The lectures offered often cover latest developments,

thus complementing the standard curriculum; at the same time, our young researchers gain valuable teaching experience.

Research Organization • The large Workshop and Seminar Program at the mpi**pks** also offers young scientists the opportunity to gain experience in the organization of meetings. Thus, they can influence a broader research agenda and grow in visibility. Between January 2013 and June 2015, junior scientists of the institute were involved in the coordination of eight out of 45 workshops (p. 139).

1.5 Diversity

The structure of the institute offers ideal conditions for the promotion of diversity. Via the unique flexibility of the visitors program, we are able to support stays of different lengths (from a few days to several years), and with different purposes (from workshop participation to collaborations, PhD training or sabbatical stays), logistically and/or financially as needed. Like this, we can tailor our support to individual needs, profiles, and backgrounds. On average the institute hosts scientists from about 40 nations at any given time.

The mpi**pks** aims to promote the advancement of women in science. It participates in the annual *Girl's Day*, invites female students from high schools to lectures and discussions about a career in science, and encourages female scienstist to apply for positions. We have thus increased the percentage of female researchers to 11% of all postdocs and 14% of all predocs holding a contract of more than three months.

To accomodate the requirements of researchers with young children the institute provides a *parent & child apartment* in one of the guest houses. This facility gives scientists who travel with children the opportunity to participate in workshops and seminars while their children are cared for on the premises. Qualified staff is organised by the institute upon request. When not booked for workshop participants, the *parent & child apartment* can be used by members of the mpi**pks** who need to bring their young children during working hours.

1.6 Public Relations and Outreach

The institute endeavours to bring science, and our contribution to it, closer to the general public.

Each year, we reach about 4000 people with public evening lectures offered in connection with scientific workshops, the institute's acitivities at the *Long Night of the Sciences* (p. 175), and the lecture series *Science in the City Hall* (p. 175).

In early 2015, the institute hosted an art exhibition exploring the contrasting role of the riddle as a problem in mathematics versus its various cultural forms, which many external visitors used to engage in discussion with mpi**pks** scientists.

A particular focus of the outreach efforts is to acquaint children and teenagers with the sciences and encourage them to approach scientific topics with confidence (p. 176): Our contributions to the program *Junior Doctor* aim to arouse the curiosity of young children in a playful way. The school contact program addresses high school students, who we hope to inspire through direct contact with young researchers.

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 TU Dresden is mirrored in the Max Planck Fellow Group *Chaos and Quantum Chaos* headed by *Prof. R. Ketzmerick*, as well as in the mpi**pks** participation in the cluster of excellence *Center for Advancing Electronics Dresden*, the collaborative research center *Correlated Magnetism: From Frustration To Topology*, the graduate school *Cell, Developmental and Systems Biology*, and the research training group *Itinerant Magnetism and Superconductivity in Intermetallic Compounds*. The mpi**pks** has particularly close contacts to the Institute of Theoretical Physics and the Institute of Biophysics and is involved in a number of joint

projects (p. 169). The division *Biological Physics* is in close collaboration with the Max Planck Institute of Molecular Cell Biology and Genetics. The cooperation between both institutes has institutionalized in 2012 by the foundation of the Intersectional Center for Systems Biology Dresden (p. 10). The division *Condensed Matter* cooperates with the Leibniz Institute for Solid State and Materials Research Dresden and runs a joint Junior Research Group with the neighbouring Max Planck Institute for the Chemical Physics of Solids (p. 11). Further collaborations connect the mpi**pks** with the Biotechnological Center and the newly founded Center for Regenerative Therapies.
National and International • The numerous different national and international collaborations and contacts are listed in the research group reports (Chapters 1.8 – 1.11, and 3.4). The joint workshop program, which is run in cooperation with the New Zealand Institute for Advanced Studies, is described in Chapter 3.3.4.

1.7.1 Center for Systems Biology Dresden

The Center for Systems Biology Dresden is a joint initiative of the mpi**pks** and the MPI-CBG. The Center was established by the Max Planck Society as an inter-sectional collaboration. Building on the strong and long-standing partnership between the mpi**pks** and the MPI-CBG, the center continues and extends the previously existing research program on the physics of biological systems of the two institutes. The establishment of the Center for Systems Biology brought the opportunity to add approaches from computer science to the previously existing research activities linking physics and biology.

The Center for Systems Biology was founded in 2013 with the signing of an operational agreement between the mpi**pks** and the MPI-CBG. Both institutes administer the Center together. The Max Planck Society provides funds for three research groups and for a new division. The new division of Eugene Myers at MPI-CBG focusses on novel approaches to image analysis combined with the development of microscopy techniques that are optimized for automated image analysis. Furthermore, new group leaders were hired. Three research groups of the Center are headed by Ivo Sbalzarini, Michael Hiller and by Jan Brugués. Michael Hiller and Jan Brugués have their administrative homes at mpi**pks** and are also affiliated with MPI-CBG. Ivo Sbvalzarini has his administrative home at MPI-CBG and collaborates closely with mpi**pks**. In 2014 he also became W3 professor in computer science at the TU Dresden. The Center for Systems Biology thereby also fosters strong collaborations with the TU Dresden. Further members of the Center are groups at mpi**pks** and MPI-CBG that share a common interest in theoretical, computational and quantitative approaches to biology. These are in particular the groups of Anthony Hyman (MPI-CBG), Jan Huisken (MPI-CBG), Frank Jülicher (mpi**pks**), Moritz Kreysing (MPI-CBG), Guillaume Salbreux (mpi**pks**), Pawel Tomancak (MPI-CBG), Vasily Zaburdaev (mpi**pks**), Marino Zerial (MPI-CBG) as well as the group of Stephan Grill (TU Dresden, Biotec).

The Center investigates integrated biological systems with a focus on spatio-temporal processes in cells and tissues. This research involves quantitative experiments on normal and perturbed systems to study complex patterning processes in biology. Theoretical approaches play a key role to identify principles and to propose mechanisms that underlie the self-organization of such dynamic patterns. State of the art microscopy techniques provide data in three space dimensions and in time. Their analysis requires the development of novel algorithms for image analysis and computer vision. This combination of computer science, theoretical physics and experimental biology, with the goal to understand how cells form tissues, is the main mission of the Center.

A steering committee is responsible for the scientific management of the Center. The Center also funds the ELBE postdoc program which attracts postdoctoral researchers that work across disciplines from physics and computer science to biology and between experiment and theory. This program is modelled on the visitors program of mpi**pks** and administered by mpi**pks**. The ELBE postdoc program has the

important role to also foster collaborations between experimentalists and theorists. Therefore, ELBE postdocs are affiliated with two research groups, typically one experimental and one theoretical. Furthermore, the Center also organizes the ELBE PhD track that funds cross-disciplinary PhD students.

In order to host the new division and the three research groups of the Center, a new building is currently being constructed. It will also provide space for the TU Dresden by hosting the group of Ivo Sbalzarini. This building is funded by the state of Saxony. It is designed by the Finnish architects Heikkinen and Komonen. With the construction of the new building, the Center for Systems Biology Dresden will soon be fully operational. It provides a unique research environment, bringing together experimental biology, theoretical physics, bioinformatics and image informatics to shed light on the physical principles that underlie living systems.

CSBD building construction, August 14, 2015. Picture by K. Boes, MPI-CBG.

Visualization of the planned building by Heikkinen-Komonen architects.

1.7.2 Joint research group with MPI-CPfS

Since its very inception, mpi**pks** has had a strong research activity in condensed matter theory, in particular the physics of strongly correlated electronic systems. Similarly, the neighbouring Max Planck Institute for the Chemical Physics of Solids (MPI-CPfS) has a strong emphasis on correlated quantum matter. This has led to a broad range of collaborations between the two institutes.

Shortly after the appointment of Roderich Moessner as a new director at mpi**pks**, a joint research group between the institutes was established, in order to provide an organisational framework combining the respective expertise of the institutes, in particular enabling a young scientist to benefit from both access to experimental work at MPI-CPfS and the theory environment at mpi**pks**. It organises and bundles a range of activities, and joint seminars between the two institutes feature theorists working in the broad area of strongly correlated electron physics, superconductivity and magnetism.

The joint group was initially funded for five years by the Innovationsfond of the President of the Max Planck Society. After an evaluation of the group, which was first headed by Stefan Kirchner on the topic "Collective Phenomena in Solid State and Materials Physics", and with the new appointment of Andrew Mackenzie as director at MPI-CPfS, it was decided to turn this into a long-term arrangement.

With Stefan Kirchner having moved on to a Professorship, the resulting vacancy has attracted Takashi Oka to move from University of Tokyo to Dresden to head the joint group "Nonequilibrium quantum matter" in the second half of 2015.

1.8 Divisions and Research Groups

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

Condensed matter physics deals with physical processes and phenomena on many scales and levels – from their microscopic basis all the way to applications in daily life. One of its central attractions lies in the possibility of pursuing a research programme covering, and linking, many of these.

In this spirit, the condensed matter division studies the collective behaviour of inanimate matter. 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. For this, we strive to identify models exhibiting interesting phenomena, as well as materials where these may be observed.

On the methodological side, a broad scope of research goals in turn requires a versatile and flexible set of approaches. The work of the division is thus dedicated to a considerable degree to method development. Regarding numerical approaches, this covers e.g. Monte Carlo, exact diagonalisation or DMRG algorithms and their descendants. Analytically, the mature toolbox of many-body theory is used and extended, for example in extending the X-ray edge problem to the case of Majorana Fermions in Kitaev spin liquids. On top of all of this, much attention is devoted to developing 'heuristic' approaches to discover and describe new phenomena in new settings.

Three research themes stand out for the period covered by this report. One is the longstanding interest in what has become known as topological condensed matter physics: the discovery, and description of states of matter beyond the Landau-Ginzburg paradigm. A second one is the study of disorder combined with interactions and/or topology, in particular the search for new degrees of freedom as well as their collective behaviour. Finally, a more recent addition to research activities is the collective dynamics of many-body systems in a wide variety of settings, such as the coherent quantum dynamics of driven systems or the behaviour of topological systems after a quench.

Research Topics

Glassiness and topology. Already in the very first experiments on highly frustrated magnets, the concurrent appearance of a cooperative paramagnetic regime and an instability to a spin glass phase were noted. We now understand the former as a classical topological (Coulomb) spin liquid, but the latter has remained mysterious, with the tantalising possibility of disorder-free glassiness inherent in the spin liquid state. For the case of the Coulomb phase of spin ice, we have demonstrated that dilution with non-magnetic ions induces a bona-fide spin glass transition; that the effective degrees of freedom which freeze are highly unusual 'ghost dipoles', related to regular spins in a way analogous to the relation between holes and electrons in a filled band; and that the freezing transition scales with the density of these ghost dipoles, a result of interest for dipolar spin glasses more generally.

Coherent quantum dynamics. The advent of experiments capable of reaching long coherence times, especially in cold atomic systems, have opened a window on the collective coherent dynamics of quantum many-body systems. We have studied the behaviour of such systems subject to periodic driving, as a simple instance of non-equilibrium behaviour realisable experimentally. We have found a first classification of the resulting behaviour, comprising a small number of distinct cases, including a periodic version of the generalised Gibbs as well as, in many-body localised systems, a transition as a function of driving frequency out of the localised regime to "generic" behaviour, which is maximally featureless.

Thermalisation in quantum systems. We have established statistical properties of matrix elements of operators in families of Hamiltonians incorporating both integrable and non-integrable members, allowing insights into the underpinnings of eigenstate thermalisation.

Electro- and mangetolyte physics. The magnetic monopole picture for spin ice permits formulating the behaviour of this topological magnet in terms of concepts familiar from electrolyte physics. We have analysed the venerable Wien effect of electrolytes both starting from Onsager's original solution and in lattice-based simulations, in order to obtain the non-linear AC susceptibility of spin ice over an unprecedented window of frequencies and amplitudes. This has also produced new insights into the AC version of the classic Wien effect.

Dynamical signatures of quantum spin liquids. We have obtained the first exact solution of the full dynamical structure factor of non-trivial quantum spin liquid in $d > 1$. This contains direct signatures of its emergent degrees of freedom, Majorana Fermions and emergent gauge fluxes, which we have analysed for ESR, neutron scattering and Raman experiments.

Pauli percolation. We have identified a model with a discontinuous percolation transition involving only a minimal amount of non-locality. Unlike the much-studied problematic case of explosive percolation, this transition is reversible.

Magnetic, superconducting and topological materials. We have continued our extensive research activities in these fields. Salient results include the first fully analytical computation of the proton correlations in water ice; the identification of the phase diagram of dipoles on the kagome lattice; an analysis of the role of multiferroicity in the crystallisation of magnetic monopoles; signatures of quantum fluctuations in spin ice; the properties of mobile holes in the Kitaev model; and the connection of large Chern number bands on the pyrochlore lattice with the physics of Weyl semimetals.

Perspectives

The condensed matter division at the mpi**pks** was constituted in late 2007 with the arrival of Roderich Moessner as director. Two group leaders - Andreas Läuchli and Emmanuel Gull, both computational physicists - have already come and gone to take up professorships in Austria and the USA. 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. Jens Bardarson joined in 2013 to head the group *Quantum Matter - Transport and Dynamics*, who investigates disordered and low-dimensional systems, in particular with view to manifestations of phenomena such as Weyl semimetals and many-body localised states.

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

The coherent quantum dynamics of many-body systems will be investigated, both with view to understanding its basic properties but also in order to identify the settings in which interesting phenomena can best be observed experimentally.

One strand of work will be to continue to identify possible extensions, and limits of, the concepts of thermodynamics to non-equilibrium systems. In particular, we are interested in possible definitions of phases, and the existence of sharp transitions between them, in situations where not even the equilibrium concepts as fundamental as that of internal energy remain well-defined.

Building on our recent theoretical progress, we plan to work together with experimental groups in the search for topological magnetic materials, with an emphasis on identifying new fractionalised excitations on top of the deceptively featureless background provided by a topological spin liquid ground state.

More broadly, in continuation of our more 'conceptual' activities, we aim to further the integration of previously distinct fields of correlated electron physics, such as the physics of frustrated lattices and the study of novel electronic states such as Weyl semimetals.

Finally, our activites in quantum information theory will centre on the attempt to understand better many-body wavefunctions and the structures they form in Hilbert space, for example by analysing the possibility of defining concepts such as the clustering of wavefunctions, or the planting of solutions to computational problems.

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* had a research activity centred on the field of quantum phase transitions, which substantively complements the research undertaken in the condensed matter division. Its head Stefan Kirchner has taken up a full professorship in Hangzhou (China). This collaboration is being continued with the newly appointed director Andrew Mackenzie at the MPI-CPfS.

- *Manifold cooperations with theory groups internationally, e.g.:*
  - Austria: Universität Graz (Hans Gerd Evertz); Universität Innsbruck (Andreas Läuchli)
  - Canada: Simon Fraser University (Igor Herbut); University of Toronto (Yong-baek Kim; Sung-Sik Lee)
  - France: Université de Bordeaux (Jerôme Cayssol); CEA Grenoble (Mike Zhitomirsky); École Normale Supérieure Lyon (Peter Holdsworth); Université Paris VI-Jussieu (Benoît Douçot)
  - Great Britain: University of Cambridge (Claudio Castelnovo; Dima Kovrizhin); University College London (Steve Bramwell); Oxford University (John Chalker); St. Andrew's (Chris Hooley)
  - Hungary: Budapest University of Technology and Economics (Balazs Dora)
  - India: IACS Kolkata (Arnab Das, Arnab Sen); Tata Institute for Fundamental Research (Kedar Damle)
  - Italy: ICTP Trieste (Antonello Scardiccio)
  - Japan: Okinawa Institute for Science and Technology (Nic Shannon)
  - United States: Google (Sergei Isakov); Los Alamos National Laboratory (Gia-wei Chern); University of Minnesota (Natalia Perkins); Princeton University (Shivaji Sondhi); University of Washington (Chris Laumann)

- *Cooperations with experimental groups, e.g.:*
  - Argentina: UNLP-Conicet La Plata – Santiago Grigera (non-equilibrium behaviour in spin ice)
  - Germany:
    * High magnetic field laboratory, Helmholtz Zentrum Dresden-Rossendorf – Sergei Zherlitsyn, Jochen Wosnitza (ultrasound studies on frustrated magnets)
    * IFW Dresden – Bernd Büchner, Sabine Wuhrmehl (correlated materials)
    * TU Dresden – Hans-Henning Klauss (novel superconductors)
  - United States: Oak Ridge National Laboratory – Steve Nagler, Alan Tennant (spin liquids)

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

The research group *Topology and Correlations in Condensed Matter* was established at the **mpipks** in January 2011. It currently consists of five postdocs (Yin-Chen He, Adolfo Grushin, Rajeev Singh, Jean-Marie Stephan, Yohei Fuji) and six PhD students (Johannes Motruk, Krishanu Roy Chowdhury, Siddhardh Chandra Morampudi, Giuseppe DeTomasi, Johannes Hauschild, and Ruben Verresen). We have also hosted two summer students (Sanjay Moudgalya and Yi-Hao Jhu).

Our group is interested in a variety of problems in Condensed Matter Theory. The focus lies mainly 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 and many-body localization, charge and spin degrees of freedom on geometrically frustrated lattices, as well as the applications of quantum-information concepts to strongly correlated systems. Over the past two years, our group focused particularly on the following topics:

Realization of topological orders in physical lattice models. Condensed matter is found in a variety of phases, the vast majority of which are characterized in terms of symmetry breaking. A notable exception to this rule was provided by the discovery of the quantum Hall effects which exhibit new kinds of topological orders not associated with any symmetry breaking. In this context, we studied the emergence of topologically ordered phases in strongly correlated electron and spin-systems: (i) We introduced an exactly solvable quantum dimer model that realizes a double semion phase and numerically proved its stability (ii) Using the infinite density matrix renormalization group method on an infinite cylinder geometry, we characterized the $1/3$ fractional Chern insulator state in the Haldane honeycomb lattice model at one-third filling. (iii) We studied a bosonic model with correlated hopping on a honeycomb lattice, and showed that its ground state is a bosonic integer quantum Hall phase, a prominent example of a symmetry protected topological phase.

Infinite density matrix renormalization group for fractional quantum Hall systems. Quantum Hall systems have a plethora of experimentally observed phases which have yet to be definitively identified, such as

the plateaus at $\nu = 5/2$ and $\nu = 12/5$. Numerical simulations, in particular exact diagonalization (ED), have long played an important role as a bridge between our theoretical and experimental understanding. We introduced the infinite density matrix renormalization group method as a new tool to study fractional quantum Hall systems on infinitely long cylinders. This method allows us to consider systems that are considerably larger than those accessible to ED – which turns out to be very important in understanding the subtle physics of some of the plateaus. With this new method, we have addressed two long standing questions: (i) We found clear numerical evidence that at filling $\nu = 12/5$ a Read-Rezayi phase is stabilized by Coulomb interactions at finite layer thickness. (ii) At filling factor $\nu = 5/2$, we found that Landau level mixing at the Coulomb point energetically prefers the anti-Pfaffian state.

Frustrated systems. Strongly correlated systems on frustrated lattices can exhibit very interesting physics at low temperatures. In such systems, the competition between different interactions often results in multiple low-energy states which are degenerate or nearly degenerate with each other. Consequently, quantum fluctuations become very important at low temperatures and can lead to emergent phases of matter with exotic properties: (i) We studied an extended Hubbard model on the kagome lattice at filling factor $n = 1/6$ and found that spin fluctuations can induce a transition into a charge ordered state. (ii) We studied the stability of the $U(1)$ spin liquid in quantum spin ice under realistic long range interactions. (iii) We considered hard-core bosons on the kagome lattice in the presence of short range repulsive interactions and focused particularly on the filling factor $n = 1/3$ for which we observe a transition from a nematic to a spin-liquid phase.

Many-body localization. Many-body localization (MBL) occurs in isolated quantum systems when Anderson localization persists in the presence of finite interactions. The study of MBL is very challenging because we need to understand the physics of eigenstates of quantum many-body systems at finite energy densities. Thus new theoretical and numerical tools need to be developed: (i) We explored entanglement properties that are promising for the study of the MBL transition in excited states. In particular, by measuring the variance of the bipartite entanglement entropy, we observed a conjectured MBL mobility edge. (ii) We introduced a unitary matrix-product operator based variational method that approximately finds all the eigenstates of fully many-body localized one-dimensional Hamiltonians.

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 setup for non-equilibrium investigations due to the high degree of control over various dissipation mechanisms. We studied a number of different model systems which are motivated by different optical lattice experiments: (i) We studied slow (linear) quenches in homogeneous and inhomogeneous Luttinger Liquids and showed the absence of an orthogonality catastrophe for local interaction quenches. (ii) We studied real-time dynamics in the one-dimensional Hubbard model. (iii) Using recently developed numerical techniques for the time evolution of two-dimensional quantum systems, we studied the expansion of bosonic clouds. (iv) We performed a detailed analysis of the breakdown of thermalization in disordered spin chains.

Cooperations

- *University of California, Berkeley*: Collaboration with Joel Moore and several members of his group on simulating the dynamics of long ranged Hamiltonians using matrix-product states and topological phases of matter
- *University of California, Riverside*: Collaboration with Kirill Shtengel on frustrated spin- and fermionic systems
- *The Institute for Solid State Physics, Kashiwa*: Collaboration with Masaki Oshikawa on topological phases of matter
- *National Taiwan University, Taipei*: Collaboration with Kao Ying-Jer and several members of his group on the development of tensor-product state based numerical methods
- *Research Institute for Solid State Physics and Optics, Budapest*: Collaboration with Karlo Penc on the study of frustrated magnets
- *Budapest University of Technology and Economics*: Collaboration with Balazs Dora on quenches in one-dimensional systems
- *Okinawa Institute of Science and Technology*: Collaboration with Nic Shannon on the study of frustrated magnets
- *University of Bordeaux*: Collaboration with Jerome Cayssol on Majorana bound states

- *Princeton University*: Collaboration with Shivaji Sondhi on efficient simulations of many-body localized systems

Research Group: Quantum Matter - Transport and Dynamics
(Head: Dr. Jens H. Bardarson)

The research group "Quantum Matter – Transport and Dynamics" was established in September 2013. It currently consists of two postdocs (Jacopo Viti and Soumya Bera) and four PhD students (Emmanouil Xypakis, Jan Behrends, Talía Lezama and Younes Javanmard). The group has also hosted three master level interns (Sarthak Chandra, Darek Kajtoch and Shang Liu).

We understand "quantum matter" to stand for condensed matter which properties are strongly influenced by quantum mechanical effects. The major quantum phenomena are interference, entanglement and topology. Interference is induced by scattering of impurities or by chaos, entanglement by correlations between identical particles, and topology is induced by strong spin-orbit coupling. It is this connection between the quantum mechanical spin and topology that justifies including topology in the list of major quantum phenomena. The study of quantum matter is therefore broadly the study of the interplay between disorder, interactions and spins. The combination of topology and disorder leads to topological states of matter. When gapped this gives rise to topological insulators and superconductors, while the gapless case includes Weyl and Dirac semimetals. Many-body localization is the study of the combined effects of interactions and disorder, and topological order is obtained when topology and entanglement mix. The research of our group aims at developing an intuition and understanding of all these and related states of matter. Below we give more details of some our main research directions.

Physics is at the core an experimental science. Our research is accordingly strongly motivated by experimental reality, and at the same time focused on developing fundamental theoretical understanding. Some of our work is in direct collaboration with experimental groups, both helping with interpretation of existing data and suggesting experiments that probe the most fundamental physical properties of the materials under study. In the absence of such direct experimental verification of our analytic understanding, we employ computer experiments to verify and deepen our intuition of physical systems. To that end we both adapt and adjust existing numerical algorithms, as well as developing our own simulations schemes. This synergy between analytical modeling, numerical and lab experiments, reflects the working mode of physics itself and nicely summarizes the ideals according to which we conduct our research.

Topological insulators and superconductors. Topological insulators are bulk insulators with a metallic surface described at low energies by Dirac fermions. Topological superconductors, similarly, are insulating in the bulk for quasiparticles and host a surface state described by Majorana zero modes. When a 3D topological insulator is made into a wire, the surface is gapped out due the nontrivial Berry phase a Dirac fermion picks up upon encircling the circumference of the wire. This gap is readily closed by a magnetic field along the wire when the corresponding Aharonov-Bohm flux through the wire is equal to half a flux quantum, π-flux, and therefore exactly cancels the Berry phase. This leads to the emergence of a perfectly transmitted mode and a characteristic Aharonov Bohm oscillations in the conductance of the wire which we have discussed theoretically.

When the wire is brought into proximity with an s-wave superconductor, the perfectly transmitted mode is transformed into a Majorana state, and the wire becomes an induced topological superconducting wire. One way to probe this wire is to measure the NS conductance in the single mode limit, obtained by a perpendicular magnetic field in the normal part, which induces a chiral mode which can be thought of as an edge state of a quantum Hall state, despite the absence of a physical edge. Essentially, the curvature of the wire is such that part of it effectively see a positive magnetic field and the other part a negative magnetic field, giving arise to an interface between two distinct quantum Hall states.

In a collaboration with experimental colleagues at IFW Dresden, we have studied the conductance fluctuations of such topological insulator nanowires in the normal state. We have found that there is a large parameter region far from the Dirac point where non-universal conductance fluctuations are obtained, which can be modulated by a magnetic field, giving rise to Aharonov-Bohm oscillations in the conductance fluctuations. Such modulations are unusual in mesoscopic systems and reflect the robustness of Dirac fermions to disorder. In addition we have theoretically studied the conductance fluctuations close to the Dirac point when the transport is dominated by the emergence of the magnetic field induced chiral mode mentioned above.

Weyl and Dirac semimetals. In a Weyl semimetal the conduction and valence bands touch in a set of isolated points which correspond to a monopole of Berry flux and are therefore topologically stable. As a consequence, a unique surface state, often referred to as Fermi arcs, appears. We have studied the properties of this surface state. First, we have discussed if and when it can coexist with a Dirac fermion when a Weyl semimetal is interfaced with a topological insulator. Second, we have discussed how the surface state can be used a direct signature of the chiral anomaly in photoemission spectroscopy studies. The chiral anomaly leads to a chiral chemical potential difference in the presence of parallel electric and magnetic field that causes a characteristic note-shaped pattern to emergence in angular resolved photoemission spectra.

Another theoretically predicted consequence of the chiral anomaly is negative magnetoresistance in the presence of parallel electric and magnetic fields. In collaboration with the group of Prof. Felser at the Max Planck Institute for Chemical Physics of Solids we have reported on the experimental observation of such a negative magnetoresistance in the Weyl semimetal TaP. Theoretically, there is an ongoing discussion in the literature, to which extend such negative magnetoresistance is directly related to the chiral anomaly, as the combination of magnetic field and disorder can in certain cases also lead to the same effect in the absence of the chiral anomaly. This is an added motivation for other probes of the chiral anomaly, such as the photoemission spectroscopy mentioned above.

Many-body localization. Many-body localization refers to the stability of an Anderson localized phase in the presence of interactions. We have been studying both the properties of this many-body localized phase as well as the properties of the associated transition into a delocalized and ergodic metallic phase. We have adopted two main approaches to this, both based on exact diagonalization numerical studies. The first is the study of entanglement, which follows an area law in the localized phase, a volume law in the delocalized phase and has diverging fluctuations at the transition. The second is the eigenvalues (occupations) and eigenvectors (natural orbitals) of the one particle density matrix. In the localized phase the occupations are close to a step function with a fermi-liquid like singularity, reflecting the fact that the eigenstates are Fock space localized and close to a product state. This step function gets smeared and approaches a constant when entering the delocalized phase, in agreement with delocalization in Fock space.

The field of many-body localization got a boost this year from the publication of several cold atom experiments. Both the entanglement and one particle density matrix just mentioned, are obtained from the eigenstates of a given system, which is not directly experimentally accessible. A major future direction of research in many-body localization is therefore that of experimental signatures of many-body localization, both in dynamics after quantum quenches and in transport. In line with our general philosophy we closely follow and participate in the progress towards experimental verification of many-body localization physics.

Collaborations

- Jérôme Cayssol, Université Bordeaux et CNRS, France
- Romain Giraud and Joseph Dufouleur, Leibniz Institute for Solid State and Materials Research, IFW Dresden, Germany
- Fabian Heidrich-Meisner, Ludwig-Maximilians-Universität München, Germany
- Roni Ilan, University of California Berkely
- Fernando de Juan, University of California, Berkeley
- Teemu Ojanen, Aalto University, Finland
- Henning Schomerus, Lancaster University, United Kingdom
- Jörn W. F. Venderbos, MIT, USA
- Binghai Yan and Claudia Felser MPIPKS and Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Division: Finite Systems
(Head: Prof. 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). Light from intense pulses to correlated single photon interaction provides another, quite

universal kind of environment. Thirdly, noise forms an important class of environment, also studied at mpi**pks** 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 and Rydberg-many particle systems (project leader *Michael Genkin* 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 is pursued in collaboration with *Alexander Eisfeld* and his research group *Quantum aggregates*. 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. Through the new research group from the Max Planck Center for Attosecond Science, *Ultrashort light-matter interaction*, headed by *Alexandra Landsman*, also the strong field part of the group will have a closely related counterpart for exchange of ideas and methods within the institute.

Research topics

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.

The Envelope Hamiltonian. Starting from the Kramers-Henneberger formulation, where the coordinate system moves with the (laser driven) electron, we have succeeded in formulating a zeroth order Hamiltonian which allows one to formulate a time-dependent perturbation theory for the number of absorbed photons irrespectively of how short the pulse is. Although it can be numerically expensive to calculate the zeroth order Hamiltonian (which depends parametrically on the evolution of the laser pulse envelope), this is a major advance since short-pulse interactions become susceptible to perturbation theory.

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 experimental observations of a surprisingly rich structure in the low energy photo-electron spectrum of strong field ionization, we have established "soft recollisions" driven by the laser field as the origin of both of the experimentally identified low energy features which also describe in a very simple way the complementary dependence on the pulse length.

With the formulation of the so called envelope hamiltonian (see above) we have identified another source of slow electrons which are non-adiabatically "spilled" into the continuum by ultrashort XUV pulses.

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 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 Schrödinger cat state on the micrometer scale represented by an entangled pair of atom clouds, mesoscopically separated through internal electronic forces, and most recently the stirring of coherent dynamics along different directions

at intersecting atomic chains.

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. Apart from exploring the applicability of machine-learning concepts, we will concentrate on two aspects: The dynamical origin and behavior of slow electrons in light-matter interaction. Here, the formulation of a new time-dependent perturbation theory based on the envelope hamiltonian will give us a handle for disentangling different processes keeping a full quantum description. A complementary approach based on classical mechanics has lead us to the discovery of soft recollisions and their universal character, whose consequences for electron-strong-field interaction have only started to become clear. The second aspect is the ejection of (fast protons) from X-ray illumination of hydrogen rich matter (basically all biologically relevant large molecules). Following our identification of this peculiar phenomenon in hydride clusters, we will investigate its effect in large, inhomogeneous molecules, e.g., Lysozyme.

Our interest in ultracold Rydberg dynamics is shifting towards questions about how this coupling manifests itself in optomechanical nano systems, where the Rydberg character provides a match regarding the spatial scale while maintaining ultra low temperatures with appropriate design of the interaction.

Cooperations

We have cooperations with

- Prof. M. Beims (Curitiba, Brazil) on semiclassical theory,
- Prof. Berrah (Storrs, 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. Richter (BESSY) regarding ionization in XUV pulses,
- Prof. Singh (ITER, Mohali, India) on attosecond ionization .
- 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.

Local cooperations

With Dr. Großmann from the TU Dresden we have enjoyed an ongoing collaboration on *semiclassical propagation techniques*.

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

The group was established in October 2012 and currently consists of three PhD students (Alan Celestino, David Schönleber, Pan-Pan Zhang). During the evaluation periode two students finished their PhD (Sebastian Möbius, Gerhard Ritschel) and the group hosted several postdoctoral guest scientists (Sebastiaan Vlaming, Gennady Chuev, Pablo Lopez, Xiaoqing Wang).

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.

Stochastic Schrödinger equations for open quantum system dynamics. Open quantum system approaches are widely used in the description of physical, chemical and biological systems to handle the coupling of electronic degrees of freedom to vibrations. A structured vibrational environment consisting of internal

molecular modes and solvent modes 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 in the electronic subspace. Unfortunately, the derived evolution equation 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 have recently succeeded to derive an exact hierarchy of coupled stochastic equations that provides trajectories of pure states. Besides the appeal for weak measurement interpretations this hierarchy also provides a numerically exact and efficient method. We could show that it is superior to common approaches based on hierarchies for the reduced density operator. We have applied our method to treat absorption and energy transfer in light harvesting aggregates. In this context it is worth mentioning that to describe absorption only a single trajectory is needed, even at finite temperatures. At the moment we are extending the formalism to time-dependent Hamiltonians with the aim to treat multidimensional femtosecond spectroscopy in a non-perturbative way.

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 chromophores with the protein environment and its role for the transport. To this end reliable information about energy-levels of the chlorophyll molecules are needed, which depend sensitively on the local protein surrounding. In addition one needs to know the coupling of an electronic transition of the chlorophyll to vibrational modes. We use mixed molecular dynamics and quantum chemical simulations to obtain these quantities which we then use as input in open quantum system approaches to calculate transport and optical properties.

Self-assembled organic-dye aggregates. In the recent years we focussed on organic dyes on surfaces. Dielectric materials like KCl or NaCl can be used as templates to induce specific arrangements of adsorbed molecules. Our main interest is the appearance of superradiance and its interplay with non-radiative relaxation mechanisms like exciton fission. These studies are carried out together with the experimental groups of Prof. Sokolowski (U. Bonn; monolayers of the organic semiconductor PTCDA on a KCl surface) and Prof. Stienkemeier (U. Freiburg; molecules on neon-droplets).

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. We focus on finite dimensional systems interacting with a structured environment. In collaboration with Dr. Wüster and the experimental group of Dr. Whitlock (U. Heidelberg) we have recently shown that ultra-cold Rydberg aggregates embedded in a laser driven background gas are promising candidates for this task.

Nano-electromechanical devices. We have proposed a nano-rotor which is driven by single electron tunneling. It consists of two charge islands (e.g. quantum dots, metallic nano-clusters, etc.), placed at the ends of a rigid rod. Electrons from a source-lead can tunnel on the dots and leave the dots at the drain-lead. A time-independent field gradient (bias voltage) can lead to a self-excitation of oscillations or even continuous rotatory motion, depending on the ratio between the driving field and damping processes. Considering the current through the device, we found a regime of strong negative differential conductance. Furthermore, for an oscillating bias voltage the device can for certain frequencies work as a rectifier. While in the previous investigations the rotor was treated classically, we now aim at a full quantum treatment to describe charge transport through *molecular* rotors. This work is done in collaboration with the PKS-fellow Dr. Croy.

Cooperations

- Prof. Aspuru-Guzik (Harvard University, Cambridge, USA): Quantum simulators.
- Dr. Croy (mpi**pks**): Nano-electro mechanical devices; quantum rotors.
- Prof. Engel (University of Würzburg, Germany): Molecular dimers, 2D spectroscopy.

- Prof. Hauer (Wien, Austria): Spectroscopy of organic dye aggregates.
- Prof. Knoester (University of Groningen, Netherlands): Unconventional disorder and localization.
- Prof. Sokolowski (University of Bonn, Germany): PTCDA monolayers on dielectric surfaces, superradiance.
- Prof. Stienkemeier (University of Freiburg, Germany): Spectroscopy in helium nano-droplets.
- Prof. Strunz (TU Dresden, Germany): Stochastic Schrödinger equations.
- Dr. Whitlock (Heidelberg, Germany): Monitoring of Rydberg excitation.
- Dr. Wüster, Prof. Rost (mpi**pks**): Rydberg aggregates.

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

The group was established in September 2008, and currently consists of four PhD students: Wildan Abdusallam, Laura Gil, Callum Murray and Valentin Walther, as well as five postdoctoral guest scientists: Jörg Götte, Dario Jukic, Rick van Bijnen, Gaoyong Sun and Christopher Gaul. We also hosted two visiting Master students: Patrick Donnan (from Auburn University) and Erik van der Wurff (from Utrecht University), and two senior guest scientists Prof. Massimo Boninsegni (from the University of Alberta, Canada) and Prof. Asaad Sakhel (Al-Balqa' Applied University, Jordan). We have been in close contact with a number of international groups through several EU-funded networks such as the Marie-Curie ITN "COHERENCE", the STREP-project "QuILMI", the FET-Open (Xtrack) project "HAIRS" and the recently established FET-PROACTIVE network "RySQ".

Our research interests cover a range of problems at the intersection of quantum optics, atomic and molecular physics and many-body physics. A major focus is devoted the search for generic principles behind the coupling of light to strongly interacting matter systems which on the one hand, can give rise to tuneable light-induced interactions between the matter constituents or govern the emergence of optical nonlinearities on the other. While a strong emphasis is and has been placed on ultracold atomic gases, the scope of our research has expanded to a broader diversity of problems from hot vapour and solid-state settings to synthetic quantum matter such as trapped ion assemblies. Understanding the mutual influence of light and matter excitations in such systems, with an eye towards scientific and technological applications, lies at the core of our research. Besides addressing related fundamental and methodological problems, we aim to devise suitable schemes to implement specific applications and work closely together with experimental groups towards actual realizations in the laboratory. Current lines of our research include:

Synthetic quantum magnets. The pursuit of synthetic systems for quantum simulations of quantum magnetism represents an exciting frontier in AMO research. Ultracold atoms in optical lattices, cold polar molecules or trapped ion crystals are among the most promising candidates under active investigation theoretically as well as experimentally. In our group we explore an alternative route based on the controlled laser-excitation of high lying Rydberg states in an atomic lattice. Here, the general idea is to utilize the strong interaction between Rydberg atoms to generate tuneable interactions between artificial spins encoded in the discrete levels of the atoms. Through few-body calculations of atomic interactions and simulations on larger scales, we are exploring different ideas towards realizing spin models of various kinds with complete laser-control over synthetic interactions and external fields. First experimental steps towards this goal have been recently made in close collaboration with the group of Prof. Immanuel Bloch at the MPQ in Garching. Along a complementary direction, we are studying laser-excitation of two-electron atoms exploiting the additional spin degree of freedom of the coupled electron pair for new approaches to strong effective interactions. Initial ideas are currently being put to test jointly with the group of Prof. Thomas C. Killian at Rice University in experiments on Bose-Einstein condensates of Strontium atoms.

Open quantum systems. For the above settings, environmental decoherence and decay processes often present an inevitable limitation that one often tries to mitigate, e.g., through clever coupling schemes or short operation times in order to preserve coherent quantum dynamics. On the contrary, it emerged that dissipation may also serve as a powerful resource, e.g., for the robust generation of many-body entanglement. Generally, the many-body physics of such driven dissipative systems is of inherent interest, as it can

give rise to phases and transitions that have no counterpart in their equilibrium equivalent. One central aim is to understand the complex interplay between unitary interactions (generating coherence and entanglement) and decoherence (potentially destroying it), and its effects on the nature of non-equilibrium phases and transitions. Inspired by the aforementioned synthetic spin systems, we studied cold-atom realizations of simple open quantum magnets, and found that long-range order can indeed emerge for certain spin models in the limit of strong decoherence. Currently, we are investigating highly dissipative, disordered ensembles, and in particular the role of strong spin correlations and atomic motion for the emergence of bistable behaviour suggested by recent experiments. Building on this work, future interests include the important but likewise more challenging question about the transition from this semi-classical regime to the deep quantum limit.

Photon-photon interactions. The undisturbed propagation of photons in vacuum constitutes a distinguishing property of light that forms the basis for applications in optical communication. Yet, the realization of photonic interactions strong enough to act on a single quantum level remains an outstanding goal of major scientific and technological significance. Major efforts have been made to implement such interactions by coupling single emitters to light that is tightly confined, e.g., in optical cavities or nanophotonic structures. Recent developments to which we have continuously contributed in the past exploit strong matter interactions in large ensembles of emitters enabling strong interactions between freely propagating photons without the need of tight mode confinement. We are studying the few-body propagation dynamics of photons in such settings to uncover the nature and basic mechanisms behind the emergence of photon interactions in such settings. A current emphasis is placed on the exploration of alternative approaches towards new types of nonlinearities that will eventually enable their application, e.g., for all-optical quantum information processing.

Many-body quantum optics. For many interacting photons, such optical media can provide a platform for unconventional quantum fluids of light and matter in a new regime where strong correlation effects defy common perturbative pictures. Further interest stems from the intrinsic non-equilibrium nature of the underlying physics, as photons are constantly entering and leaking out of the system. On the one hand, we are exploring specific situations that permit analytical treatments or effective photon-field descriptions, seeking intuitive insights into the non-equilibrium many-body dynamics. On the other hand, we use numerical approaches, such as, e.g. Quantum Monte Carlo techniques, to obtain a broader understanding of the basic mechanisms that drive the coupled dynamics of quantum matter and quantum light acting on equal footing. Besides addressing fundamental questions in a new regime of light-matter interactions, such an understanding may ultimately be valuable for engineering correlations of multi-photon states in a collective fashion rather than sequentially creating entanglement by stringing together binary operations. Moreover, our initial work on strongly interacting Rydberg atoms, has now led to explorations of a broader range of settings and questions such as the effects and utility of weak spin interactions in mesoscopic assemblies (such as ion crystals) in optical cavities or long-range interacting excitons in new types of semiconductors that are strongly driven by quantum light.

Cooperations

- Local cooperations:
  - Dr. Robert Johne (pks-fellow), [cavity-QED with ion crystals]

- Cooperations with experimental groups:
  - Prof. Immanuel Bloch (MPQ, Germany), [synthetic quantum magnets]
  - Prof. Vladan Vuletic (MIT, USA), [interacting photons]
  - Prof. Thomas C. Killian (Rice University, USA), [two-electron Rydberg gases]
  - Prof. Charles Adams (Durham University, UK), [driven dissipative spin systems]
  - Prof. Alexander Szameit (Jena University, Germany) [optical chips]

- Cooperations with theory groups:
  - Prof. Mikhail D. Lukin (Harvard, USA), [quantum nonlinear optics]
  - Prof. Michael Fleischhauer (University of Kaiserslautern, Germany), [dissipative spin lattices]

– Prof. Massimo Boninsegni (University of Alberta), [long-range interacting quantum fluids]
– Prof. Stefan Skupin (University of Bordeaux, France), [nonlocal nonlinear optics]
– Prof. Wieslaw Krolikowski (Australian National University, AU) [nonlocal nonlinear optics]

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 a postdoctoral scientist (Dr. Laurent Mercadier) and a bachelor student (Miguel Angel Silva Toledo). Former group members are Dr. Victor Kimberg (now researcher at the KTH Stockholm), Dr. Marcus Dahlström (now researcher at Stockholm University), Dr. Wen Te Laio (now assistant professor at the National Central University of Taiwan), Dr. Song-Bin Zhang (now assistant professor at Shaanxi Normal University, Xi'an, China), and Felix Aviat and Miguel Angel Silva Toledo (former Bachelor students). Our group is located at the Center for Free-Electron Laser Science (CFEL) at the DESY campus in Hamburg and was formally integrated in the Max Planck Institute for the Structure and Dynamics of Matter (MPSD) in April 2015. Our group focuses on theoretical and experimental studies on quantum optical and nonlinear x-ray processes in atoms, molecules, liquids and clusters and leads 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).
Nonlinear x-ray spectroscopy
With the advent of short-wavelength free-electron lasers, delivering femtosecond x-ray pulses of unprecedented high intensity new opportunities in the field of nonlinear quantum optics with x-rays arise, a field that hitherto was virtually unexplored. So far, the entirety of x-ray based diagnostic techniques in solid-state physics, structural biology, plasma physics, atomic and molecular physics etc. are based on a linear, single-photon interactions with matter. Among those processes are coherent diffractive imaging of biological molecules, femtosecond serial nano-crystallography, time resolved photo absorption spectroscopy, resonant inelastic x-ray scattering and Thomson scattering. The invention of XFELs, however, sets the scene for the observation of the first nonlinear x-ray optical effects. A particularly promising aspect of nonlinear x-ray interaction is the transfer of coherent femtosecond nonlinear pump-probe spectroscopies from the optical to the x-ray domain. In the optical and UV spectral range, these techniques are powerful methods to study processes such as photocatalytic reactions, long-range coherent charge and energy transfer in biologically relevant systems. Their strength lies in the combination of femtosecond time resolution and high energy resolution and their ability to differentiate between coherent and incoherent nuclear dynamics. A transfer of these methods to the x-ray domain would widen the applicability of the method to measure coherent electron motion (electronically excited wave packets), the coherent interplay between electronic and nuclear degrees of freedom and would add high spatial resolution of these processes, by the ability of x-rays to target specific elements, for example transition metal-based catalytic centres in biological systems. The core activity of the group centers around the development of such nonlinear x-ray spectroscopic techniques and the fundamental nonlinear x-ray interaction processes that are building blocks of these techniques, both in theory and experiment. In the funding period from 2011-2015, our group made seminal contributions in the field of nonlinear x-ray science. The most important milestones towards developing nonlinear x-ray spectroscopy were:

- First demonstration of stimulated x-ray emission following inner-shell photoionization of an atomic target(realization of an x-ray laser based on stimulated emission on an inner-shell atomic transition in neon) and detailed theoretical studies and comparisons to the experiment
- First demonstration of stimulated electronic x-ray Raman scattering in an atomic system,the process that is the building block for nonlinear x-ray pump-probe spectroscopies
- Theoretical studies to transfer these scheme to molecular targets, including vibrational and rotational degrees of freedom, and two experimental studies of stimulated x-ray Raman scattering in diatomic molecules
- Theoretical studies to nonlinear quantum beat Auger-electron spectroscopy, an alternative to read-out nonlinear pump-probe signals in optically thin samples
- First demonstration of stimulated x-ray emission in the hard x-ray regime in liquids and solid targets, demonstration of chemical shifts in stimulated K-α emission of different Manganese-containing chemical compounds in solution and in solids

- Stimulated EUV emission following inner-shell ionization at soft x-ray wavelengths in atomic gases and clusters

Wave mixing effects of few-cycle visible laser and attosecond XUV pulses
A second focus in our research are nonlinear optical processes induced by mixing of few-cycle optical lasers and attosecond extreme-ultraviolet (XUV) pulses. A method to achieve optical x-ray wave mixing is by combining the high-harmonic generation (HHG) process initiated by strong optical fields with attosecond XUV pulses. Thereby, 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, that have an impact on the emitted HHG spectrum: An extension of the HHG plateau is predicted and certain spectral regions can be assigned to specific coherent processes. Theoretical methods have been developed in our group 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. A possible new HHG process, involving coherent coupling of different electronic states within the HHG process ("cross-channel coupling") was recently theoretically investigated in one of our collaborations with experimentalists from ETH Zürich. In that case the HHG process evolves from an electronic spin-orbit and rotational wave packet, and coherently connects pairs of different states by the tunnel-ionization and recombination steps in the HHG process. This coherent method is extremely sensitive to small excitation fractions of the wave packet and will serve as an effective method to characterize rovibronic wave packets. In the future this cross-channel pathway of HHG will be explored in combination with XUV assisted processes.
The interplay of coherent wave packets involving valence excited states, or continuum wave packets with XUV light was recently explored also in terms of photo electron spectroscopy. In a recent theory study, we investigated the effect of nearly resonant core to valence excitation induced by XUV light in the residual ion on a continuum electronic wave packet that was formed by short-pulse ionization. Excitation of an inner-shell electron in the parent ion by a slightly detuned pulse results in a shearing (re-shaping) of the electronic continuum wave packet, that can be detected in the photo electron spectrum. A first application of this continuum electron dynamics induced by manipulation of the parent ion was recently proposed by our group to characterize the phase of attosecond pulses. The method will be extended in the future, to study coherent electron dynamics in highly-correlated atomic and ionic systems.

Current cooperations

- Uwe Bergmann (SLAC National Accelerator Laboratory, Menlo Park, USA) and Vittal Yachandra, Junko Yano (Lawrence Berkeley National Laboratory, Berkeley, USA) on stimulated hard x-ray emission for chemical analysis of transition metallo-enzyme model compounds
- Christoph Bostedt (Argonne National Laboratory, Argonne, Illinois, USA) and Thomas Möller (TU Berlin) on XUV superradiance and stimualtex XUV emission of clusters
- José Crespo Lopez-Urrutia (Max Planck Institut für Kernphysik, Heidelberg) on high-resolution spectroscopy of XUV lasers in Xenon and Krypton
- Daniel Rolles and Artem Rudenko (Kansas State University, Manhattan, Kansas, USA) on stimulated XUV emission in atomic gases
- Jan-Erik Rubensson, Joseph Nordgren (Uppsala University, Uppsala, Sweden) on high-resolution spectroscopy and stimulated resonant electronic Raman scattering
- Hans Jakob Wörner (Eidgenössisch Technische Hochschule Zürich, Switzerland) on cross-channel high-harmonic spectroscopy
- Alberto Lutman (SLAC National Accelerator Laboratory) on the development of FEL settings for two-color stimulated electronic Raman scattering
- Tim Laarmann (DESY, Hamburg) on fluorescence spectroscopy on high-intensity cluster experiments at FLASH

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

The division *Biological Physics* focusses on the study of active processes and spatiotemporal 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 unconventional material properties. Biological dynamics typically combines active mechanical processes with chemical regulation. The theoretical analysis of such mechano-chemical pattern formation opens original lines of new research in biophysics and can also lead to new physics.

In addition to the investigation of the physical principles of active processes, we study current problems of cell and developmental biology in close cooperation with biologists. These projects aim at a theoretical and quantitative understanding of biological processes in cells and tissues. The goal is to develop theoretical approaches and concepts to unravel principles that underly the function and the spatio-temporal organization of living systems.

The division *Biological Physics* started its activities in 2002. The research of our division 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 between both institutes that led in 2012 to the creation of the Center for Systems Biology Dresden (CSBD) which is jointly operated by the two Max Planck Institutes. The CSBD consists of the three research groups headed by Michael Hiller, Ivo Sbalzarini and Jan Brugues. 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 as well as sequence bioinformatics to the center. In addition to the CSBD, a variety of collaborative projects exist between our division 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. Within the Dresden campus, our group interacts in particular very closely with the Biotec Center and the Center for Regenerative Therapies (CRTD) of the TU Dresden. More recently, the excellence cluster "Center for advancing electronics Dresden" was established in 2012. Within this cluster, our group is interacting with engineers and computer scientists.

Current research topics include:

Theory of active matter. The dynamics of cells is driven by active processes on the molecular scale such as the motion of molecular motors along filaments of the cytoskeleton. Such active processes on small scales lead on large scales to emergent out-of equilibrium phenomena such as spontaneous flows and oscillations, active stresses and unconventional material properties that can be captured by generic hydrodynamic equations. The theory of active matter is generic and applies to many different systems in biology but also to possibly an increasing number of artificial systems. For example, tissue dynamics that results from active cellular behaviours can be studied in the same spirit using continuum limits and hydrodynamic descriptions of active matter.

In recent years, we have studied the consequences of active processes with chirality on the material properties of active gels. Such processes introduce torque dipoles in a material that can give rise to chiral flows and movements. Such active chiral processes can give rise to rich dynamics near surfaces. In collaboration with the group of Stephan Grill (Biotec, TU Dresden) we have shown that chirality of the actin cytoskeleton plays a key role for the left-right symmetry breaking of the body plan of the worm C. elegans. Symmetry is broken in this case by chiral rotations of the cell division axis at early stages of the embryo.

Spatial organization of cells. We are interested to understand the spatial organisation of cells and of cellular processes. For example, cells are organised in distinct compartments which provide different chemical environments in the cell. While many such compartments such as classical organelles are separated from the cytoplasm by a membrane, a many cellular compartments have no membrane. A particular exciting development is the discovery that such membrane-less compartments often have liquid like properties and are essentially liquid droplets in the cell. These droplets coexist with the surrounding cytoplasm which implies a coexistence between phases of different composition. The spatial organization of the cell cytoplasm then involves liquid-liquid demixing combined with chemical reactions. The physics

of active droplets that localize chemical reactions in space is an emerging research field with relevance to cell biology. A recent example concerns the physical nature of centrosomes, which play a key role during cell division. Our work suggested that centrosomes are droplets that grow by an autocatalytic process.

Other examples of structures that are involved in the spatial organisation of cells are the mitotic and the meiotic spindle. These are self-organized structures that are formed by dynamic microtubules. To understand the shape and size of such spindles, we investigate the dynamic organization of many interacting microtubules. Interestingly, the meiotic spindle can be understood as a droplet of a liquid crystal made of short microtubules. Because of the presence of molecular motors, active stresses have also to be taken into account.

Morphogenetic processes and mechano-chemical patterning. A fundamental question in biology is how a complex organism forms, starting from a fertilized egg. This process called development involves the collective organization of many cells that are generated by subsequent cell divisions. We are interested in the physical principles that underlie tissue morphogenesis. The combination of two aspects is important. First, tissues represent an active material in which cellular force generation together with cell division and cell death drive tissue remodeling. Second, cellular behaviors are organized with the help of signaling systems. Morphogenesis thus is a fundamentally mechano-chemical patterning process.

Generic features of mechano-chemical pattering processes can be studied in simplified models that combine reaction-diffusion processes with active fluids. A diffusing molecular species regulates the magnitude of active stresses. The resulting flows advect molecular species. We have shown that such mechanochemical systems can generate spatial patterns already with one diffusing stress activator and can generate oscillations and waves with only two stress regulators. Such systems generalize the paradigm of Turing patterns to mechanically active systems.

Collective dynamics of oscillators in biology and engineering. Interacting dynamic oscillators play important roles in many biological systems. For example, 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 a cochlear amplifier which performs nonlinear frequency-selective amplification. It is based on the generic properties of dynamic oscillators at a critical point. We study the collective nonlinear waves that emerge in the cochlea as a consequence of coupling between critical oscillators. These behaviours of dynamic oscillators play a key role for the generation of so called oto-acoustic emissions of most human ears. Interestingly, nonlinear wave phenomena that result from coupling of oscillators occur in many biological systems. Other examples that we currently investigate are the genetic waves that govern vertebrate segmentation and the mechanical bending waves of the ciliar beat.

The study of genetic oscillations revealed that time delays in the coupling of oscillators play an important role for stable synchronisation. We are now applying these concepts to engineering, where distributed electronic clocks could provide synchrony in multi-core architectures and in communication networks. Because of the high clock rate of such systems (GHz), centimetre distances at the speed of light imply significant communication delays that can help synchronisation.

Perspectives

We have now obtained a good understanding of the basic properties of active matter, however the mechanisms by which active processes are coordinated in living systems are still poorly understood. In general, morphogenetic processes and the formation of structures and patterns in cells are mechano-chemical in nature and closely integrate chemical signals and mechanic events. Such mechano-chemical systems exhibit rich behaviors that we are just beginning to understand. Early work shows that systems in which active mechanical stresses are regulated by diffusing signaling molecules can give rise to pattern formation that extend and generalize the concept of Turing patterns in reaction-diffusion systems. The dynamics of the cell cortex in the C. elegans embryo is an ideal model system to understand how cells make use of the physics of mechano-chemical systems for pattern formation. We expect that studies of mechano-chemical patterning will reveal novel mechanisms of pattern formation in biology.

Another very promising future line of research is the study of liquid phases of proteins and RNA in cells. Such protein droplets provide chemical microreactors for the spatial organization of cellular processes. There is a steadily growing number of such liquid compartments which have important roles in cellular function and in diseases. These structures are built by elementary physics of multicomponent phase

separation but are driven far from equilibrium by chemical reactions. In the coming years we expect many exciting new developments on this emerging problem.

Finally, cells are information processing systems that detect external signals (often chemical) which are transduced and processed by the cell. An important goal is to understand how information is processed and how decisions are taken by cells. Concepts from information and decision theory that have been useful in engineering are well suited to investigate principles of cellular computations and decisions. On the other hand, biological systems provide original and novel paradigms for information processing that could stimulate the development of technologies. In the excellence cluster "center for advancing electronics Dresden" we are interacting closely with computer scientists, engineers and biologists to understand how information processing in cells and in engineering differ. A recent success is the idea to use the collective behaviors of dynamic oscillators to build distributed clocks in multi-core computer architectures and in communication networks. This idea is motivated by the use of distributed clocks in cellular biological systems. The collaborative environment in Dresden is ideal to pursue these challenges in the coming years.

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 Gene Myers on the dynamic organization of epithelia.
  - Collaboration with Andy Oates on the segmentation of vertebrates through oscillating and spatio-temporal gene expression patterns.
  - Collaboration with Marino Zerial on the dynamics of endosomal transport and signaling networks in cells.
- TU Dresden
  - Collaboration with Christian Dahmann on interfaces in two-dimensional tissues.
  - Collaboration with Stefan Diez on the collective behaviors of molecular motors.
  - Collaboration with Gerhard Fettweis on the use of distributed clocks in multi core systems and on decision theoretical approaches to biophysics.
- 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 College London
  - Collaboration with Andy Oates on the segmentation of vertebrates through oscillating and spatio-temporal gene expression patterns.
- 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 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. In collaboration with the group of Ewa Paluch at UCL we have explored the role of the friction coefficient between the cell and its surrounding environment in setting the cell velocity, and we have shown that cells can move while exerting forces orders of magnitudes smaller than previously measured. 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. We have shown theoretically that animal cells moving with run and tumble motion can adjust their run time to optimise target search by chemotaxis.

Physics of nuclear migration. 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. In collaboration with the group of Caren Norden at MPI-CBG, we investigate forces involved in these processes with the help of physical models of cell mechanics.

Actomyosin oscillation and filament ordering 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. In collaboration with the group of Stephan Grill at TU Dresden, we have investigated the ordering of actin filaments occurring during actomyosin cortical flows in the *C. elegans* embryo. We have shown that a simple flow-alignment coupling, similar to couplings known to exist in liquid crystal physics, can explain filament alignment and the early steps of a furrowing invagination of the embryo. These findings are relevant for the mechanics of cell division, where a combination of filament ordering and molecular motor recruitment at the equator of the cell is responsible for the constriction of the cell into two daughter cells.

Physics of the actin cortex and membrane. We are also interested in the mechanical coupling between the membrane and the cellular actin cortex and its influence on cell mechanics. Little is understood on how the actin cytoskeleton at the cell surface mechanically constraints the lipid membrane. Recent experiments have shown that the cell membrane can adopt surprisingly complex folded shapes, presumably due to its attachment to cortical filaments. We develop models to describe the shape and mechanical state of the cell membrane, incorporating forces exerted by the cytoskeleton, as well as knowledge on mechanisms regulating the cell membrane surface area.

Three-dimensional 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. In collaboration with the experimental group of Anne 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. We are also interested using the same tools in understanding the mechanics of gastrulation in *Drosophila*.

Developmental mechanics at the embryo scale. In collaboration with Carl-Philip Heisenberg at the IST Austria, we have developed a physical model of the forces involved during zebrafish doming, one of the first step in the development of the zebrafish embryo, during which a roughly hemispherical tissue becomes thinner and spreads over the yolk of the embryo. The mechanical description we have proposed uses a coarse-grained description of tissue flows, and allows to investigate how the interplay of forces exerted by different tissues drives embryonic flows and deformations.

Cell and tissue shape. We are also interested in the mechanics of epithelia, which are two-dimensional layers of connected cells. In collaboration with Frank Jülicher and Suzanne Eaton, we are exploring the relationship between cell shape and tissue shape during the morphogenesis of the *Drosophila* pupal wing. We are developing a hydrodynamic theory of tissue flows that takes into account cellular stresses, cell planar polarity and the role of topological transitions in the tissue. By applying our framework to the study of the pupal wing, we have investigated the role of spontaneous oriented neighbour exchanges in driving changes in cell and tissue shape during morphogenesis, and we are exploring how these events are regulated during development.

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 dorsal closure
- Anne Classen, LMU Munich, on cyst formation in the Drosophila wing disc
- Carl-Philipp Heisenberg, IST Vienna and S. Grill, MPI-CBG, Dresden on the mechanics of zebrafish doming
- 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 in 2012 and since then has grown to host 9 scientists. Our focus is on developing and applying methods of statistical physics to biological problems. Most of our projects are interdisciplinary and collaborative. Several of our postdocs and PhD students are jointly supervised and combine theoretical and experimental work. In 2015, we co-organized two conferences at mpi**pks** and for two consecutive years we actively participated in the Long Night of Science, a Dresden-wide event helping to achieve a broader public exposure of our research. Currently the group works on many exciting problems, and below we present some of them.

Lévy walks. Random walk is a fundamental concept with applications ranging from quantum physics to econometrics. Remarkably, one specific model of random walks appears to be ubiquitous across many fields as a tool to analyze transport phenomena in which the dispersal process is faster than dictated by Brownian diffusion. The Lévy-walk model combines two key features, the ability to generate anomalously fast diffusion and a finite velocity of a random walker. Recent results in optics, Hamiltonian chaos, cold atom dynamics, biophysics, and behavioral science demonstrate that this particular type of random walk provides significant insight into complex transport phenomena. In our group, we further develop this model to better understand its properties and make it suitable for a broad range of applications. The mathematical machinery involved goes beyond standard central limit theorems and requires some extra effort. Recently, however, we have shown that an elegant mathematical approach, originally developed for renewal processes, could be used to compute the asymptotic shapes of the probability density function of Lévy walks in the ballistic regime. Interestingly, although there is a large body of work devoted to Lévy walks, most if not all theoretical results so far were derived for one dimensional systems. In stark contrast, many real life phenomena, which researchers try to quantify by using the Lévy walk concept, happen in

two dimensions. Somewhat surprisingly, generalizations of the Lévy walk concept to two dimensions are still virtually unexplored. It is the goal of an ongoing project to extend the model of Lévy walks to two dimensions and provide researchers across disciplines with this powerful tool to describe anomalously fast, superdiffusive dispersal processes. As an intermediate summary of our work we should mention a review by V. Zaburdaev, S. Denisov, and J. Klafter recently published in Reviews of Modern Physics (2015).

Physical properties of the cell cytoplasm. Cells can enter into a dormant state when faced with unfavorable conditions. However, how cells enter into and recover from this state is still poorly understood. Our collaborators, the lab of Simon Alberti at the MPI-CBG, have found that dormancy in different eukaryotic organisms is associated with a significant decrease in the mobility of organelles and foreign tracer particles – a phenomenon which can be termed cytoplasmic freezing. They also showed that cytoplasmic freezing is caused by a marked acidification of the cytoplasm, which leads to widespread macromolecular assembly of proteins and triggers a transition of the cytoplasm from a sol to a gel state with increased mechanical stability. We performed an advanced analysis of trajectories of foreign tracer particles in normal and dormant cells. Experimental data for the mean-squared displacement of particles, power-spectrum of displacements, density and correlation functions of displacements are in good agreement with the theoretical model of fractional Brownian motion. Remarkably the negative correlations, leading to the overall subdiffusive behavior of particles, are strongly increased for dormant cells, indicating a transition to a more mechanically stable gel-like state. Broad variation of the diffusivity of particles suggests a pronounced inhomogeneous structure of the cytoplasm in acidified cells. We could show that gel formation is required for cellular survival under conditions of stress. These findings have broad implications for understanding alternative physiological states, such as quiescence and dormancy, and create a new view of the cytoplasm as an adaptable fluid that can reversibly transition into a protective gel state. This research project is really just a beginning of our collaborative activities directed towards understanding the physics of cytoplasm.

Chromatin dynamics in fission yeast. Together with the group of Iva Tolić at the MPI-CBG (currently at Ruder Bošković Institute, Croatia) we investigated how the oscillatory movement of the nucleus during meiosis in fission yeast could facilitate the process of recombination. During recombination, DNAs of parents exchange their genetic information to give rise to a genetically unique offspring. For recombination to occur, homologous chromosomes need to find each other and align with high precision – mistakes in recombination are usually fatal for the offspring. Fission yeast, a model organism in cell biology, solves this problem by folding chromosomes in loops and pulling them through the viscous nucleoplasm, similar to doing washing in a river. However, the physical mechanisms underlying this process are poorly understood. In our recent work, we proposed a theory of pulled polymer loops that quantifed the effect of viscous drag forces on the alignment of chromosomes. To solve this problem we utilized the concept of Brownian bridges, which is well known in statistical physics, and generalized it to include the effects of an external force. Furthermore, for the one-dimensional model example we noticed an analogy between the orientation of monomers in the polymer chain and the occupation probabilities in the fermion system governed by the Fermi-Dirac distribution. The combination of Brownian bridges and Fermi-Dirac statistics allowed us to describe the statistics of polymer loops analytically. We could generalize this solution to a three-dimensional case and even more complex geometries taking into account additional inter-connections between the chromosomal loops. Remarkably, we can predict the pulling force required for alignment of the chromosomes which is in agreement with existing experimental measurements. We continue to work on this project in two complementary directions. We develop realistic computer simulations of chromosome alignment in the cell and further explore the analytical results to generalize them for the case of a periodic driving force.

Cooperations

- Dr. Simon Alberti (MPI-CBG, Dresden) experiments on physical properties of the cytoplasm.
- Prof. Eli Barkai (Bar Ilan University, Israel) theory of Lévy walks.
- Prof. Carsten Beta (University of Potsdam, Germany) experiments on bacterial motility.
- Prof. Nicolas Biais (CUNY Brooklyn College, New York, USA) experiments on clustering of *N. gonorrhoeae* bacteria.
- Prof. Sergey Denisov (Augsburg University, Germany) theory of Lévy walks, game theory.
- Prof. Stephan Grill (TU Dresden) theory and experiments on RNA polymerase translocation.

- Prof. Peter Hänggi (Augsburg University, Germany) theory of stochastic processes.
- Prof. Joseph Klafter (Tel Aviv University, Israel) theory of Lévy walks.
- Prof. Thomas Pfohl (Basel University, Switzerland) experiments on X-ray microscopy of living cells.
- Prof. Iva Tolić (Ruder Bošković Institute, Zagreb, Croatia) experiments on chromosome organisation.
- Dr. Nadine Vastenhouw (MPI-CBG, Dresden) experiments on genome activation during early embryo development.

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

This group was established in 1995 with a research programme in nonlinear dynamics and time series analysis. Over the years the focus has shifted 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 driven by 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 the mean pose the real challenges. More precisely, in these settings we aim for the characterization, modeling, understanding, and prediction of fluctuations, e.g., in terms of their magnitude distributions and temporal or spatial correlations. Particular motivation arises from the study of extreme events, which often occur as natural disasters and then have large impact on human life. Extreme events in driven systems are very large but rare fluctuations, where the research goal is to identify dynamical mechanisms (feedback loops) which first drive the system far off its normal state, but then terminate these excursions making them short lived and rare.

Fluctuations in atmospheric physics. The atmosphere is one of the most complex physical systems, with dynamics on many spatial and temporal scales. Climate change and the concequences of rising greenhouse gas concentrations are nowadays indisputable facts, however, details of which changes in particular on the regional scale are to be expected are still unclear. One specific claim is that extreme weather conditions might occur more frequently and that weather events might become more severe. We investigate recordings of temperature, precipitation, and river levels by methods from record breaking statistics and non-stationary extreme value statistics in order to explore on the observational level the significance of trends in the frequency and magnitude of extreme weather. A statistically significant finding is that the number of hot days in Germany is indeed increasing, although the fluctuations around this trend are huge.

In precipitation data of Germany we have till now no indication of changes in the past few decades. Instead, they are of interest due to their statistical properties, which can be approximately described by power laws. Self organised criticality (SOC) has been proposed as a way to explain these. In a joint project with meteorologists from Reading we look into model output for a better understanding which, if successful, will lead to better parametrizations to be used in climate models.

Fluctuations in atmospheric variables are caused by the interplay of local dynamics and global transport due to advection. Hence, barriers to transport are of high interest. In advection, they are caused by particular structures in velocity fields which cause Lagrangian particles to be trapped in eddies. We started a project to detect, follow, and predict the breakdown of these so called Lagrangian coherent structures in 2-dimensional velocity fields. Also, in time dependent velocity fields, these structures form only partial barriers. It is a challange to determine the rate at which trajectories can leak from such a confined region in a quantitative way.

Time averages, short and long range correlations. We have exactly one Earth, and hence information about the state of our planet can only be obtained by time averages, not by ensemble averages. A natural question is how close a single finite time average typically is to the (unknown) ensemble average, or, from the opposite point of view, how the particular "initial" condition at the beginning of the measurement time influences the mean value thus found. The theory of large deviations makes statements about how probable it is that a single time average is far from the ensemble mean for uncorrelated processes. We extend these results to selected short range and long range correlated processes (AR and ARFIMA) and

find slower than exponential decay in sample size of probabilities to be far off the ensemble mean, when data are long range correlated. But when are data long range correlated? An extremely popular method to detect such correlations is the detrended fluctuation analysis DFA, which, however, has not found a sound theoretical basis, yet. Because of inconsistencies reported in the literature we decided to look into that in great detail. First and unexpected results of our analysis are summarized in our report in Sec. 2.22.

Weak ergodicity breaking, ageing, and fractional derivatives. In a larger collaboration with colleagues from Potsdam, Charkov, Tel Aviv, and Skopje, we investigate stochastic processes with anomalous behaviour, namely Continuous Time Random Walks and fractional Fokker Planck equations. These are models for very slow transport leading typically to sub-diffusion and hence to anomalous behaviour of the mean squared displacement. In addition, weak ergodicity breaking and ageing phenomena can be observed. Another look at these systems is to interprete these as extreme cases of intermittent behaviour, and there are examples of dynamical systems with equivalent properties, e.g., the Manneville-Pomeau map. We contribute with the detailed analysis of various aspects in the rich phenomenology and the attempt to trace back real world phenomena to such processes.

Predictions and forecasting. We all need reliable forecasts for decision making and planning. Forecasting the short term evolution of dynamical systems has been part of our research for two decades. Currently, we are concerned with spatially extended systems. In a project funded by the Volkswagen foundation, we applied a novel state space reconstruction scheme to predict extreme events in a spatially extended excitable system. The forecasts are used to apply tiny local perturbations to the system's dynamics prior to an extreme event and thereby suppress it. Details are reported in Sec. 2.21. This work is part of a network which studies harmful algal blooming and epileptic seizures as extreme events in excitable systems, with colleagues from Oldenburg, Bonn, and Potsdam.

Non-equilibrium fluctuations and irreversibility. In very small systems such as nano-devices or biological cells, thermodynamic fluctuations become relevant and experimentally measurable. For thermodynamic systems out of equilibrium, where classical statistical ensembles are meaningless, 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 isothermal non-equilibrium processes which are strictly non-stationary since they are driven by the change of some control parameter. We eventually succeeded to analyse a particular experimental setting operated at the ENS in Lyon, where the initial macro-state of the system is different from the final state after the backward process. This situation has never been considered before, neither numerically nor experimentally. We show how to interpret the fluctuation theorem in this case and could demonstrate its validity using the experimental observations.

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. Through this centre, we collaborate with Katrin Padberg-Gehle (Computer Science) on Lagrangian Coherent Structures.
- Roland Ketzmerick, Physics Department, Technical University of Dresden and PKS Max Planck Fellow: Chaos and intermittency in Hamiltonian systems.
- Ulrike Feudel (Oldenburg), Helmut Hillebrand (Oldenburg), Klaus Lehnertz (Bonn), Jürgen Kurths (PIK Potsdam), Dave Caron (University of Southern California, USA): VW-project Extreme events in excitable media.
- Eli Barkai (Bar Ilan, Israel), Aleksei Chechkin (Charkov, Ukraine), Ralf Metzler (Potsdam), Trifce Sandev (Skopje), Alexander Iomin (Haifa): CTRW, Sinai model, Fractional Fokker Planck Equation, weak ergodicity breaking and ageing.
- Sergio Ciliberto (ENS Lyon), Léo Granger (Madrid), Jumna Mehlis (Halle), Edgar Roldan (PKS): experimental test of a nonequilibrium fluctuation theorem.
- Robert Plant and Christopher Holloway (Meteorology Department, Reading, UK): high resolution regional precipitation simulations for SOC analysis of precipitation.

Research Group: Self-Organization of Biological Structures
(Head: Dr. Jan Brugués)

The group Self-organization of Biological Structures started in September 2013 and uses the mitotic spindle and the nucleus in Xenopus laevis egg extract and zebrafish Danio rerio embryos as model systems to study how the large-scale patterns and behaviors of biological structures emerge from the collective behaviors of molecules. The mitotic spindle is a protein-machinery composed of long polar polymers of microtubules, and associated molecules such as molecular motors, cross-linkers, and regulatory proteins. Although spindles retain their overall shape for hours, their components are very dynamic and turnover within few seconds. This rapid turnover allows spindles to adapt their shape according to cell size and to rapidly recover after perturbations. The nucleus, in contrast to spindles, lacks structural components with intrinsic polarity. Structures within the nucleus, however, are partitioned into specific regions, such as chromosome territories or transcription factories. Moreover, recent studies have shown that the spatial organization of nuclear structures plays a major role in gene expression. The physical and molecular principles behind this organization are unknown and must be fundamentally different to those acting on spindles, where the polarity of microtubules dictates the bipolar symmetry and spatial organization of spindle components. We aim to use the mitotic spindle and the nucleus as two complementary systems to uncover the physical principles of self-organization in biological structures by integrating theory and experiments. We will perform the experiments in Xenopus laevis egg extract and zebrafish embryos. Egg extract allows for excellent imaging, easy manipulation and biochemistry, whereas zebrafish allows studying these processes in the context of the development of a living organism. Our general approach consists mainly of two steps. First, we characterize the large-scale behavior of spindles and nuclei (microtubule nucleation, spindle morphology and size, and chromatin organization). Then, we use these measurements together with theory and biochemical perturbations to reveal the underlying molecular mechanisms. To this end, we design new multi-scale quantitative methods that can resolve the local dynamics of soluble proteins, dissect the architecture of cellular structures, and characterize the mechanical properties and dynamics at large scales.

Design of new quantitative methods: wide-field fluorescence correlation microscopy. We currently know many of the molecules involved in the formation of biological patterns and structures, yet we lack a bottom-up understanding of how the collective activities of these molecules give rise to the formation of large structures such mitotic spindles and nuclei. At the microscopic level, these processes arise ultimately from the local molecular activities, interactions, and diffusion processes. Characterizing the spatial and temporal dynamics of these molecules is therefore essential to understand large-scale pattern and structure formation. Existing methods, such as fluorescence correlation spectroscopy (FCS), cannot properly characterize these processes. These methods are limited to small samples and small structures, or compromise the spatial resolution of the measurements to achieve the necessary temporal resolution. To overcome these limitations, we are developing a new method capable of obtaining the concentration and local dynamics of molecules simultaneously in the whole area detector (wide-field) at time scales below microseconds, regardless of the detector speed. Our method is based on modulating the intensity of the emission laser, and can be generally used with any microscope capable of confocal-sectioning (TIRF, spinning disk, laser scanning, and light-sheet). We plan to build our method around a customized light sheet microscope capable of sectioning the mitotic spindle and nucleus. **Collaborators:** Gene Myers (MPI-CBG Dresden)

Mechanisms of microtubule nucleation in mitotic spindles. The mitotic spindle is a highly dynamic steady-state structure that is continuously rebuilt. Its main components, microtubules and associated proteins, turnover every few seconds whereas the spindle lasts for several minutes to hours. This rapid turnover requires a continuous supply of microtubules that have to be nucleated throughout the spindle. It is still not clear, however, what is the mechanism of microtubule nucleation in spindles and how it contributes to their morphology, size, and architecture. This partly stems from the lack of methods to directly measure microtubule nucleation because there are no means to fluorescently label the site of a nascent microtubule and because microtubules are too dense in spindles to be resolved individually using optical microscopy. In this research line, we aim to study microtubule nucleation in the Xenopus laevis egg extract. Our first goal is to measure the profile of microtubule nucleation in spindles using a method developed in the lab based on femto-second laser ablation. This method allows to measure the minus end densities, which correspond to the location of microtubule nucleation. Additionally, it also reveals the plus ends, polarity and length distribution of microtubules, which allows characterizing the relationship between

microtubule nucleation and spindle architecture. We will complement this method with measurements of the microtubule dynamics in spindles (life time, growth velocity and depolymerization velocity) by imaging single molecule fluorescent tubulin speckles and fluorescent proteins that co-localize with the growing plus ends (Eb1-GFP). With these measurements at hand, we will test the contribution of the different mechanisms of microtubule nucleation by perturbing each one separately and measuring their effect on the nucleation profile. Finally, using our experimental data we will build a generic mathematical model of microtubule nucleation in terms of microtubule dynamics, density of nucleators, and spindle architecture. We expect this research line to provide a better understanding of how the mitotic spindle if assembled, and more generally how cells regulate the architecture, size, and shape of cytoskeletal structures. **Collaborators:** Frank Jülicher (mpi**pks** Dresden)

Mechanisms of spindle morphology and scaling during early development. It has been known for a long time that there is a correlation between the size of a cell and the size of its organelles, including the spindle and the nucleus. This relationship is perhaps most striking during the first stages of embryogenesis, when cells change in size and shape several fold in the absence of growth. During this process, the spindle adapts its size and shape accordingly to accurately segregate chromosomes over a wide range of length scales. These changes in size and shape are ultimately related to chromosome position, define the cleavage plane, and are therefore crucial for the proper development of the embryo. The mechanisms that regulate spindle scaling and its relation to the cell boundary, and more generally how cells control organelle size and shape, remain elusive. To gain insight into these questions, we will investigate spindle scaling during the early development of the zebrafish Danio rerio.

Our first aim will be to simply characterize how spindles scale in terms of their main structural component, the microtubules. To this end, we will systematically measure the architecture of spindles across zebrafish development using our two-cut laser ablation method that we recently developed. Our preliminary results show that these spindles are made of short microtubules similar to spindles assembled in Xenopus laevis egg extract. We will test, for the first time, whether spindles scale by (i) reducing the microtubule lengths while maintaining the overall architecture, (ii) rearranging the microtubules throughout the spindle while maintaining their lengths and dynamics, or (iii) a mixture of both. This architectural information will be crucial, as it will dramatically constraint the possible underlying mechanisms behind spindle scaling. Assuming spindles decrease in size due to the depletion of a limiting component, the scaling relationship between the amounts of this component (set by the cell volume) and spindle size will depend dramatically on the way the microtubule architecture changes during scaling. As examples of possible limiting components, we will investigate tubulin and microtubule nucleators by measuring their concentrations using our wide-field FCS (see previous research line), and microtubule associated proteins by measuring microtubule dynamics using single molecule measurements during scaling. We will then combine these measurements with a model for spindle scaling that predicts the changes of spindle size upon biochemical and genetic perturbations in the embryo (together with the Norden lab). Taken together, these studies will not only advance our understanding of spindle scaling, but also advance our understanding of organelle scaling in biology and its role during embryo development. **Collaborators:** Caren Norden (MPI-CBG Dresden), Jan Huisken (MPI-CBG Dresden)

Dynamics of chromatin organization in the nucleus. Our work on spindles is leading us to a better understanding of the physical principles of self-organization of cellular structures. Mitotic spindles are one example of a structure made of polar cytoskeletal filaments. The polarity of these filaments together with the local activities of molecules gives rise to the bipolar axial shape of spindle, and the spatial organization of its components. In contrast, other organelles, like the nucleus, lack structural components with intrinsic polarity, yet the sub-compartments of these organelles, such as chromosome territories, active genes or transcription factories, are localized at specific regions within the organelle. The answer to the question of how the large-scale organization of the nucleus arises for the local activities of its components would therefore appear to be fundamentally different as in the case of spindles. We aim to apply and expand the methodology we developed for spindles to understand the large-scale organization of the nucleus. In particular, in this new research line we initially will study how transcription factors, RNA polymerases, and other molecules are partitioned in the nucleoplasm, and how they contribute to the establishment of structures such as transcription factories, chromosome territories or chromatin states. **Collaborators:** Moritz Kreysing (MPI-CBG Dresden), Nadine Vastenhouw (MPI-CBG Dresden), Tony Hyman (MPI-CBG Dresden), Jochen Guck (Biotec, TU Dresden)

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. Our main interest is to apply these ideas to complex social systems. This is motivated by the recent availability of large databases of human activities, a by-product of new technologies and of the digitalization of communications. Examples of databases investigated in our group include the popularity of items on the Internet (e.g., of millions of online videos or scientific papers) and records of language usage over the last two centuries. The main scientific interest in such databases is that they allow for quantitative investigations of old and new problems. Beyond the traditional analogies between social and natural complex systems, it is now possible to quantitatively compare models to data. Here we build on the long Physics tradition in both modeling and data analysis to obtain a mechanistic understanding of problems of technological and societal interest.

As clear from the name of the group, a distinguishing feature of our approach is the focus on the dynamics of the system. This requires analyzing data at different times, but also proposing models (equations) for the temporal behavior that can be used in forecasts. For instance, when analyzing databases of natural language we look not only at their (universal) statistical properties, but also on models of how these property emerge and how languages change. The dynamical models typically have a combination of (non-linear) deterministic and stochastic terms. Here applications to traditional physical systems are also investigated in the group, in particular of non-linear dynamical systems with transiently chaotic dynamics. 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.

Specific problems which have been investigated in the last two years include:

Universality and dynamics in language. 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. On the one hand, we are interested in universal features observed in such data: the applicability and foundations of statistical laws, the role of fluctuations and how they can be explored to extract information about texts and used to improve data-mining methods (e.g., topic models). On the other hand, we are interested in the dynamical side of language, e.g., to understand language change and to trace the dynamics of ideas, opinions, and behavior expressed through the tracked words. We model these phenomena using stochastic growth models (e.g., for the vocabulary as a whole), methods from complex networks (e.g., stochastic block models), and models of population dynamics (e.g., words competing for the same meaning).The goal is to obtain models with predictive power which also provide a mechanistic understanding of the origin of the observations.

Predictions and fluctuations 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.

Computation of rare configurations in complex systems. The dynamics of complex systems is often dominated by extraordinary events which, despite being rare, are responsible for the most interesting phenomena. One example are extreme events, which can be several orders of magnitude larger than the typical events and are responsible for most economical impact. We are interested in developing computational methods to find rare trajectories in chaotic dynamical systems (e.g., in transient chaos) and rare network configurations (e.g., random networks with motifs). We adapt Importance Sampling Monte Carlo methods used in statistical physics (e.g., multicanonical simulations) and apply them to cases which could not be explored with alternative methods.

Science of Science. The propagation of scientific ideas happens mainly through scientific publications

which are increasingly available for automated studies. In a collaboration with the Max Planck Digital Library, we have been granted access and are investigating the collection of all papers indexed by the ISI Web of Science since 1980. The spreading of ideas can be quantified by looking at the dynamics and network of citations between the different papers. One of our interests is to investigate how such properties relate to information that can be extracted automatically from the text of the papers (e.g., the topics of a paper).

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.
- J. Scharloth (TU Dresden, Germany) on corpus linguistics.
- M. Beims (Curitiba, Brazil) on high-dimensional chaos.
- T. P. Peixoto (Bremen, Germany) on topic models and complex networks.
- M. Palzenberger (Max Planck Digital Library, Germany) on bibliometrics.

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 was 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 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 2014, Stefan Skupin got permanently employed by the French CNRS at the Centre Lasers Intenses et Applications (CELIA) in Bordeaux and left the mpi**pks**, and no new group members were recruited.

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.

Another aspect of high intensity laser matter interaction we are currently looking at is its application to material processing. In particular, we are interested in exploiting spatio-temporal pulsed-beam shaping techniques to optimize the material modifications induced by the laser. This is, among others, important for precise ophthalmic fs-surgery.

On this topics, we collaborate with Luc Bergé (CEA/DAM, Arpajon, France), Ihar Babushkin (Leibniz Universität Hannover), Eduardo Cabrera Granado (Universidad Complutense Madrid), and the group of Stefan Nolte (Friedrich-Schiller-Universität Jena).

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 or patterns.

On this topic, we collaborate with the group of Thomas Pohl (mpi**pks**), Wieslaw Królikowski (TAMUQ, Doha, Quatar), and Fabian Maucher (University of Durham, UK).

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 electron and ion acceleration (see also 2). On these topics, we collaborate with the groups of Vladimir Tikhonchuk (CELIA, Bordeaux, France) and Malte Kaluza (FSU Jena).

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.

As of October 1st 2013, my group has moved to the Biotechnology Center (BIOTEC) of TU Dresden. However, we are grateful to enjoy continued collaborations with various groups at mpi**pks**, continued support, and continued engagement with the scientific life at mpi**pks**.

Morphogenetic Mechanochemical Pattern Formation. 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. Bio- chemical 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 characterized the mechanochemical pattern generator that is at the heart of polarization of the C. elegans zygote. In work that was performed in collaboration with Frank Jülicher, we showed that the actomyosin cortical layer is capable of generating active torques to drive chiral flow. In theoretical work we have characterized the force and torque balance that underlies such chiral rearrangements, and we discovered that the C. elegans embryo utilizes active torque generation to undergo left/right symmetry breaking in development. This is a major step forward, giving us the change to understand the fundamental physical mechanisms by which organisms choose their left/right body axis.

Single Molecule Transcription. 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, moves backwards in a process called backtracking. We have also worked out how backtracking and diffusive proofreading ensure that a minimum number of copy mistakes are made. In combined theoretical and experimental work, we have recently shown that both RNA polymerase I and II exit a backtracking event in a kinetic competition between diffusive recovery and transcript cleavage. Through this we have identified the distinct backtrack recovery strategies of Pol I and Pol II, shedding light on the evolution of cellular functions of these key enzymes.

Cooperations

- E. Betzig, J. Farm, Virginia, U.S.A.: Bessel Beam SPIM Microscopy
- 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: Computational Biology and Evolutionary Genomics
(Head: Dr. Michael Hiller)

Our group focuses on the development of computational biology and comparative genomics approaches to link observable characteristics of species (phenotypes) to the underlying loci in the DNA (genotype). Since the DNA sequence determines the phenotypes of a species, differences in phenotypes must be due to differences in their DNA. Today, the genomes of hundreds of animals have been sequenced, including more than 100 mammals. These sequenced genomes provide an unprecedented opportunity to discover which genomic changes underlie particular phenotypic changes between species. This is the overarching scientific question we address in the lab by combining both computational as well as experimental approaches.

The complexity and difficulty of this question is illustrated by the fact that mammalian genomes have billions of base pairs and species differ by many millions of genomic changes. Even accurately comparing the entire genome of just two species poses a big challenge. Nevertheless, our previous research has established a proof-of-concept that makes it possible to detect genomic loci that underlie a particular phenotypic difference. Key to this so called Forward Genomics method is that the independent loss of a phenotype during evolution should lead to sequence divergence of the underlying genomic loci. By quantifying the divergence of a genomic locus between a species and its ancestral sequence that we reconstruct with a maximum-likelihood approach, we could show on both simulated and real data that these genomic loci harbor enough statistical signal that they can be pinpointed in a background of several other hundred thousand unrelated loci. This phenotype-genotype question can also be addressed by a "reverse" approach that starts with systematically detecting genomic differences that likely have functional consequences and uses exploration-driven approaches as well as statistical enrichment tests to predict phenotypic changes associated with individual or sets of genomic differences in these species. It should be noted that in contrast to other research groups, our focus is explicitly on differences *between* species and not on differences *within* a species (between individuals or populations).

In the last $\sim$2.5 years, one focus was on improving the methods that form the basis for our research. In particular, we have developed new methods to detect functional genomic differences. First, we are developing a computational pipeline that systematically detects gene losses without needing manual curation. While a number of case studies have manually investigated gene losses, a computational approach that systematically detects gene losses at high accuracy does not exist. Our gene loss detection approach integrates a Hidden Markov Model re-alignment approach to resolve alignment ambiguities, genome alignment filtering steps to remove non-orthologous alignments, and a method that determines which isoform of each gene consists entirely of ancestral exons (detailed in the research report). Second, we have started to develop a method tailored to the genomic loci that regulate the expression of genes. This method incorporates changes in the binding sites of the transcriptional regulators (gains, losses, changes in their strength) across a phylogeny to yield a computational measure of binding divergence on a per-species basis. Our final goal here is to develop a method that can detect both the regulators and the regulatory elements that are associated with a given phenotypic change. Third, we improved the detection of statistical associations between genomic and phenotypic changes by explicitly taking the relatedness of species and differences in evolutionary rates into account (detailed in the research report). Most of these methods-development projects will be completed in near future. Together, these improved and new approaches give us an extensive toolbox for analyzing and mining genomic data, for detecting biologically important differences for various classes of genomic elements, and for addressing the important phenotype-genotype question.

In parallel to developing methods, a smaller focus was to already apply these methods to clades that have many sequenced genomes and accessible phenotypic differences. This has led to the discovery of candidate loci that we are now experimentally investigating. Finally, with the help of the CSBD ELBE PhD stipends, we have recently started a new collaboration with experimentalists to address the mystery of why the experimental deletion of genomic regions that are under extreme purifying selection (indicating clear functional importance) gives viable mice without any detectable phenotypic consequences. By iterative cycles of computational analysis and experimental screening approaches in cell lines, we will investigate the role of genetic redundancy and robustness, which are key properties of biological systems and networks.

In future, our research will shift more and more from methods development to application. Numerous new genomes make it possible to apply our approaches to new clades, exemplified by birds with now

48 sequenced genomes and a spectacular phenotypic diversity. Also, the joint affiliation with the MPI-CBG gives us the opportunity to not only make bioinformatics predictions but to also experimentally test if manipulating such a locus affects the predicted phenotype in a model organism, thus establishing a causal link between genomic and phenotypic change. Finally, a main limitation right now is digital access to phenotypic data of all sequenced species. To this end, we have started to build a consortium of zoologists to address the pressing need to convert existing phenotypic knowledge into a digitally accessible database and to fill this phenotype gap for sequenced species, which is a key prerequisite to address the phenotype-genotype question systematically and to learn how biological systems evolve.

Our research group is jointly affiliated with the mpi**pks** and the MPI-CBG as part of the Center for Systems Biology Dresden (CSBD), which is a joint initiative of both Max Planck Institutes. The group started in Oct 2011 and most PhD students/postdocs started in early 2013. Michael Hiller was awarded the German Life Science Award in 2013.

Collaborations

- Wieland Huttner (MPI-CBG)
- Pavel Tomancak (MPI-CBG)
- Jochen Rink (MPI-CBG)
- Federico Calegari (CRTD, Dresden)
- Michael Brand (CRTD, Dresden)
- Marius Ader (CRTD, Dresden)
- Stefan Diez (BCUBE, TU Dresden)
- Frank Buchholz (Medical Faculty, TU Dresden)
- Heiko Stuckas (Senckenberg Naturhistorische Sammlungen Dresden)
- Matthias Platzer (Leibniz Institute for Age Research, Jena, Germany)
- ChulHee Kang (Washington State University, USA)

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 a joint group of the mpi**pks** and the MPI-CPfS and is co-sponsored by *Innovationsfond* of the President of Max Planck Society. Its primary goal was to enhance the synergy between and improve collaborations among the two MPIs, mpi**pks** and the MPI-CPfS. The group ceased to exist and at the time of writing, *i.e.* May 2015, only one PhD student is left at mpi**pks** (and MPI-CPfS).

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 MPI-CPfS 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.

Cooperations

In addition to the projects between the mpi**pks** and MPI-CPfS, the group enjoyed a few external collaborators. Joint projects currently existed primarily 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. 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. Douglas Natelson from Rice University on transport characterization of nano-scale devices.
- Prof. Qimiao Si from Rice University, Houston and Prof. 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. 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. Emanuel Gull from University of Michigan on a dual fermion description for the charge order transition in the Falicov-Kimball model.
- Prof. 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. 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 **mpipks**. The group is co-headed by Dr. André Eckardt. Further group members currently are four PhD students (Felix Fritzsch, Alexander Schnell, Christoph Sträter, Daniel Vorberg), one associated guest scientist (Arul Lakshminarayan), as well as two external members (PD Arnd Bäcker from TU Dresden, Prof. Holger Schanz from Hochschule Magedeburg-Stendal).

The interests of the group range from quantum signatures of regular and chaotic dynamics, with the current focus on 4D symplectic maps; over non-equilibrium steady states of driven-dissipative quantum gases; to ultracold atomic quantum gases with a special interest on fermionic spinor dynamics, Floquet systems, 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. 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 Arnold 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. 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. Finally, we are extending the semiclassical theory of regular-to-chaotic tunneling to the case of resonance-assisted tunneling and have stimulated its first experimental observation by designing a suitably shaped microwave cavity.

Non-equilibrium steady states of driven-dissipative quantum gases. We are studying the properties of bosonic and fermionic quantum gases that are driven into a steady state far from equilibrium. Specifically, we concentrate on periodically driven systems in weak contact to a thermal bath and on systems with weak coupling to two baths of different temperature or chemical potential. The non-equilibrium steady state to which such a driven-dissipative system relaxes corresponds neither to a Gibbs state nor does it obey detailed balance. It depends on the very details of the system-bath coupling and not only on a few thermodynamic variables, like temperature or chemical potential. On the one hand, this makes the treatment of such non-equilibrium steady states a true many-body problem already for ideal quantum gases of non-interacting particles. On the other hand, it offers new opportunities to tailor the state and the properties of a system beyond the constraints of equilibrium. The main focus of our work lies on investigating the consequences of the bosonic or fermionic quantum statistics. For that purpose, we employ Floquet-Markov theory in combination with both numerical and analytical methods (quantum-jump Monte-Carlo simulations, mean-field theory). Remarkably, we found that bosons undergo a generalized form of Bose condensation, when reaching the quantum degenerate regime. Namely away from equilibrium several Bose selected states can acquire extensive occupations. This effect can be used to control the heat conductivity of a system, which significantly depends on the number of selected states. Future plans concern, among others, the role of interactions, the application of our theory to photonic many-body systems (exciton-polariton fluids, photons in dye-filled cavities), and the question whether Bose condensation can be achieved using baths of temperatures well above the equilibrium critical temperature.

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. 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. These systems are extremely clean, highly tunable (also in a time-dependent fashion during the experiment) and well isolated from coupling to the environment. This makes them a unique platform for the investigation of many-body quantum dynamics. One main theme of our work is the spinor dynamics of fermionic quantum gases. Here differences with respect to the standard situation of condensed matter physics arise both from having particles with large spin ($> 1/2$), allowing for spin-changing collisions, and the presence of the trap. In close collaboration with experimentalists from Sengstock's group in Hamburg, we have investigated spin-wave excitations, giant long-lived spin-oscillations, and the different time scales governing the relaxation towards equilibrium in a system of trapped ^{40}K atoms with a spin of 9/2. Another major theme is the physics of interacting quantum gases in periodically driven optical lattices. Here the aim is to engineer the time-independent effective Hamiltonian that governs the time evolution of such Floquet systems, in order to realize artificial magnetic fields or to coherently open orbital degrees of freedom. Our work includes the design of novel schemes for this type of *Floquet engineering*, the many-body physics of the engineered systems, as well as the investigation of detrimental heating processes that limit Floquet engineering.

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. U. Kuhl (University of Nice) and 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 lattices, spinor dynamics in quantum gases of fermionic atoms with large spin, and multiphoton interband transitions in periodically driven optical lattices.

- 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 the creation of artificial gauge fields in optical lattices and fermionic spinor dynamics.
  - Prof. Gediminas Juzeliūnas and Prof. Egidijus Anisimovas (Insititute for Theoretical Physics and Astronomy, Vilnius University, Vilnius, Lithuania) on Floquet engineering of optical-lattice systems.

1.11 Advanced Study Groups

Advanced Study Group 2012/2013: Topological band structures and their instabilities
(Convenor: Igor Herbut, Simon Fraser University, Vancouver, Canada)

Background

There exists today an entire class of solid state systems that display non-trivial electronic band structures, such as Dirac points, quadratic band touching, Dirac lines, or flat bands in the bulk or on the surface. Probably the best known such a general "Dirac material" would be graphene, but there are many others, both in two and three dimensions: Weyl semimetals, gapless semiconductors such as gray tin, bilayer graphene, and surfaces of topological insulators. These systems are often unusually robust for reasons

of non-trivial band topology, and exhibit a plethora of exotic properties, such as the anomalous Hall or spin-Hall effects, non-localizing surface states, and other transport anomalies.

People and activities

The Advanced Study Group focused on the effects of electron-electron interactions and disorder on these Dirac systems. It started in November 2012 and ended in December 2013, and consisted, besides the convenor, of Fakher Assaad (Wurzburg), Balázs Dóra (Budapest), Ken Imura (Hiroshima), Christopher Mudry (Paul Scherrer), and Larz Fritz (Utrecht), who all stayed for more than two months each at the institute. Besides these long-term members, there were a number of short-term visitors, who stayed in the institute between one and three weeks. During their stay they would present a longer informal seminar, and collaborate with one or more of the group members. This latter group included Akira Furusaki (Riken), Masaki Oshikawa (Tokyo), Oskar Vafek (Florida), Martin Hohenadler (Wurzburg), Flavio Nogueira (Bochum), Babak Seradjeh (Indiana), Lukas Janssen (Jena), Bitan Roy (Maryland), Doru Sticlet (Bordeaux), Francesco Parisen Toldin (Wurzburg), Leticia Tarruell (Zurich), and Jerome Caysoll (Bordeaux). The group has also benefited from and participated in two topically closely related conferences held at the **mpipks** during this time: "Flat bands: design, topology, correlations" (6 - 9 March, 2013), and "Spin-orbit entanglement: exotic states of quantum matter in electronic systems" (15 July - 2 August, 2013).

Results

The time during and long after the meetings of the Advanced Study Group was very exciting and productive, with a number of new collaborations started, various directions explored, and some promising results found. This resulted in a number of publications, with more still in preparation. Some of the highlights so far are:

- New understanding of the nature of the quantum criticality in two dimensional Dirac systems [1–4]: a combination of new quantum Monte Carlo approach to interacting electrons on honeycomb lattice and of the state-of-the-art finite size scaling analysis has resulted in significantly improved understanding of the quantum criticality in presence of gapless (Dirac) fermions. The first paper in the series [1], has been highly visible, and even labeled as a "highly cited paper" by the Web of Science.
- Quantum criticality at the semimetal-metal transition of disordered three dimensional Dirac fermions [5]: we proposed that in contrast to the usual Anderson localization transition, the semimetal-metal quantum phase transition at finite disorder in three dimensions should display universal critical scaling, with a new set of critical exponents and universal scaling functions. These were computed using the "kernel polynomial method", developed earlier by T. Ohtsuki and collaborators for the Anderson transition. The reference [4] has also, incidentally, been labeled as a "highly cited paper" by the Web of Science.
- The interplay of the electron-electron interactions and the quadratic band touching: we have generalized the quadratic band touching Hamiltonian in two dimensions to situations that lack the time reversal symmetry, and studied the competition between the anomalous quantum Hall and nematic instabilities in this system. [6, 7] It was argued that in three dimensions the expected non-Fermi liquid state is unstable to nematic instability via a novel mechanism of "fixed-point collision". [8]
- Persistent currents in one-dimensional Dirac systems: we focused on the effect of a single magnetic or nonmagnetic impurity in two cases, in the continuum and on the lattice. In the continuum Dirac model, an analytical expression for the persistent current flowing along a ring with a single delta-like magnetic impurity is obtained after a regularization of the unbounded negative energy states. The predicted decay of the persistent current agrees with the lattice simulations. The results have also been generalized to finite temperatures. [9]
- The Loschmidt echo in Luttinger liquids after a spatially homogeneous and inhomogeneous interactions quench: in spite of the non-equilibrium nature of the problem, the Luttinger model still describes reasonably well the short and long time dynamics in the XXZ Heisenberg chain, studied numerically using matrix product state based methods. [10, 11]
- Instabilities in the partially filled flat band induced by strain in graphene: the mean-field and the Monte Carlo calculations point indicate a new magnetic state for the Hubbard model in presence

of the pseudo magnetic field, which is locally both a ferro- and an antiferromagnet, but globally only has the Neel order surviving. [12, 13]
- Interaction induced topological insulator: in an exact diagonalization study on a small honeycomb lattice we found that a large next-nearest-neighbor repulsion leads to a topologically non-trivial state, in contrast to other numerical studies, but in accord with a mean-field calculation. The difference in the conclusion is attributed to different boundary conditions used in our study. The result is confirmed on larger systems by using the entangled-plaquette ansatz method. [14]

Publications

[1] F. Assaad, I. Herbut, Pinning the order: the nature of quantum criticality in the Hubbard model on honeycomb lattice, Phys. Rev. X **3** (2013) 031010.

[2] M. Hohenadler, F. Parisen Toldin, I. Herbut, F. Assaad, Phase diagram of the Kane-Mele-Coulomb model, Phys. Rev. B **90**, (2014) (Editor's suggestion) 085146.

[3] L. Janssen, I. Herbut, Antiferromagnetic critical point on graphene's honeycomb lattice: A functional RG approach, Phys. Rev. B **89** (2014) 205403.

[4] F. Parisen Toldin, M. Hohenadler, F. Assaad, I. Herbut, Fermionic quantum criticality in honeycomb and pi-flux Hubbard models, preprint, arXiv:1411.2502.

[5] K. Kobayashi, T. Ohtsuki, K. Imura, I. Herbut, Density of states scaling at the semimetal to insulator transition in three dimensional topological insulators, Phys. Rev. Lett. **112** (2014) 016402.

[6] B. Dóra, I. Herbut, R. Moessner, Coupling, merging, and splitting Dirac points by electron-electron interaction, Phys. Rev. B **88** (2013) 075126.

[7] B. Dóra, I. Herbut, R. Moessner, Nematic, topological and Berry phases when a flat and a parabolic band touch, Phys. Rev. B **90** (2014) 045310.

[8] I. Herbut, L. Janssen, Topological Mott insulator in three-dimensional systems with quadratic band touching, Phys. Rev. Lett. **113** (2014) 106401.

[9] D. Sticlet, B. Dóra, J. Cayssol, Persistent currents in Dirac fermion rings, Phys. Rev. B **88** (2013) 205401.

[10] B. Dóra, F. Pollmann, J. Fortágh, G. Zaránd, Phys. Rev. Lett. **111** (2013) 046402.

[11] B. Dóra, F. Pollmann, preprint, arXiv:1410.5954.

[12] B. Roy, I. Herbut, Topological insulators in strained graphene at weak interactions, Phys. Rev. B **88** (2013) 045425.

[13] B. Roy, F. Assaad, I. Herbut, Zero-modes and global antiferromagnetism in strained graphene, Phys. Rev. X **4** (2014) 021042.

[14] T. Djuric, N. Chancellor, I. Herbut, Interaction-induced anomalous quantum Hall state on the honeycomb lattice, Phys. Rev. B **89** (2014) 165123.

Advanced Study Group 2013/2014: Co-evolution: A proving ground for non-equilibrium statstical mechanics

(Convenor: Prof. Kevin E. Bassler)

Scientific Aims, Procedures and Products

Unlike the firm foundation laid by Boltzmann and Gibbs a century ago for equilibrium statistical mechanics, there are no similar overarching principles for non-equilibrium statistical mechanics (NESM). Understanding NESM has become more urgent in the last decade or two, as the scientific community turned to more quantitative aspects of biological and/or social systems, and at the same time, recognized that none of these systems can exist in equilibrium. Exploring systems in this category helps us along the path towards the ultimate goal: the establishment of fundamental principles for NESM.

Co-evolution is a term for describing a system with two or more distinct components (e.g., nodes and links) that evolve in an inter-dependent manner. Furthermore, it can also refer to systems in which the constituents and the dynamics (i.e., rules of evolution) can change in response to each other. This phenomenon is ubiquitous, ranging from biological systems to global networks. The focus of our ASG was on two classes of such NESM systems: (a) adaptive, dynamic networks and (b) competition between many species and game strategies.

The ASG brought together experts in the two relatively disjoint areas in an effort to develop fruitful collaborations across disciplines. Additionally, some biologists and biophysicists that are experts in evolutionary biology also visited the group with the goal of broadening the scope of the work and to apply our understanding of NESM and of co-evolution to experimental biological systems. A number of related topics also arose during the course of the group's activities that were pursued collaboratively by the core group members and/or the short-term visitors.

The group interacted largely informally with frequent, often spirited discussions on the application of NESM to a variety of topics that ranged from simple models of co-evolution that can be easily simulated and at least partially understood analytically, to more complicated realistic studies of neural networks and of biological evolution. We also worked to understand the current limitations in our knowledge of

fundamental NESM and to develop some methods and tools to help address those limitations. A number of talks were given by the members and visitors in an effort to stimulate discussion and interaction. Many collaborative projects have emerged from the ASG. Thus far there are sixteen papers [1–15] that have resulted from work done at the ASG that have either been published, submitted, or are near to being submitted. There are a number of other ongoing projects that have developed because of the group that have not yet resulted in papers, but that are expected to do so in the near future.

Schedule and Personnel

The ASG was convened in two different periods. The first period was from April 15 to August 15, 2013, and the second period was from September 1 to October 15, 2014. The core, long-term members of the ASG were Charo I. Del Genio (U. Warwick, UK), Erwin Frey (LMU, Munich), Zoltan Toroczkai (U. Notre Dame, USA), and Royce K. P. Zia (Virginia Tech, USA). The group also benefited from 17 short-term visitors, including Ricardo Azevedo (U. Houston, USA), Tom Chou (UCLA, USA), Jia-Jia Dong (Bucknell Univ., USA), Peter L. Erdos (Hungarian Academy of Sciences, Hungary), Thilo Gross (U. Bristol, UK), Markus Gumbel (Mannheim University of Applied Sciences, Mannheim), Oskar Hallatschek (MPI for Dynamics and Self-Organization, Göttingen), Gyorgy Korniss (Rensselaer Polytechnic Institute, USA), Michael Lässig (U. Cologne, Cologne), Joachim Krug, (U. Cologne, Cologne), William Mather (Virginia Tech, USA), Istvan Miklos (Hungarian Academy of Sciences, Hungary), Madeleine Opitz (LMU, Munich), Richard Neher (MPI for Developmental Biology, Tübingen), Beate Schmittmann (Iowa State, USA), Leah B. Shaw (College of William and Mary, USA), and Eve Wurtele (Iowa State, USA). The interactions with the short-term visitors was extremely valuable as it worked to substantially broaden the scope of the group's research, and resulted in a number of on-going collaborations.

Selected notable scientific results

We formulated a simple model for co-evolution [15]. Referred to as the ABC-XIE model, it combines two paradigmatic models: (i) ABC, a stochastic rock-paper-scissors game of cyclic competition played by N nodes in which every pair of nodes can interact, and (ii) XIE, with fluctuating dynamics of links between extreme (X) "introverts" (I), who act to sever links, and "extroverts" (E), who act to establish links. Each of these NESM models individually displays remarkable properties – "survival of the weakest" in the former and an extraordinary mixed order transition in the later. Combining the two, we ask: Are there further surprises when the node and link dynamics are interwoven? It is well-known that in stochastic ABC games and in conserved Lotka-Volterra models, that extinction occurs at times of O(N). However, by introducing a novel feature – where individuals can cut/add links to the others – through the XIE dynamics, we find a surprising new state of the system: long living coexistence of all species. Remarkably, much of the new non-equilibrium phenomena is captured in a simple theoretical description. However, an intuitive understanding of this effect of co-evolution remains an open issue.

We have studied the extraordinary phase transition in the XIE model [6, 9]. In common descriptions of phase transitions, first order transitions are characterized by discontinuous jumps in the order parameter and normal fluctuations, while second order transitions are associated with no jumps and anomalous fluctuations. Outside this paradigm are systems exhibiting 'mixed order transitions' displaying a mixture of these characteristics. When the jump is maximal and the fluctuations range over the entire range of allowed values, the behavior has been coined an 'extreme Thouless effect'. We have found such a phenomenon, in the context of dynamic, social networks. Defined by minimal rules of evolution, it describes a population of extreme introverts and extroverts, who prefer to have contacts with, respectively, no one or everyone. From the dynamics, we derived an exact distribution of microstates in the stationary state, and studied collective variables of interest, including the total number of I-E links and the degree distributions.

Among the novel methods we have developed is a solution to long-standing problem in Network Science [10]. Many real-world networks exhibit correlations between the node degrees. For instance, in social networks nodes tend to connect to nodes of similar degree. Conversely, in biological and technological networks, high-degree nodes tend to be linked with low-degree nodes. Degree correlations also affect the dynamics of processes supported by a network structure, such as the spread of opinions or epidemics. Proper modeling of these systems requires the sampling of networks with a specified set of constraints. We have found a solution to the sampling problem when the constraints imposed are the degree correlations. In particular, we have developed an efficient and exact algorithm to construct and sample graphs with

a specified joint-degree matrix. A joint-degree matrix determines the number of edges between all the sets of nodes for each degree, thus completely specifying all pairwise degree correlations. Our algorithm always produces independent samples in polynomial time, without backtracking. Our results allow highly accurate modeling of complex systems of wide societal interest.

We have also developed a fast spectral algorithm for community detection in complex networks [5]. It searches for the partition with the maximum value of the modularity via the interplay of several refinement steps that include both agglomoration and division. We have validated the accuracy of the algorithm by applying it to several real-world benchmark networks. On all these, our algorithm performs as well or better than any other known polynomial scheme. This allowed us to extensively study the modularity distribution in ensembles of Erdos-Rényi networks, and to obtain accurate theoretical predictions for means and variances inclusive of finite-size corrections. This provides a way to accurately estimate the "effect size" of modularity, providing a z-score measure of it and enabling an informative comparison of networks with different numbers of nodes and links.

Most species are kept distinct by incompatibilities between the genes they carry. These genetic incompatibilities cause hybrids between the species to have low fitness. We have proposed that combinations of several genetic incompatibilities can collectively cause the origin of species, although they cannot do so acting alone a mechanism we call emergent speciation [11]. Using a simple model that captures the essence of the phenomenon, we find that emergent speciation can, indeed, occur through the combined effects of multiple genetic incompatibilities. We have also shown that emergent speciation is a robust mechanism that can take place in the presence of migration. We conclude that the interaction between genetic incompatibilities may be a root cause of the origin of species.

Publications

[1] N. T. Markov, M. Ercsey-Ravasz, D. C. Van Essen, K. Knoblauch, Z. Toroczkai, H. Kennedy, Cortical High-Density Counterstream Architectures, Science 342, 578 (2013).

[2] M. Ercsey-Ravasz, N. T. Markov, C. Lamy, D. C. Van Essen, K. Knoblauch, Z. Toroczkai, H. Kennedy, A Predictive Network Model of Cerebral Cortical Connecitivity Based on a Distance Rule, Neuron 80, 184 (2013).

[3] C. I. Del Genio and T. House, Endemic infections are always possible on regular networks, Phys. Rev. E **88**, 040101 (2013).

[4] S. Hossein, M. D. Reichl, K. E. Bassler, Symmetry in critical random Boolean network dynamics, Phys. Rev. E **89**, 042808 (2014).

[5] S. Trevino III, A. Nyberg, C. I. Del Genio, K. E. Bassler, Fast and accurate determination of modularity and its effect size, J. Stat. Mech. P02003 (2015).

[6] K. E. Bassler, W. Liu, B. Schmittmann, R. K. P. Zia, Extreme Thouless effect in a minimal model of dynamic social networks, Phys. Rev. E **91**, 042012 (2015).

[7] A. Nyberg, T. Gross, K. E. Bassler, Mesoscopic structures and the Laplacian spectra of random geometric graphs, J. Complex Networks cnv004 (2015).

[8] P. L. Erdős, I. Miklós, Z. Toroczkai, A decomposition based proof for fast mixing of a Markov chain over balanced realizations of a joint degree matrix, SIAM J. Discr. Math. 29, 481-499 (2015).

[9] K. E. Bassler, D. Dhar, and R. K. P. Zia, Networks with preferred degree: A mini-review and some new results, J. Stat. Mech. P07013 (2015).

[10] K. E. Bassler, C. I. Del Genio, P. Erdos, I. Miklos, Z. Toroczkai, Exact Sampling of Graphs with Prescribed Degree Correlations, New J. Phys. 17, 083052 (2015).

[11] T. Paixao, K. E. Bassler, R. B. R. Azevedo, Emergent Speciation by Multiple Dobzhansky-Muller Incompatibilities, submitted, bioRxiv preprint http://dx.doi.org/10.1101/008268.

[12] C. I. Del Genio, M. Romance, R. Criado, S. Boccaletti, Synchronization in time-varying networks, submitted, preprint arXiv:1505.00188

[13] R. Chauhan, P. Datta, S. Trevino III, D. Schnappinger, K. E. Bassler, G. Balazsi, M. L. Gennaro, Reconstruction and topological features of the sigma factor network of Mycobacterium tuberculosis, submitted.

[14] C. Orsini, M. M. Dankulov, A. Jamakovic, P. Madahevan, P. Colomer-de-Simon, A. Vahdat, K. E. Bassler, Z. Toroczkai, M. Boguna, G. Caldarelli, S. Fortunato, D. Krioukov, How random are complex networks, to appear in Nature Comm. (2015).

[15] K. E. Bassler, E. Frey, R. K. P. Zia, Co-evolution of nodes and links: Diversity driven coexistence in cyclic competition of three species, in preparation.

Advanced Study Group 2014: Optical rare events: A challenge in Laser Dynamics

(Convenor: Prof. Jason Gallas)

Scientific context

An outstanding problem attracting ever increasing interest in recent years is predicting when catastrophes, rare events, will strike. In this context, the interest of the Advanced Study Group (ASG) was to explore how several quantitative aspects of rare events – outgrowing the quintessential rogue waves that capsize large ships – can be studied with lasers and other dissipative systems far from equilibrium. Classically, turbulence arises as fluid motion spawns swirls that break into smaller and smaller swirls, leading to vortices at all length scales. Under appropriate conditions, this superfluid turbulence resembles the one in the classical ideal fluid and can be realized experimentally in optics, e.g. with ultra-cold bosons. Rare

events are definitely a cross-disciplinary topic burgeoning in many disciplines and subfields. Such growth has also triggered some level of confusion between the various communities involved, which is quite natural since the viewpoints/interests involved are sometimes very different. On the whole, scientists concentrated on modeling and predicting their specific areas, working yet disjointly. Even though problems can be addressed with analogous mathematical frameworks, much confusion is present within the physics of rare events. Traditionally, rare events are described by considering the full spatio-temporal dynamics. More recently, there were proposals of addressing them by looking just at the temporal evolution. The ASG brought together experts from fairly distinct areas, to explore the implications of new findings in a more holistic view, with emphasis on optical instabilities. These heterogeneous expertise contributed and profited from the complementary of their work to pin-point common open problems and efficient strategies to proceed. Nevertheless, there was also a clear recognition that, although some degree of "universality" exists, much remains to be clarified.

Structure and summary of activities

The ASG *Optical Rare Events: A Challenge in Laser Dynamics* took place over three and a half months beginning July 14, 2014. Its convener was Jason Gallas (Universität Erlangen & UFPB, Brazil) and the invited long-term members were Cristina Masoller (Universidad Politécnica de Catalunya, Spain), Marcus W. Beims (UFPR, Brazil), Vassilios Kovanis (Virginia Polytechnic Institute and State University, USA).

The efforts and activities addressed the following topics:

1. *Attempt to unify different views concerning spiking and bursting in optical media.* Brain-storming to summarize the growing literature and mentioned conflicting aspects of rare events in optical media, e.g. pump-modulated, mode-locked, and optically injected lasers, particularly for laser diodes. Of interest was to extract useful signatures valid across the disciplines of the experts attending.

2. *Extreme events in semiconductor lasers.* Recently, the study of laser systems had revealed solutions where recurrent laser pulses of great amplitude arise apparently randomly. These phenomena were named Optical Rogue Waves Extreme Pulses (EPs) and argued to be Extreme Events. Legitimate or not, an effort was made to understanding the origin of large laser pulses in time-dynamics, specially by mapping parameter intervals where such pulses should be expected. This problem is generic for class-B laser models, e.g. CO_2 lasers, systems known for their rich dynamical diversity.

3. *Spiking and bursting in biochemical oscillators.* Oscillations occur in a number of enzymatic systems as a result of feedback regulation. Currently, regulation is studied assuming Michaelis-Menten kinetics to influence the oscillatory behavior in enzyme systems, notably in models for oscillations in the activity of phosphofructokinase (PFK) in glycolysis and of cyclin-dependent kinases in the cell cycle. The model for the PFK reaction is based on a product-activated allosteric enzyme reaction coupled to enzymatic degradation of the reaction product. During the ASG, it became clear that, in fact, Michaelis-Menten kinetics has much in common with the feedback regulation proposed originally by Lotka in 1910-1920, when suitably extended. This mathematically simpler alternative opens interesting possibilities which are now being actively pursued.

4. *Possibility to detect extreme events using cold atoms.* The nonlinear Schrödinger equation describes the propagation of a light field in the paraxial approximation in presence of Kerr effect and plays a key role in the study and design of microstructured optical fibers. In condensed matter, it describes the flow of a superfluid – ^{4}He being the most used one experimentally – in which context it is known as Ginzburg-Landau equation. In atomic physics, it describes the dynamics of a weakly interacting ultracold quantum-degenerate gas of Bosons (which also presents superfluid characteristics) – a Bose-Einstein condensate – where it is called Gross-Pitaevskii equation. Therefore, all these domains are experimental playgrounds for the study of complex phenomena like wave condensation, superfluidity, Bose-Einstein condensates, quantum and classical turbulence, and so on. Such possibilities are being considered for experiments to be done in France.

The ASG activities proceeded by focusing periods of one- to two-weeks on subjects overlapping with the expertise of the visitors. Informal seminars and discussions were held, including the ASG participants and Institute members. General seminars were also presented for general audience of the Institute.

A weekly activity was organized in the form of a Wednesday Forum, very informal in spirit, moderated by an ad-hoc colleague responsible for providing introductory material and catalyzing discussions. These

activities were quite successful and rarely did a talk last less than 2 hours due to the lively atmosphere and the extensive questioning. In fact, discussions lasted the whole morning period and it was not uncommon to spend the whole day on them.

Special visitor

Prof. Yoshisuke Ueda (Waseda University, Japan) was a surprising and delightful participant of the ASG. As it is known, Prof. Ueda was a student in Chihiro Hayashi's laboratory [Kyoto University] experimenting with analog computers when he noticed on Nov. 27, 1961 – before Lorenz's famous 1963 paper – what Ueda called "randomly transitional phenomena". Prof. Hayashi was not fond of his conclusions and did not allow him to report his findings until 1970. Prof. Ueda gave a well-attended public seminar at the Institute and actively participated in a week of discussion, having travelled from Japan solely for this purpose. He was born December 23, 1936. The ASG is indebted to him and to Prof. Yuzuru Sato, Hokkaido University, Sapporo, Japan, for sharing their expertise.

Extra activity

Since Prof. Riccardo Meucci could not attend the ASG as originally planned, the Convener spent the second week of September at the *Istituto Nazionale di Ottica*, in Florence, Italy. This visit allowed to complete the papers later published as Refs. [8] and [1]. In addition, it was possible to discuss aspects of the PhD work of Dr. Eugenio Pugliese (defended in Florence, Italy, March 2015).

Publications and unpublished documents

List of works resulting from ASG acitivities are:

[1] J. Ahuja, D.B. Nalawade, J. Zamora-Munt, R. Vilaseca, and C. Masoller, Optics Express, **22**, 28377-82 (2014).
[2] M.J.B. Hauser and J.A.C. Gallas, J. Phys. Chem. Lett. **5**, 4187-4193 (2014).
[3] Michelle R. Gallas, Marcia R. Gallas, J.A.C. Gallas, Eur. Phys. J. Special Topics **223**, 2131-2144 (2014).
[4] O.J. Brison and J.A.C. Gallas, Physica A **410**, 313-318 (2014).
[5] B. Vermersch and J.C. Garreau, Phys. Rev. A **91**, 043603 (2015).
[6] M.W. Beims, M. Schlesinger, C. Manchein, A. Celestino, A. Pernice, and W.T. Strunz, Phys. Rev. E **91**, 052908 (2015).
[7] R.M. da Silva, C. Manchein, M.W. Beims, and E.G. Altmann, Phys. Rev. E **91**, 062907 (2015).
[8] E. Pugliese, R. Meucci, S. Euzzor, J.G. Freire, and J.A.C. Gallas, Nature Sci. Rep. **5**, 08447 (2015).
[9] J.E. Kollmer, T. Pöschel, and J.A.C. Gallas, New J. Phys. **17**, 013036 (2015).
[10] L. Junges and J.A.C. Gallas, New J. Phys. **17**, 053038 (2015).
[11] M.A. Nascimento, H. Varela, and J.A.C. Gallas J. Solid State Electrochem. DOI 10.1007/s10008-015-2800-4
[12] Marcia R. Gallas and J.A.C. Gallas, Invited contribution in the Irving Epstein *Festschrift*: Chaos **25**, 064603 (2015).
[13] J.G. Freire, R. Meucci, F.T. Arecchi, and J.A.C. Gallas. Invited paper, 25th Anniversary Focus Issue: Chaos **25**, 097607 (2015).
[14] J.A.C. Gallas, Invited chapter in the *Festschrift Bai-Lin Hao*, World Scientific (2015).
[15] J.A.C. Gallas, Modeling the complex dynamics of lasers, Invited chapter in *Advances in Atomic, Molecular, and Optical Physics*, (2015)

Chapter 2

Selection of Research Results

2.1 AC Wien effect in spin ice, manifest in non-linear, non-equilibrium susceptibility

VOJTĚCH KAISER, RODERICH MOESSNER

Introduction. The non-linear response to an applied field can be as varied as it is interesting – even for the vacuum of QED, a strong electric field produces electron-positron pairs via the Schwinger mechanism [1]. More complex collective 'vacua' are provided by weak electrolytes, whose conductivity enhancement via the Wien effect also involves pair creation and unbinding, as first analysed by Onsager [2].

Our work [3, 4] addresses the Wien effect as a phenomenon occurring in the class of magnetic materials known as spin ice [5], as well as studying in detail its AC version, also applicable to conventional electrolytes. In spin ice, the emergent (and magnetic) Coulomb charges [6] are attached to 'Dirac strings' carrying fluxes of the corresponding emergent gauge field [7]. We find that this completely destroys the steady state known from electrolytes but – remarkably – leaves behind a frequency window in which an analogous quasi-steady state can be observed. We provide a combined quantitative analytical-numerical study of the time-dependent Wien effect. Our study extends the conventional theory to include the effect of vacuum polarisation, such as occurs, for example in water ice, via the Jaccard field [8, 9], as well as exposing the dynamical suppression of the Wien effect at high frequency.

The charge creation process of the Wien effect couples to a non-linear susceptibility, which provides a clear signature of the field-driven changes to internal correlations. We obtain a description of the non-linear uniform AC susceptibility of spin ice over an unprecedented window of frequencies, amplitudes and temperatures – a rare possibility for any non-trivial magnet. The wide parameter range of our predictions also underscores the role of spin ice as an electrochemical model system, providing in particular a perfectly symmetric electrolyte.

The underlying mechanism of the Wien effect is the generation by an external field of an excess – often very sizeable – of free charge (number density n_f), as shown in Fig. 1 for both a lattice electrolyte and its magnetic equivalent, the magnetolyte. The excess magnetic charge, in turn, amplifies the magnetic response. We have devised an accurate kinetic model for both the Wien effect and the magnetic response observed in simulations and we propose an experimental protocol for detecting the AC Wien effect in $Dy_2Ti_2O_7$ (DTO).

Model. We treat spin ice as a network of corner-sharing tetrahedra of Ising magnetic moments μ constrained to point along the axis connecting the centers of neighboring tetrahedra (at distance a). Ground state configurations satisfy the ice-rules of two spins pointing in and two out of each tetrahedron. Monopoles represent a violation of the ice rules corresponding to magnetic charges $Q_\mathrm{m} = \pm 2\mu/a$ (Fig. 1a).

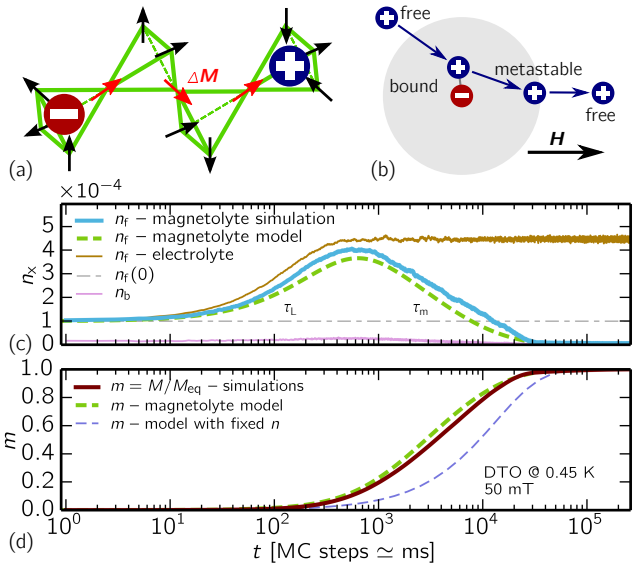

Figure 1: (a) Monopoles move via spin flips and their current magnetizes the ice manifold; (b) The second Wien effect involves the field enhanced dissociation of bound pairs. Non-linear response: (c) After a field quench, the Wien effect increases the free charge density, n_f, in an electrolyte. In a magnetolyte with the same initial density and temperature, the free monopole density increase is only transient, counteracted by the growing magnetization m of the system, which eventually even reduces monopole density for unrelated reasons (d). The increased monopole density is observable in the faster rate of magnetization m compared to a magnetization process at fixed density n. The response is well described by our kinetic model. The bound charge density (n_b) is only weakly influenced. Magnetolyte parameters are $T = 0.45$ K, $n_\mathrm{tot}(0) \simeq 1.1 \times 10^{-4}$, $n_\mathrm{f}(0) \simeq 1.0 \times 10^{-4}$, and $\mu_0 H_0 = 50$ mT; electrolyte parameters are set to obtain the same zero field density.

Wien effect and non-linear response. By analogy to electrolytes, we expect the Wien effect to occur [5] in DTO below ~ 1.5 K, where $\mu_0 Q_\mathrm{m}^2/4\pi a > 2k_\mathrm{B}T$ [10]. Our first and central result is that dynamical Monte Carlo simulations do indeed show the Wien effect in the increase in monopole density at a time scale τ_L (Fig. 1c)! However, this is only transient because the monopole currents magnetize the system (Fig. 1d) at a longer time scale τ_m, which halts the Wien effect.

Monopoles can be separated into free monopoles and bound 'Bjerrum' pairs (number density n_b), treated as distinct chemical species. Combining this with the creation of bound pairs from the ice manifold (quasi-particle vacuum), we have a double equilibrium: *vacuum* $\rightleftharpoons$ *bound* (n_b) $\overset{K(H)}{\rightleftharpoons}$ *free* (n_f) [2], which is

shifted by the applied field, H. In dilute magnetolytes, a *universal* field variable $b = \mu_0^2 Q_\mathrm{m}^3 H_0 / 8\pi (k_\mathrm{B} T)^2$ appears [2]

$$\Delta n_\mathrm{f}(b)/n_\mathrm{f}(0) = [\gamma(0)/\gamma(b)]\sqrt{F(b)} - 1\,, \qquad (1)$$

where $F(b) = 1 + b + \mathcal{O}(b^2)$. The activity coefficient γ, gives the modification of the free charge density due to internal correlations [10]. At fields sufficiently strong to remove the screening atmosphere $\gamma(b) \to 1$ [11] ('Onsager's theory'); in lower fields, a crossover $\gamma(b) \to \gamma(0)$ occurs to the zero-field value [3], found e.g. from the Debye–Hückel–Bjerrum theory.

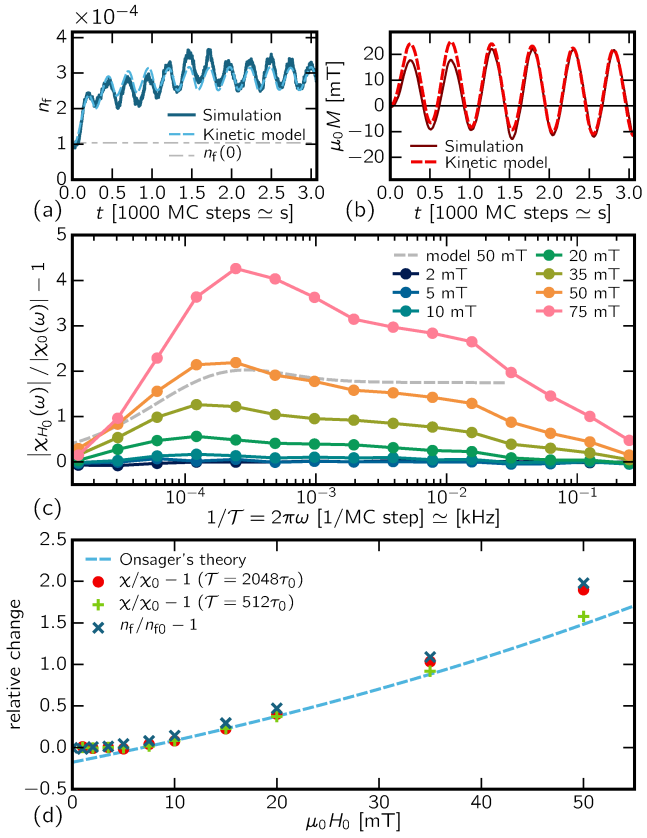

Figure 2: The free monopole density increase (a) due to sine driving enhances the magnetic response (b). The enhanced density leads to an increase in the absolute value of the non-linear susceptibility; the relative change in χ_{H_0} is shown in (c) revealing additional features in the Wien effect plateau compared to the density increase. The amplitude dependence (d) stays close to Onsager's theory of the DC Wien effect (with mean modulus of the field $\langle |H_0 \sin(\omega t)| \rangle = 2H_0/\pi$ and $\gamma(b) \to 1$ for $\mu_0 H_0 \gtrsim 3$ T) despite the approximations made, which include rewriting eq. 4 as $\Delta\chi_{H_0}(\omega)/\chi_0(\omega) \overset{\omega \gg \tau_\mathrm{m}}{=} \Delta \langle n_\mathrm{f}(H_0) \rangle_\mathcal{T} / n_\mathrm{f}(0)$. The kinetic model (results for $\mu_0 H_0 = 50$ mT) captures the time evolution of density and magnetization (dashed lines in a–b); the low-frequency transition in density and susceptibility (grey dashed lines in c); and the structure of the susceptibility increase. However, it does not include the high-frequency cutoff due to pair reorientation. Magnetolyte parameters are $T = 0.45$ K, $n_\mathrm{tot}(0) \simeq 1.1 \times 10^{-4}$, $n_\mathrm{f}(0) \simeq 1.0 \times 10^{-4}$.

Magnetization dynamics. Changes in magnetization are coupled to the current density of free (mobile) monopoles. Our kinetic model, detailed in Ref. [4], relates the charge-density increase $\zeta(t) = \Delta n_\mathrm{f}(t)/[b n_\mathrm{f}(0)/2]$, above the zero-field value $n_\mathrm{f}(0)$, to the magnetisation, taken relative to the equilibrium value $m = M/M_\mathrm{eq} = M/(\chi_T H_0)$, with χ_T the isothermal susceptibility and H_0 driving amplitude,

$$\mathrm{d}\zeta/\mathrm{d}t = \left(|h(t) - m| - \zeta\right)/\tau_\mathrm{L}^{(0)}\,, \qquad (2)$$

$$\mathrm{d}m/\mathrm{d}t = (1 + b\zeta/2)(h(t) - m)/\tau_\mathrm{m}^{(0)}\,. \qquad (3)$$

where $\tau_m \propto 1/n_\mathrm{f}$ and $\tau_L \propto 1/\chi_T n_\mathrm{f}$ is the Langevin time. Numerical integration gives quantitative agreement with our numerical data, Figs. 1 and 2a–b!

Non-linear susceptibility. For a susceptibility $\chi_{H_0}(\omega)$ comparing H_0 with the amplitude of magnetization at the same frequency $M(\omega)$, eq. (3) implies

$$\chi_{H_0}(\omega) = \frac{M(\omega)}{H_0} = \frac{\chi_T}{1 - i\omega\tau_\mathrm{m}} = \frac{\chi_T}{1 - 3i\omega\tau_0/2\,\langle n_\mathrm{f} \rangle}\,, \qquad (4)$$

where τ_0 is the hopping rate. We compute $\chi_{H_0}(\omega)$ in our simulations and observe that this approach is remarkably successful (Fig. 2d); especially so at frequencies $1/\tau_\mathrm{m} \lesssim \omega \lesssim 1/\tau_\mathrm{L}$ (Fig. 2c) where density fully relaxes as the field changes (even from zero field, as in Fig. 1c). Further, the effect persist beyond $1/\tau_\mathrm{L}$, albeit in a reduced form, as the related correlations relax faster than the density.

Similarly, the response $M(l\omega)$ at multiples of the base frequency yields higher harmonics $\chi_{H_0}^{(l)}(\omega)$ [4]. Both the magnitude of the field response and the occurence of higher harmonics are characteristic of the Wien effect, as it couples a scalar (density) to the *modulus* of an applied vector field [13].

Conclusions. Our main proposal for experiment concerns the strong amplitude dependence of a non-linear susceptibility which serves as a novel observable for the Wien effect.

The results are also the most detailed modeling of the AC Wien effect in any material system. They enable its study in an 'electrolyte' which is perfectly symmetric under the interchange of the sign of the charges, and provide access to more delicate aspects of the second Wien effect such as the reorientational dynamics of bound pairs at high frequencies.

[1] J. Schwinger. Phys. Rev., 82(5):664–679, 1951.

[2] L. Onsager. J. Chem. Phys., 2(9):599–615, 1934.

[3] V. Kaiser, S. T. Bramwell, P. C. W. Holdsworth, and R. Moessner. Nat. Mat., 12(11):1033–1037, 2013.

[4] V. Kaiser, S. T. Bramwell, P. C. W. Holdsworth, and R. Moessner. PRL, 115(3):037201, 2015.

[5] S. T. Bramwell, S. R. Giblin, S. Calder, R. Aldus, D. Prabhakaran, and T. Fennell. Nature, 461(7266):956–959, 2009.

[6] C. Castelnovo, R. Moessner, and S. L. Sondhi. Nature, 451(7174):42–45, 2008.

[7] S. V. Isakov, K. Gregor, R. Moessner, and S. L. Sondhi. PRL, 93(16):167204, 2004.

[8] C. Jaccard. Phys. kond. Mat., 3(2):99–118, 1964.

[9] I. A. Ryzhkin. JETP, 101(3):481–486, 2005.

[10] W. J. Moore. *Physical Chemistry*. Prentice-Hall, 5 edition, 1999.

[11] A. Patterson and H. Freitag. J. Electrochem. Soc., 108(6):529, 1961.

[12] L. D. C. Jaubert, M. J. Harris, T. Fennell, R. G. Melko, S. T. Bramwell, and P. C. W. Holdsworth. PRX, 3(1):011014, 2013.

[13] R. G. Pearson. Discuss. Faraday Soc., 17:187, 1954.

2.2 Maximally simple magnetic quantum simulators

ANDREAS LÄUCHLI, IOANNIS ROUSOCHATZAKIS, RODERICH MOESSNER

Quantum spin liquids and other exotic magnetic states are among the theoretically most interesting yet experimentally elusive instances of collective quantum phenomena, underpinning the counterintuitive emergence of new particles from the 'decay' of electrons in a magnet [1], such as holons and spinons which carry the electric and magnetic properties of an electron independently, or the new Majorana fermions involved in topological quantum computing, protected from noise from the + environment [2].

Some of the earliest proposals for quantum simulators have thus aimed at generating such exotic spin physics. The challenges facing such a programme are manifold and formidable. Firstly, it is necessary to generate the requisite degrees of freedom; secondly, they need to inhabit a suitable optical lattice; thirdly, their interactions must be nontrivial and satisfy symmetries of the target Hamiltonian; and finally, the system in question must be cooled to a temperature at which the target many-body states are stable.

Here we identify a class of particularly simple spin one-half model Hamiltonians which go along with particularly – we believe, maximally – simple experimental settings, for which the first three challenges are all comfortably in the realm of current technology. Our striking underlying observation is that some of the most interesting collective phenomena predicted for S=1/2 Heisenberg (HB) spin models are in fact not predicated on the SU(2) symmetry of Heisenberg models at all. Rather, they persist across a wide swathe of exchange anisotropy parameters. In cases of interest this includes XY models. These lend themselves to cold atomic settings, as the S=1/2 degree of freedom can simply be represented by the presence or absence of a particle. This requires only moderate *on-site* interactions to forbid multiple occupancy which are much easier to generate than interactions between neighbours. Given widespread experimental availability of the bosonic atoms ^{87}Rb and ^{133}Cs, and the fact that in our proposal the spin *exchange* energy scale is equivalent to the strength of the bosonic *hopping* matrix element – a one-body term not involving interactions at all – the energy scales are favourable for atomic quantum simulations.

The respective spin and bosonic Hamiltonians read

$$\mathcal{H}_{\rm spin} = J \sum_{\langle i,j \rangle} \left[(S_i^+ S_j^- + S_i^- S_j^+)/2 + \Delta\, S_i^z S_j^z \right] \quad (1)$$

$$\mathcal{H}_{\rm boson} = J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_i b_j^\dagger) + \frac{U}{2} \sum_i n_i (n_i - 1)\,,$$

where S_j^z, $S_j^\pm = S_j^x \pm i S_j^y$ are spin-1/2, and $b_j^\dagger$, $n_j = b_j^\dagger b_j$ boson operators at site j of a lattice defined by its bonds $\langle ij \rangle$. We consider antiferromagnetic spin interactions.

The anisotropy parameter $\Delta = 1$ for the HB model. Crucially, $\Delta = 0$ for the XY case, which corresponds to hardcore bosons (large U). The XY model can thus be realised via only a simple hopping term.

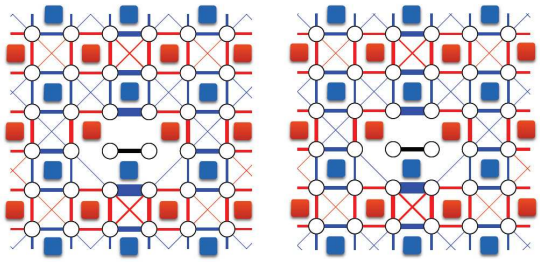

Figure 1: Valence bond crystal on the checkerboard lattice. Ground state bond correlations are essentially identical for 36 spins for XY (left) and HB (right).

The mapping between hardcore bosons and S=1/2 XY models is well known. Our main contribution is to explicitly identify and demonstrate that a number of very interesting phenomena do in fact occur in such XY models, including the physics of an emergent gauge field, the realisation of resonating valence bond physics and the appearance of quantum spin liquidity on the kagome lattice.

Origin of XY-HB equivalence: Our basic idea can already be gleaned from a fully connected cluster of q spins, where $q = 3(4)$ corresponds to a triangle (tetrahedron). Up to a constant, the Hamiltonian $\mathcal{H}_{\rm spin}$ for the cluster can be written in terms of its total spin, $\mathbf{L} = \sum_{i=1}^{q} \mathbf{S}_i$:

$$H_{HB} = \mathbf{L}^2 = L(L+1) \quad (2)$$

$$H_{XY} = \mathbf{L}^2 - L_z^2 = L(L+1) - L_z^2 \quad (3)$$

with L a (half-)integer between $L_{min} = 0\ (1/2)$ and $L_{max} = q/2$ for q even (odd), and $-L \le L_z \le L$ in integer steps.

Thus, *for both HB and XY spins*, in the ground state $L = L_z = L_{min}$. In both cases – indeed, for any value of Δ – the energies of all states follow from their values $\{L, L_z\}$, but their order in energy may differ between HB and XY – the equivalence only holds at low energy.

This HB-XY equivalence extends exactly to a number of different lattices (Fig. 1a-c in Ref. [3]), including the sawtooth and Majumdar-Ghosh chains as well as the Shastry-Sutherland lattice (where the ground state equivalence was noted when that magnet was first

studied [4]), all of which have singlet coverings as exact ground states.

Checkerboard Lattice: This consists of tetrahedra arranged to share corners, with tetrahedra projected onto a plane corresponding to squares with diagonal interactions. While not exactly solvable, the HB model is known to exhibit quantum order by disorder, yielding a plaquette valence bond crystal (pVBC). Our numerics finds essentially identical ground-state correlations for XY and HB in exact diagonalisation (Fig. 1).

We are not yet aware of an attempt to construct this magnet in an optical lattice. However, as the pVBC order is robust, it lends itself ideally for a study of non-classical order in a quantum magnet. Indeed, we have shown that it is a promising candidate for realisation via an entirely different route, utilising laser-excited Rydberg atoms [5]. These have the degree of versatility that allows engineering the angular dependence of the NN interactions necessary for distinguishing between the two different species of (crossed and uncrossed) plaquettes, and the efficient control of the (unavoidable) longer-range interactions. It will be interesting to compare these two strategies in practice.

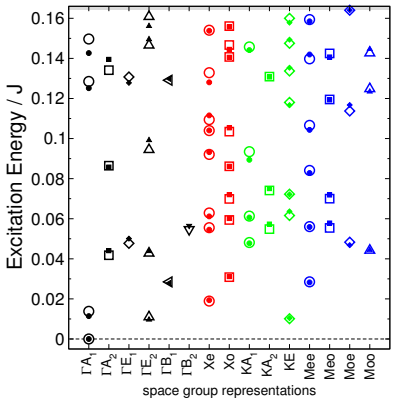

Figure 2: Kagome lattice: Low-lying many body energy spectrum of a 36 site sample for HB (open symbols) and XY (solid symbols) is identical modulo a single global shift and rescaling.

Kagome Lattice: Our most surprising case, the kagome $S{=}1/2$ HB antiferromagnet is one paradigm of quantum spin liquids. Despite intense efforts stretching decades [6, 7], the nature of its ground state and low lying excitations is still not settled. Thus, unlike the previous examples, no reliable solution of the kagome $S{=}1/2$ HB model is known, so that results from quantum simulations would be most welcome.

The XY-HB equivalence is most starkly visible in the low-energy states for a finite-size system. Compared to the case of the clusters discussed above, where the quantum numbers $\{L, L_z\}$ were used to establish a correspondence between the states for XY and HB, for a lattice system, the quantum numbers are richer. The states can be grouped into sectors, labelled by the irreducible representations of the space group of the lattice, with each sector containing an exponentially large number of states. The spectrum for a cluster of 36 sites is shown in Fig. 2, with a simple overall rescaling of the excitation energies for XY by a factor of 2.

We find a precise pairwise XY-HB correspondence between not only ground state but also *each and every* low-energy excited state in *each and every* sector! *The entire low-energy spectrum is in near-perfect correspondence!*

For constructing a quantum simulator, note that optical kagome lattices have already been obtained and studied. The required sign of the hopping can be obtained via well-understood protocols involving shaking or Raman transitions. Note that it is not even necessary to reach the ideal limit of hardcore bosons. This is true for both checkerboard valence bond crystal [5] and the kagome spin liquid where $U/J \approx 10 \sim 20$ is sufficient to obtain a high overlap with the exact XY ground state. This is easily met with either ^{87}Rb or ^{133}Cs atoms [8].

With our proposed kagome quantum simulator one can first address interesting few particle physics, such as the dynamics of caged magnons [9] (monitored by single site resolution), proceed to spontaneous pattern formation in various magnetisation plateaux [10, 11] (detected using Bragg spectroscopy), and ultimately study the nature of the spin liquid at half filling, where many theoretical questions are still open.

More fundamentally, expansions around valence bond coverings like the one by Rokhsar and Kivelson [12] to describe short-range resonating valence bond physics apply to both HB and the corresponding XY models. One then expects *gapped* phases, like a topological Z_2 HB spin liquid [13], to be stable as one perturbs away from HB towards XY.

Overall, exploring frustrated $S{=}1/2$ XY models on optical lattices has tremendous potential for advancing our understanding of, and experimental access to, the physics of quantum spin liquids, emergent gauge fields, and other exotic phenomena in magnetic and topological quantum matter.

[1] P. W. Anderson, Science **235**, 1196 (1987).
[2] A. Kitaev, Annals of Physics **303**, 2 (2003).
[3] A. M. Läuchli and R. Moessner, arXiv:1504.04380
[4] B. S. Shastry and B. Sutherland, Physica B+C **108**, 1069 (1981).
[5] A.W. Glaetzle, M. Dalmonte, R. Nath, I. Rousochatzakis, R. Moessner, P. Zoller, Physical Review X **4**, 041037 (2014)
[6] V. Elser, Phys. Rev. Lett. **62**, 2405 (1989).
[7] S. Yan, D. A. Huse, and S. R. White, Science **332**, 1173 (2011).
[8] I. Bloch et al., Rev. Mod. Phys. **80**, 885 (2008).
[9] J. Schulenburg et al., Phys. Rev. Lett. **88**, 167207 (2002).
[10] S. Nishimoto et al., Nat Commun **4**, 2287 (2013).
[11] S.Capponi et al., Phys. Rev. B **88**, 144416 (2013).
[12] D. S. Rokhsar and S. A. Kivelson, Phys. Rev. Lett. **61**, 2376 (1988).
[13] K. S. Raman et al., Phys. Rev. B **72**, 064413 (2005).

2.3 Domain walls and detection of the chiral anomaly with photoemission in Weyl semimetals

JAN BEHRENDS, ADOLFO G. GRUSHIN, JENS H. BARDARSON

Introduction. In a topological semimetal the conduction and valence bands touch in a set of isolated points that are topologically protected. In a 3D Weyl semimetal each of the touching points are the nodal points of a non-degenerate Weyl cone and act as monopoles of Berry flux in momentum space [3]. Since the total Berry flux in momentum space is required to be zero, these points come in pairs that are separated in momentum space and have opposite monopole charge or chirality. In order to eliminate the Weyl points, therefore, it is required that they be brought together and jointly annihilated. Isolated Berry flux monopoles cannot exist in the presence of both time reversal and inversion symmetry, and therefore a Weyl semimetal necessarily breaks one or both of these symmetries [4].

An important and direct consequence of the Weyl node chirality is the existence of Fermi arcs [4–6]. In the simplest case of a Weyl semimetal with only two Weyl nodes that are separated in the k_z direction, a quantum Hall like surface state appears on the x and y surfaces. This surface state has a linear dispersion and exists only for certain values of k_z, the ones in between the two Weyl nodes, which is why it is called a Fermi arc.

Coexistence of Fermi arcs with two dimensional gapless Dirac states. The simplest Weyl semimetal, with only two Weyl nodes, is obtained in the case that time reversal symmetry is broken. When such a Weyl semimetal is interfaced with a topological insulator, one may wonder what happens to the surface state Dirac fermion, which stability requires time reversal symmetry. In Ref. [1] we have shown under what conditions a Fermi arc can coexist with a Dirac fermion. Essentially, this can occur if the two states are obtained at disconnected parts of the Brillouin zone and the separation of the Weyl nodes is perpendicular to the interface. The presence of such coexisting states can in principle be probed through the optical conductivity, which features an anisotropic Drude-like peak obtained from the Fermi arc, and a constant isotropic contribution from the 2D Dirac state.

In Figure 1 we show an example of a numerical simulation demonstrating coexisting of Fermi arcs and Dirac fermions in a representative tight binding calculation.

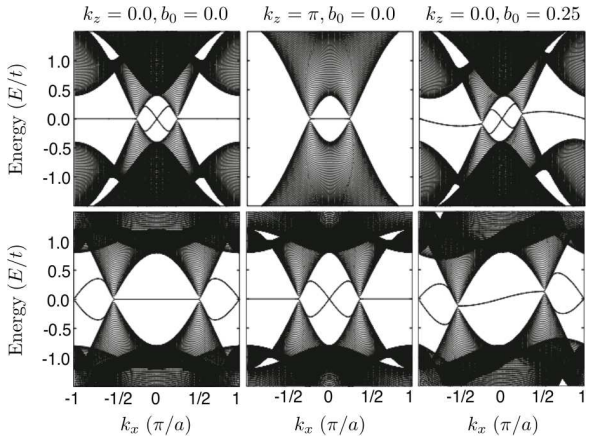

Figure 1: Band structure of a finite slab of Weyl semimetal - topological insulator interface. In the upper row the topological insulator is strong, in the lower, it is weak. The parameter b_0 shifts the two Weyl nodes oppositely in energy. For further details we refer to Ref. [1].

Visualizing the chiral anomaly with ARPES. One of the most unique features of Weyl semimetals, which at low energies is described by chiral Weyl fermions [8–10], is the chiral anomaly. In a parallel electric and magnetic field it leads to a current imbalance between two distinct species of chiral fermions [7]. Non-orthogonal electric and magnetic fields pump left handed fermions into right handed, or vice versa, so that the difference of left-handed and right-handed fermions is not conversed, while their sum is.

Angle-resolved photoemission spectroscopy (ARPES) has previously been overlooked as a diagnostic tool of the chiral anomaly, probably because the required finite magnetic field may complicate the disentangling of electron trajectories needed for angular resolution. In Ref. [2] we address different possibilities to overcome this complication and identified the main spectral signature of the chiral anomaly and its observable effect on the Fermi arcs.

The expected spectral signature is illustrated in Fig. 2 for a Weyl semimetal film with two Weyl cones. The band structure consists of both bulk cones and the corresponding surface states connecting them. Here, the grey plane represents the surface state at the film's top surface, occupied up to the equilibrium chemical potential. When parallel electric and magnetic fields are applied, the chemical potential in the left cone is shifted up to μ_L, corresponding to an increased number of left-handed fermions. Analogously, the chemical potential in the right cone is lowered to μ_R. At constant energy cuts within μ_R and μ_L, the resulting signal forms a

note-shaped pattern. In Fig. 2 (c), we support the above statements by results of numerical calculations of such an ARPES spectra, resembling the note-shaped pattern discussed before.

A similarly distinct signature is expected for Dirac semimetals since they can be seen as two copies of Weyl semimetals. Along a similar line of argument as given for the Weyl semimetal, we conclude that the ARPES signal consists of two copies of the note-shaped pattern, again supported by numerical calculations.

Naturally, these signatures can only be observed if the experimental energy resolution is sufficient to resolve the chemical potential difference. A main result of this paper is that this is indeed the case for moderate field strengths of the applied electric and magnetic fields. Detailed estimate of numbers and possibilities to minimize the influence of the external magnetic field on the electron trajectories are given in the supplemental material of Ref. [2].

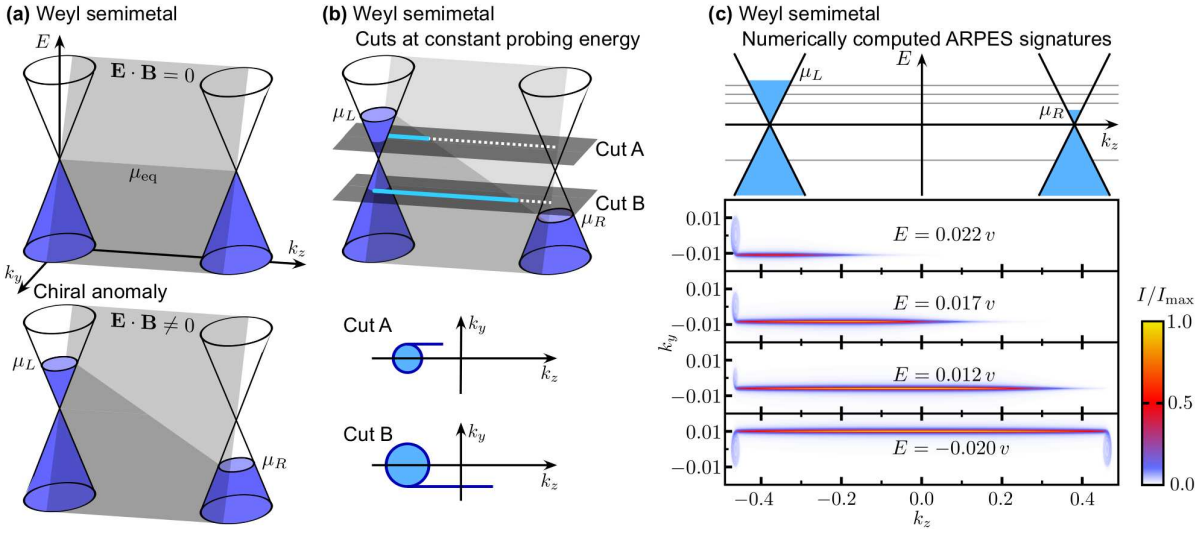

Figure 2: Visualization of the chiral anomaly in Weyl semimetals. (a) Two Weyl cones and one surface state at a given surface represent the low-energy dispersion that can be resolved with ARPES. Parallel electric and magnetic fields induce a difference in the chemical potentials that (b) gives a note-shaped pattern at constant energy cuts. (c) Numerical calculations employing a low-energy lattice model support these claims.

[1] Adolfo G. Grushin, Jörn W. F. Venderbos, Jens H. Bardarson, Phys. Rev. B **91**, 121109 (R) (2015)

[2] Jan Behrends, Adolfo G. Grushin, Teemu Ojanen, Jens H. Bardarson, arXiv:1503.04329

[3] Volovik, G. E. *The Universe in Helium Droplet* Clarendon, Oxford, UK (2003)

[4] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov Phys. Rev. B **83**, 205101 (2011).

[5] A. M. Turner and A. Vishwanath, arXiv:1301.0330.

[6] P. Hosur, and X. Qi, C. R. Physique **14**, 857–870 (2013).

[7] R. A. Bertlmann *Anomalies in Quantum Field Theories* Clarendon, Oxford, UK (1996)

[8] H. Nielsen, Phys. Lett. B **130**,389–396 (1983)

[9] G. E. Volovik, JETP Lett. **70**, 1–4 (1999)

[10] V. Aji, Phys. Rev. B **85**, 241101 (2012)

2.4 Stability of Chern insulators in strongly interacting systems

ADOLFO G. GRUSHIN, JOHANNES MOTRUK, FRANK POLLMANN

Introduction. The advent of topological phases of matter has revolutionized our understanding of condensed matter systems [1]. These phases are understood and classified with tools borrowed from the mathematical field of topology, unlike more familiar phases (e.g. crystals or magnets), that are classified in terms of symmetry breaking (e.g., space translations or spin rotations). Added to the remarkable experimental discoveries of new topological phases in both two and three dimensions, these ideas have boosted a sustained and voluminous scientific effort in the last decade that attempts to classify them and determine when and how they can emerge. Our work has addressed two concrete question regarding the emergence of topological phases in strongly interacting systems: i) Can a Chern insulating phase be stabilized by short range repulsive interactions in a time-reversal symmetric spinless fermion systems on the honeycomb tight binding model? ii) How to characterize the fractional Chern insulator phase in the Haldane lattice using efficient numerical methods?

Emergence and stability of the Chern insulator state. The Chern insulator state, first identified by Haldane [2] in the particular case of the honeycomb lattice, is a zero field analogue of the integer quantum Hall effect; the Hall conductivity contribution of each band is quantized in integer units of e^2/h and determined by a topological invariant, the Chern number. In a proof of principle, a set of mean field studies discussed how the Chern insulator can emerge from repulsive short range interactions. It was shown that spinless fermions hopping in the half-filled honeycomb lattice with nearest and next-to-nearest neighbor interactions, V_1 and V_2 respectively, displayed a Chern insulator phase as described by Haldane. Within the mean field paradigm it occurs in a region with $V_2 > V_1$ where V_2 spontaneously breaks time reversal symmetry generating complex next-to-nearest neighbor hopping strengths. The important question that still remained to be answered is whether the interaction induced Chern state survives after the effect of quantum fluctuations is included. Numerous numerical studies, mainly based on exact diagonalization techniques have provided contradictory evidence and the region where the CI phase was originally found can be occupied by competing symmetry breaking orders. Our work has therefore revisited the controversies left unsolved by previous studies using the infinite density matrix renormalization group method (iDMRG) [3]. This variational method determines the ground state of systems of size $L_x \times L_y$ where L_x is in the thermodynamic limit and L_y goes beyond what is achievable in exact diagonalization. Our main findings are summarized in the phase diagram depicted in Fig. 1. We find various charge and bond ordered phases but no indication of the emergence of the CI phase in a large parameter region. Connected to the non-interacting limit, we obtain a gapless semimetal phase that does not display any charge or bond order. For high V_1 and low V_2, a charge density wave (CDW I) with one highly and one lowly populated sublattice forms in order to minimize the interaction costs. For high V_2, a different charge pattern to compensate for the cost of the frustrated V_2 interactions occurs. The charge and bond pattern of this charge modulated (CMs) phase is depicted in Fig. 1 (a) and can be explained by a semiclassical perturbation theory. The bond but not charge ordered Kekulé phase [see Fig. 1 (b)] occurs in a much smaller parameter region than predicted by mean field and exact diagonalization studies. Finally, we find two previously undetected phases which we label CDW II and CDW III. They both display a characteristic charge ordering pattern [see Fig. 1 (c) and (d)] and their formation can, just as in the CMs case, be corroborated by semiclassical calculations.

Emergence and stability of the fractional Chern insulator state A fractional Chern insulator (FCI) state is an analogue of the fractional quantum Hall state that does not require external magnetic fields. In our work, we have studied how the fermionic FCI state associated to the $\nu = 1/3$ Haldane Chern insulator model emerges using the infinite density matrix renormalization group (iDMRG) method [4]. The hallmark of the CI (FCI) state is the integer (fractional) quantization of the Hall conductivity σ_H. The iDMRG method offers a remarkable simplification to calculate this quantity; simply by threading a flux Φ_y through the cylinder (i.e. by twisting the boundary conditions such that the electrons pick up a phase $e^{i\Phi_y}$ when circling once around it) we are able to monitor the charge pumped through an artificial (entanglement) cut through the cylinder. In Fig. 2(a) we show the charge pumped through the cut as a function of inserted flux for both the non-interacting trivial and CI cases at half filling for a cylinder with $L_y = 6$. The trivial insulator with $C = 0$ (top blue) has no charge pumping after one flux quantum and thus $\sigma_H = 0$. On the other hand, the CI state with $C = 1$ (at half-filling) shows that, after the insertion of one flux quantum, there is exactly one unit charge pumped across the boundary. Upon switching on the V_1 interaction and tuning to $1/3$ filling of the lowest band we observe that the pumped charged per

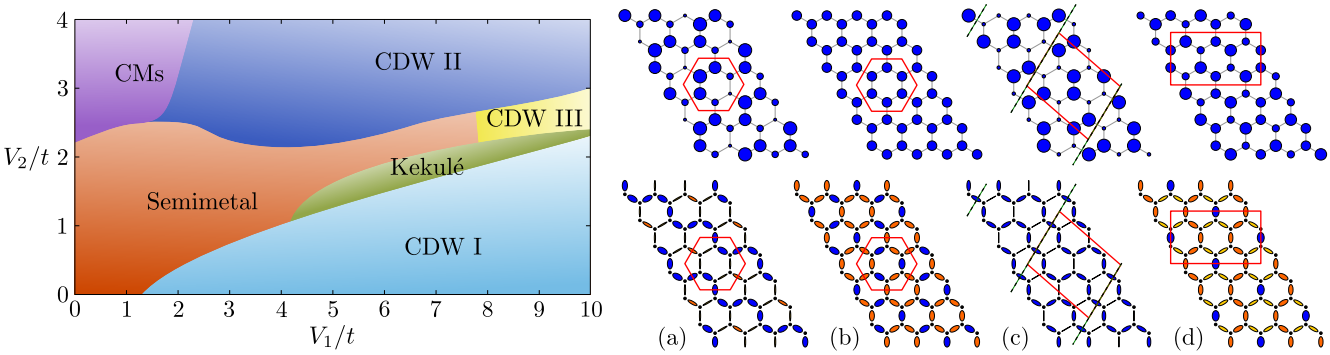

Figure 1: Left: Phase diagram obtained with iDMRG calculations on an infinite cylinder of circumference $L_y = 12$. Right: Representative charge and bond strength patterns for the four phases with largest unit cell discussed in the main text. The area of the blue circles is proportional to the particle number expectation value on the respective site and the thickness of the ellipsoids on the bonds is proportional to the hopping amplitude between nearest neighbors. The unit cells for each phase are depicted by the red polygons. These correspond to (a) CMs phase, (b) Kekulé phase, (c) CDW II phase, (d) CDW III phase.

flux is exactly $e/3$, signaling the FCI state [see Fig. 2(c)].

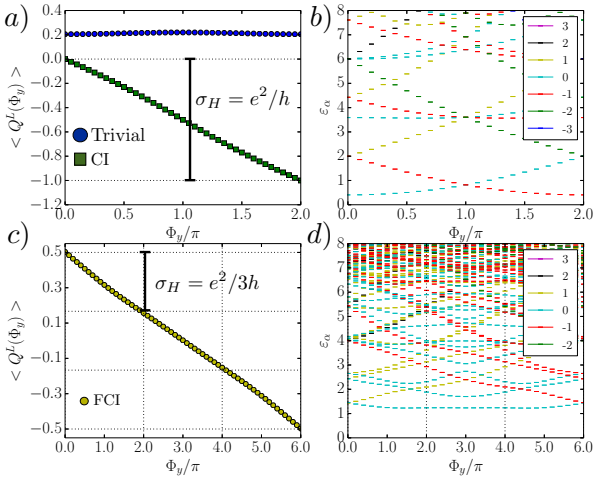

Figure 2: (a) Charge pumping after one flux insertion for a half-filled trivial insulator on a cylinder with $L_y = 6$ (blue upper curve) and a CI with (lower green curve). (b) Entanglement spectrum evolution as a function of flux for the CI. Different charge sectors Q^L are color coded. In (c) and (d) we show the charge pumping and the entanglement spectrum for the $1/3$ filled lower band of the Haldane model after *three* flux insertions for $L_y = 12$.

Alternatively, the charge fractionalization leaves also an imprint on the many-body entanglement spectrum (ES) $\{\varepsilon_\alpha\}$ as a function of Φ_y shown in Fig. 2(b) and (d). The spectrum returns to itself after one flux for a Chern insulator but shifts the charge sectors by 1. For the FCI state, the spectrum returns to itself only after three fluxes, a consequence of the fractional nature of the state.

An important advantage of the iDMRG method is that it enables us to study the emergence and stability of the FCI state under decreasing/increasing V_1 in the presence of band mixing. In particular, it can address the nature of the transition between the FCI state and possible competing orders, an issue essential for benchmarking future experiments. Using iDMRG we have computed how the entanglement spectrum and the correlation length change as a function of interaction strength V_1. The resulting phase diagram has two phases; a highly entangled phase with large correlation length at $V_1 < V_{1c}$ with zero Hall conductivity and a gapped phase with $\sigma_H = \frac{1}{3}\frac{e^2}{h}$ with small correlation length at $V_1 > V_{1c}$. The latter phase is the FCI state which is remarkably well converged within the iDMRG parameters. The former phase on the other hand strongly resembles the properties of a metallic phase. Interestingly we find no competing intermediate phase, the presence of which could not be ruled out *a priori*.

Conclusions. In our work we have addressed how the emergence of topological phases occurs spontaneously from short range electron-electron interactions. Firstly we find that the Chern insulator phase predicted in mean field theory to emerge from short range repulsive interactions is absent in the fermonic spinless half-filled honeycomb model. Furthermore we have predicted and characterized novel charge and bond ordered phases that were not captured by previous mean-field treatments. Secondly we have investigated the stability of the fractional Chern insulator phase in the honeycomb lattice and addressed the direct nature of the metal-FCI phase transition in the Haldane model at $1/3$ filling. Moreover, we have excluded the presence of competing trivial phases such as charge density wave states that could compete with the emergence of the FCI state.

[1] X.-G. Wen, Int. J. Mod. Phys. B **4**, 239 (1990).

[2] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).

[3] J. Motruk, A. G. Grushin, F. de Juan, F. Pollmann, arXiv:1505.01674 (2015).

[4] A. G. Grushin, J. Motruk , M. P. Zaletel, F. Pollmann, Phys. Rev. B **91**, 035136 (2014).

2.5 Many-body localization in a disordered quantum Ising chain

JONAS KJÄLL, JENS H. BARDARSON, FRANK POLLMANN

Introduction. The Anderson insulator is an ideal insulator in which all single particle states are localized [1]. This localization is due to quantum interference induced by elastic scattering of random impurities. It was shown in the seminal work by Basko et. al [2] that these ideal insulators can also survive in the presence of weak interactions. This quickly opened up the field of many-body localization (MBL) with many new and intriguing questions about its defining properties. First, due to the lack of transport, MBL systems do not thermalize, that is, the eigenstate thermalization hypothesis (ETH) does not hold. Second, these systems allow for a realization of topological and quantum order at finite energy densities by localizing the excitations that would otherwise melt the orders. While the Anderson insulator and MBL systems have many properties in common, one characterizing distinction is the logarithmic entanglement growth after a global quench in an MBL phase [3,4].

Disordered Ising chain. In Ref. [5], we studied the properties of eigenstates with finite energy density in a disordered Ising model using full exact diagonalization. We considered particular entanglement entropy properties that allow us to locate the transition out of the MBL phases to a higher accuracy than had previously been possible. With this improved accuracy, we find numerical evidence for the existence of different MBL phase transitions and provide the first numerical support for a many-body mobility edge. The model Hamiltonian we studied is the transverse field quantum Ising chain with disordered couplings and a next-nearest neighbor Ising term,

$$H = -\sum_{i=1}^{L-1} J_i \sigma_i^z \sigma_{i+1}^z + J_2 \sum_{i=1}^{L-2} \sigma_i^z \sigma_{i+2}^z + h \sum_{i=1}^{L} \sigma_i^x, \quad (1)$$

where σ^x and σ^z are Pauli matrices and L the number of sites in the chain. The couplings $J_i = J + \delta J_i$ are random and independent, with all δJ_i taken from a uniform random distribution $[-\delta J, \delta J]$. For the numerical results presented, we use the parameters $J = 1$ and $h/2 = J_2 = 0.3$. The Hamiltonian (1) has a global $\mathbb{Z}_2$ symmetry with respect to the parity operator $P = \prod_{i=1}^{L} \sigma_i^x$, with eigenvalues ± 1.

Phase diagram and the MBL transition. Our main results are summarized in Fig. 1, a phase diagram as a function of disorder strength δJ and energy density $\epsilon = 2(E - E_{\min})/(E_{\max} - E_{\min})$. An intuitive schematic picture of the nature of the different phases in terms of domain walls is given at the top of the phase diagram. In the high energy eigenstates studied here, the excitations are (gapped) domain walls between different ferromagnetic phases. Below some critical disorder strength δJ_c, there is a thermal phase with the domain walls extended over the whole system. In the MBL phases, the domain walls are localized.

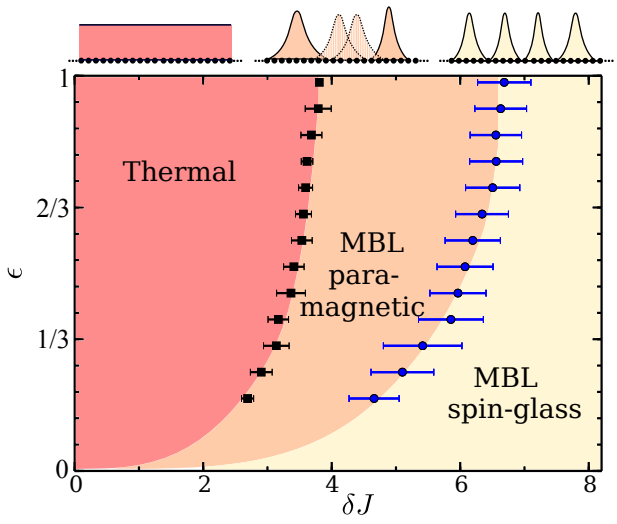

Figure 1: Phase diagram of the Ising model Eq. (1) in the $h/2 = J_2 = 0.3$ plane. The axes give the energy density above the ground state and the disorder strength. The colored areas are guides to the eye. The data is obtained from finite size scaling of entanglement entropy properties and the spin-glass order parameter. Only statistical error bars are presented. The schematic on top of the phase diagram shows a caricature of the spatial domain wall probability distribution in the different phases. The thermal phase is characterized by extended domain walls, the MBL paramagnetic phase by localized domain walls which are created and removed in pairs (dashed), and the MBL spin-glass by localized non-overlapping domain walls.

To determine the transition to the MBL phase, we study various properties of the entanglement entropy in the exact eigenstates and focus on the half-chain entanglement entropy $S = -\mathrm{Tr}_{\mathrm{L}}\, \rho \ln \rho$ of the reduced density matrix $\rho = \mathrm{Tr}_{\mathrm{R}} |\psi\rangle\langle\psi|$, where the traces are over the left and right half-chain Hilbert spaces respectively. For each disorder realization, we find the eigenstate $|n\rangle$ with energy E_n closest to a fixed energy E and thereby obtain a disorder distribution of entanglement entropies. In Fig. 2 we plot the mean (left inset) and standard deviation of this distribution, at an energy in the middle of the spectrum, as a function of disorder strength. In the thermal phase at weak disorder, the mean follows a volume law approaching the value $S = (L \ln 2 - 1)/2$ of a random state indicated by the dashed lines.

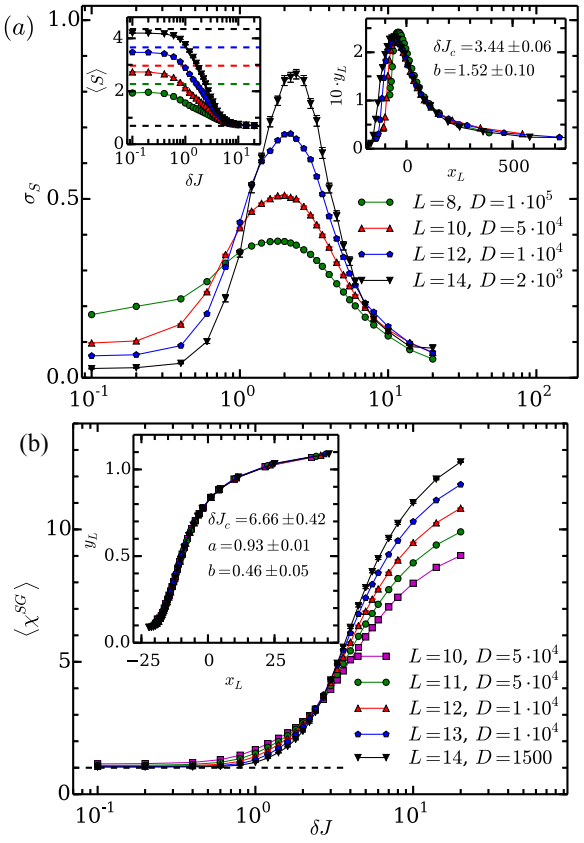

Figure 2: (a) Standard deviation of entanglement over the disorder ensemble as a function of disorder strength δJ for different system sizes L and D independent disorder realizations, at a fixed energy density in the middle of the spectrum. The left inset shows the mean entanglement entropy with dashed lines giving the values $S = (L \ln 2 - 1)/2$ and $S = \ln 2$. The right inset gives the scaling collapse of the data in the main panel. (b) Spin-glass order parameter as function of disorder strength δJ for different system sizes L and D independent disorder realization, at a fixed energy in the middle of the energy spectrum.

With increasing disorder strength, the average entanglement entropy decreases and eventually saturates at $S = \ln 2$ deep in the localized phase. The reason for this is that eigenstates become Schrödinger cat states formed by superposition of states related by parity symmetry – the domain walls are pinned by the strong disorder.

The standard deviation σ_S of the entanglement entropy goes to zero in the thermodynamic limit both deep in the thermal and localized phase, but diverges at the transition. In the thermal phase this is consistent with the eigenstate thermalization hypothesis that requires the entropy to depend on energy only, while in the localized phase all states have the same $\ln 2$ entanglement entropy. The diverging peak can be understood as follows. For a given system size, disorder amplitude δJ and energy, near the transition δJ_c, the exact value of the entanglement S_n depends on the specific disorder realization. At a fixed value of δJ close to the transition, therefore, the set of states obtained from an ensemble of disorder realizations consists of both extended and localized states giving rise to a large standard deviation in the entanglement.

To determine the location of the phase transition, we perform a scaling collapse, with a scaling function of the form $\sigma_S(L, \delta J) = g(L) f[(\delta J - \delta J_c) L^b]$, where δJ_c and b are scaling parameters and $g(L) = [(L-2)\log 2 - 1]/2$ is the difference in S between the two phases. Repeating a similar process for other quantities as well as for different energy densities we obtain the energy dependence of the critical disorder strength $\delta J_c^{\mathrm{MBL}}$ and thereby the phase boundary given in Fig. 1.

The distinction between the two MBL phases, is that for medium disorder strengths, the eigenstates have no order and form a paramagnet since the domain walls localization lengths are long enough that they frequently overlap and get created and destroyed pairwise.

A spin-glass order develops once the domain walls are strongly localized and their number fluctuations are small. The spin-glass order can be observed in the divergence of the susceptibility

$$\chi_n^{\mathrm{SG}} = \frac{1}{L} \sum_{i,j=1}^{L} \langle n | \sigma_i^z \sigma_j^z | n \rangle^2 .$$

The data for χ_n^{SG} is shown in Fig. 2 and from the scaling collapse we can determine the transition point.

Summary. We have explored a promising probe for the many-body localization transition and used it to study a disordered quantum Ising chain. The probe is obtained from the entanglement properties of exact eigenstates, namely its standard deviation of the entanglement entropy over many disorder realizations. We have obtained clear signatures of the many-body localization transition and gave evidence for the development of spin-glass order at large disorder strength. Thereby, we provided a numerical estimate of the full MBL phase diagram as a function of disorder and energy density.

[1] P. W. Anderson, Phys. Rev. **109** (1958), 1492.

[2] D. M. Basko, I. L. Aleiner, B. L. Altshuler, Ann. Phys. **321** (2006), 1126.

[3] J. H. Bardarson, F. Pollmann, J. E. Moore, Phys. Rev. Lett. **109** (2012), 017202.

[4] M. Serbyn, Z. Papić, D. A. Abanin, Phys. Rev. Lett. **110** (2013), 260601.

[5] J. A. Kjäll, J. H. Bardarson, F. Pollmann, Phys. Rev. Lett. **113** (2014), 107204.

2.6 Slow electrons from short intense laser pulses

ELIAS DIESEN, QICHENG NING, KOUDAI TOYOTA, ULF SAALMANN AND JAN M ROST

Short pulses can lead to the production of slow photo electrons for quite different reasons. We contrast here short wavelength pulses (photons of tens of eV energy) with long wavelength pulses in the mid infrared regime (typical wavelength a couple of micrometers). In the first case, slow electrons are due to non-adiabatic ionization. To isolate the phenomenon and to make it tractable with perturbation theory, we have introduced a new theoretical concept, the envelope hamiltonian. In the second case laser driven soft recollisions are responsible for peaks in the low-energy photo electron spectrum. We demonstrate in experiment and (analytical) theory that the position of those peaks becomes very sensitive to the laser pulse length for short pulses.

In XUV-short pulse ionization typically a single photon can ionize an electron far into the continuum. Nevertheless slow electrons appear for short pulses due to non-adiabatic dynamics. This is also the reason why a standard first order ($n = 1$) perturbation theory in the number n of photons is not sufficient and one has to resort in general even for one electron to full numerical solutions. Formally, e.g., in the length gauge, one needs many (unperturbed) electron orbitals of the field free hamiltonian $H = -\frac{1}{2}\nabla^2 + V$ to describe adequately the AC Stark shift. Here, we introduce the *envelope hamiltonian* (atomic units are used)

$$H_{\rm env}(t) = -\frac{1}{2}\nabla^2 + \sum_{n=-2}^{+2} V_n(\vec{r},t)\, e^{-in\omega t}, \qquad (1)$$

where the $V_n(\vec{r},t)$ are *single-cycle* averaged Fourier-components of the potential V in the Kramers-Henneberger frame, co-moving with the electron,

$$V_n(\vec{r},t) = \frac{1}{T_\omega}\int_0^{T_\omega} dt' V\left(\vec{r}+\vec{e}_x\,\alpha(t)\cos(\omega t'+\delta)\right) e^{in\omega t'} \qquad (2)$$

which constitutes an adiabatic Floquet representation: We Fourier expand the optimal oscillatory time dependence of the potential, keeping, however, the time-dependence of the pulse envelope. Thereby, the "unperturbed" Hamiltonian $H_0(t) = -\frac{1}{2}\nabla^2 + V_0(\vec{r},t)$ becomes time-dependent and its eigen functions and energies describe correctly the AC-Stark-shifted energy levels. The laser pulse is Gaussian of pulse length T and peak amplitude F_0 and is expressed via the quiver amplitude of the electron and $c = 2\ln 2$ as

$$\alpha(t) = \frac{F_0}{\omega^2}\frac{e^{-2c(t/T)^2}}{1+8\ln 2/(T\omega)^2} \equiv \alpha_0 e^{-2c(t/T)^2}. \qquad (3)$$

Applying now standard time-dependent perturbation theory to $H_0(t)$ one sees that the $V_n(t)$ are responsible for n-photon transitions. On the other hand, there is a new transition matrix element proportional to $i\partial/\partial t$, which describes non-adiabatic transitions due to the fast changing pulse enevelope. Such a transition is missing if a standard (time-independent) zeroth order hamiltonian is used. In this case, e.g., in the standard length gauge, the non-adiabatic transitions are hidden in the multi-photon transition matrix elements.

Yet, there seems to be a contradiction since the adiabatic treatment requires the time scale of the pulse envelope to be slow compared to the other time scales of the problem. A closer inspection reveals however, that for our separation of time scales we only need the pulse envelope to be slow compared to the optical frequency ω which is the case since we consider situations with well defined photon frequency. The non-adiabaticity refers to the electron dynamics and appears because the pulse envelope may vary on the same time scale as the bound orbitals.

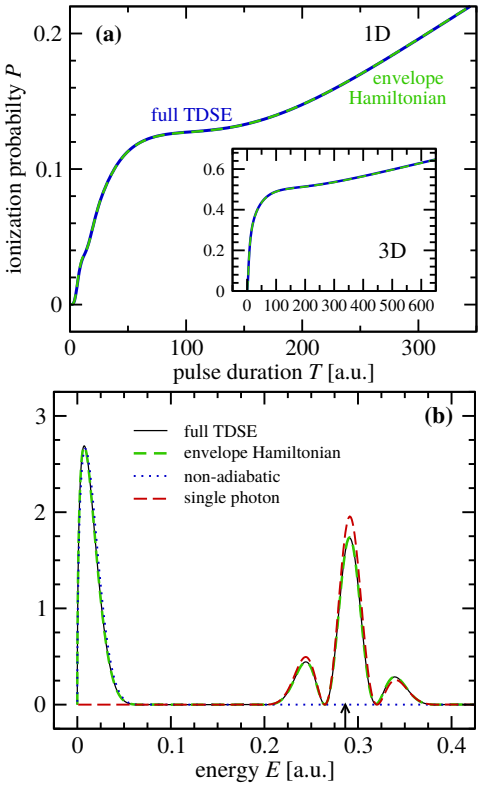

Figure 1: Ionization probability (a) as function of pulse length T and electron spectrum for $T = 100au$, 1D from the full solution (blue-solid) and for the envelope Hamiltonian (green-dashed, (1) are almost indistinguishable for short range potentials (details in [1]). The laser parameters are $\{F_0,\omega\} = \{0.5, 0.314\}$ and $\{F_0,\omega\} = \{4.5, 0.942\}$ for the 1D and the 3D case (inset), respectively.

The agreement of results from the envelope hamiltonian and an accurate numerical solution for the model system of Fig. 2 may still appear to be surprising. Even more encouraging is the fact that we can really distinguish the non-adiabatic ($n = 0$, perturbation oper-

ator $i\partial/\partial\tau$, dotted in Fig. 2b) from the single photon ($n = 1$, $V_1(t)$, red-dashed) and higher photon transitions, see [1].

Investigations to understand and explore non-adiabatic double ionization are on the way as well as exploiting the separation of the envelope time dependence for optimal control in the XUV regime.

Soft recollisions of electrons, most easily visible in mid-infrared laser fields [3], are another source of slow electrons (Fig. 2). As Fig. 3 shows, the position of the low energy peak depends sensitively on the pulse length for short pulses and on the ponderomotive potential $F_0^2/(2\omega)^2$ the pulse creates. The peaks are due to electron momentum bunching [4] when the tunnel-ionized electron returns at time t^* after 1 or 3/2 optical cycles $2\pi/\omega$ to the vicinity of the nucleus and suffers a soft recollision with a gentle "kick" from the ionic potential.

For the results in Fig. 3 it is sufficient to consider a free electron moving in one dimension in a time-dependent vector potential $A(t)$ with a Hamiltonian

$$H = \big[p - A(t)\big]^2/2\,. \tag{4}$$

Hamilton's equations produce a constant drift momentum which yields the value $p_\mathrm{d} = A(t_0)$ if we assume that the velocity $\dot{x}(t_0) = 0$ (tunneling regime). Integration of $\dot{x}(t) = p_\mathrm{d} - A(t)$ in time from t_0 to the recollision time $t^* = t_0 + \Delta t$ gives

$$x(t^*) = p_\mathrm{d}\,\Delta t + \int_0^{\Delta t} \mathrm{d}t\, A(t_0 + t)\,. \tag{5}$$

According to (5) the recollision condition $x(t^*) = 0$ requires a particular drift momentum which can be interpreted as the average of the time-dependent vector potential over Δt, the time it takes the electron from the tunnel exit to the soft recollision,

$$p = -\frac{1}{\Delta t}\int_0^{\Delta t} \mathrm{d}t\, A(t_0 + t)\,. \tag{6}$$

We obtain an analytical expression for (6) by taking the vector potential as the derivative of the quiver amplitude with Gaussian envelope (3). Expressing the pulse duration as the number n of optical cycles $T = k\,2\pi/\omega$ we get for the peak positions

$$p(k) = \frac{p_\infty}{2}\left(1 \pm e^{-c(3/k)^2}\right)\,, \tag{7}$$

where the "+(−)" sign refers to $\Delta t = \frac{3\pi}{\omega}\,(\frac{\pi}{\omega})$, the so called LES (VLES). Note that for a cw ($k\to\infty$) pulse the LES converges to $2p_\infty = 2F_0/(3\pi\omega)$ while the VLES tends to zero. The final analytical result contains laser focus averaging and a slight redshift due to the ion potential, small corrections which turn p_∞ into a factor p_∞^eff making the result target dependent shown as solid curves in Fig. 3.

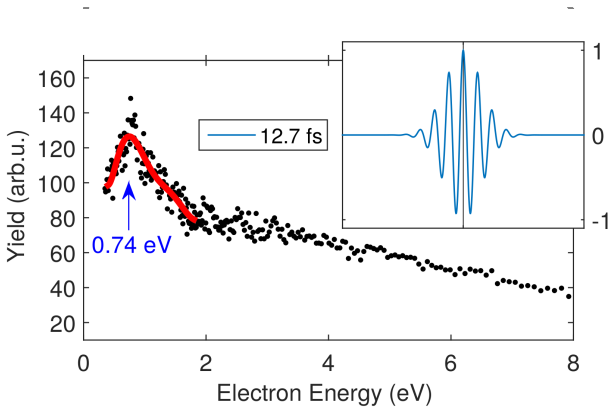

Figure 2: Photoelectron spectra of Krypton for $T = 12.7$fs with the peak position determined by a polynomial fit (red line) for a frequency of $\omega = 0.0253$ au (corresponding to a wavelength of 1800 nm); from [2].

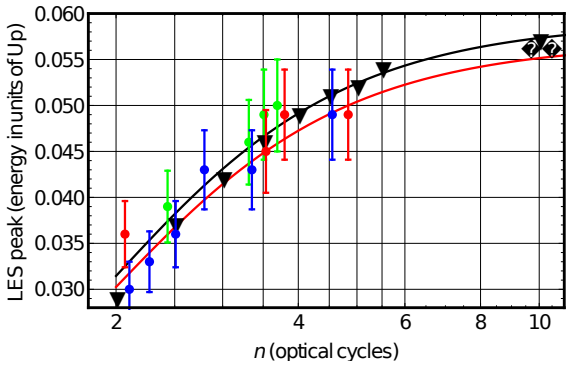

Figure 3: Low energy peak positions normalized to the peak ponderomotive energy $U_p = F_0^2/(2\omega)^2$ as a function of laser pulse duration in terms of optical cycles $k = T\omega/(2\pi)$ for ω as in Fig. 2; from [2]. Data is for Krypton ($U_p = 20$ eV, green and 25 eV, blue) and Argon (31 eV, black and 55 eV, red). Circles are from experiment, triangles are from a numerical classical calculation and lines are analytical results, see text. Theoretical results are focus averaged and shifted down by 15 % to match the experiment. The star is adopted from [3] for Argon with $U_p = 35.6$ eV.

It certainly is astonishing that a simple analytical formula can describe the experimental results. That this has been possible on the basis of classical mechanics in contrast to the non-adiabatic slow electron peak described by the envelope hamiltonian underlines the difference in origin of these two low energy electron phenomena, both of which depend sensitively on the duration of the short ionizing light pulse.

[1] K. Toyota, U. Saalmann, and J. M. Rost, New J. Phys. **17**, 073005 (2015).

[2] K. Zhang etal., submitted (2015).

[3] C. Blaga etal. Nature Physics **5**, 335 (2009).

[4] A. Kästner, U. Saalmann, and J. M. Rost, Phys. Rev. Lett. **108**, 033201 (2012).

2.7 Proton ejection from hydrogen rich molecules exposed to strong x-ray pulses

PF. DI CINTIO, A. CAMACHO, A. RUBISCH, U. SAALMANN AND J. M. ROST

Large molecules and clusters suffer considerable radiation damage by violent ionization and Auger decay when exposed to intense x-ray pulses. Here we show that in hydrogen rich systems the consequences of this damage, Coulomb explosion and a hot electron plasma, are tamed by the emission of fast protons. The emission lowers the positive charging of the system thereby reducing Coulomb explosion and the strength of the positiv back ground potential which in turn can only hold less energetic plasma electrons.

Composite clusters consisting of different atomic or molecular species can have surprising dynamical properties under intense light pulses. This has been demonstrated for so called core-shell systems where the core-cluster is formed by one sort of atoms and the hull by another one. A quite spectacular effect was predicted and experimentally verified for helium embedded rare gas clusters which absorb near infrared photons extremely efficiently [1].

Motivated by these unexpected effects we have investigated complementary "heavy-light" composite systems where the different kinds of constituents are not geometrically separated as in core-shell systems, but homogeneously mixed such as in clusters consisting of isoelectronic hydride molecules, ammonia and water clusters, augmented by the "atomic limit" of neon clusters. These systems contain the elements hydrogen, carbon, nitrogen and oxygen, omnipresent in organic molecules. A detailed understanding of their dynamics in strong X-ray pulses provides valuable information to understand the mechanisms of radiation damage [2].

Protonated large systems can eject fast protons upon absorption of X-ray pulses and this proton loss provides an effective additional channel to release the absorbed energy and acquired charge as compared to systems without protons with intriguing consequences: (i) The nano-plasma from trapped electrons is much cooler than in pristine clusters with the same number of heavy atoms. (ii) The proton ejection dynamics exhibits universal features along the isoelectronic hydrides but very different from the isoelectronic atomic cluster. (iii) The probably most surprising effect is a dynamically induced segregation of heavy ions and protons which occurs in a small but experimentally relevant intensity window around $I{\sim}10^{18}\mathrm{W/cm^2}$ where the heavy atoms (C, N or O) emerge as *neutrals* despite substantial energy deposition by the laser pulse. This is in sharp contrast to pristine clusters composed out of C or N which Coulomb explode with multiply charged ions for a comparable total charging.

Our theoretical description relies on a mixed quantum-classical approach. Electrons and ions are treated as classical particles propagated according to Newton's equations with all Coulomb interactions included. Photoionization and Auger decay, i.e., the quantum electronic processes *within* the atoms or hydrides, are described by the appropriate rates and consistently integrated into the time-evolution of the charged particles through a Monte Carlo realization.

Photons of a few-keV energy ionize mainly the K-shell ($1s$ orbitals) for the elements of the first row under consideration. For the sake of simplicity, all results presented have been obtained with photo-ionizing exclusively K-shell electrons.

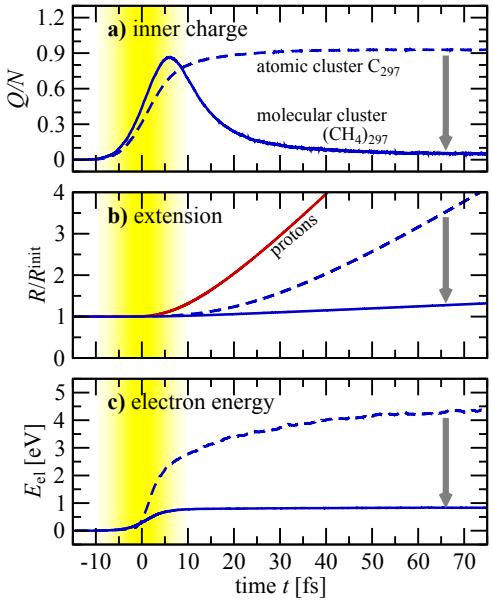

Figure 1: Time evolution for a molecular (solid lines) and an atomic (dashed lines) cluster. The yellow-shaded region marks the X-ray pulse ($I{=}10^{18}\mathrm{W/cm^2}$) with a duration of 10 fs (FWHM) centered at $t = 0$.
a) Charge inside the sphere defined by the outermost carbon ion. **b)** Radii in units of the initial radii, with the proton part shown separately (red solid line). **c)** Average kinetic energy of trapped electrons (temperature of the trapped plasma). The reduction of carbon charging, carbon Coulomb explosion and energy of trapped electrons due to proton ejection is marked by grey arrows.

Figure 1 illustrates the time evolution of relevant parameters for a cluster under the influence of the light pulse (yellow filled area). The dynamics of the pristine carbon cluster (dashed) and the methane cluster (solid) is completely different: The carbon atoms get successively charged through photo-ionization leading to more than 90% carbon ions after 90 fs with the laser pulse of peak intensity $I{=}10^{18}\mathrm{W/cm^2}$ (Fig. 1a). The

cluster ions create a deep binding potential from which most Auger electrons cannot escape but form a nano-plasma. The maximum kinetic energy of the trapped electrons is limited by the depth of the cluster potential and the average kinetic energy (Fig. 1c, dashed) is indicative of the nano-plasma temperature.

The molecular cluster, however, does not follow this scheme: While initially similarly charged as in the pristine cluster, the carbon ions in the methane cluster recombine and are in the end almost neutral on average (Fig. 1a, solid). At the same time the kinetic energy of the trapped electrons and hence the temperature of the nano-plasma remains comparatively low (Fig. 1c, solid). Both phenomena originate in the ejection of fast protons from the molecular cluster (see red line in Fig. 1b). Although the carbon K-shells are initially photo-ionized, the charge distribution of the doubly charged methane after Auger decay is such that the carbon ion is screened and the positive charge is dominantly localized on two hydrogen atoms which are likely to be ejected from the entire cluster as protons. These protons take away the excess positive charge created by photo-ionization which is of course not possible in the pristine carbon cluster. The remaining positive charge in the cluster is small giving rise to a weak potential which can only trap low energy electrons. Therefore, the temperature of the nano-plasma is by a factor of four smaller than for the pure carbon cluster after 80 fs (grey arrow); this holds also true for the Coulomb explosion of the carbon ions (Fig. 1b) with the charging of the carbon ions even more dramatically reduced, almost by an order of magnitude (Fig. 1a).

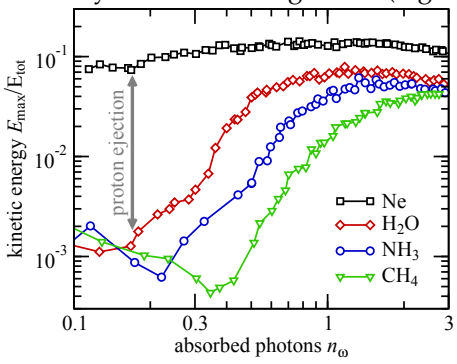

Figure 2: Kinetic energy of the fastest ion E_{max}, 0.5 ps after the peak of the pulse, versus the average number of photons absorbed per atom/molecule $n_\omega = N_\omega/N$. The kinetic energies are normalized with the total energy $E_{tot} = N_\omega\omega$ absorbed by the cluster.

One may expect that the absolute difference in velocity of heavy and light ions gets larger with increasing intensity and therefore higher charging of the cluster. Figure 2, however, reveals that the ratio of the kinetic energy for the fastest heavy ion E_{max}, relative to the energy of all ions E_{tot}, exhibits a non-monotonic behavior as a function of photons absorbed with a dip at a critical number n_ω. The latter depends moderately on the species considered, as can be seen in Fig. 2, but is otherwise a universal feature of hydride clusters in obvious contrast to the isoelectronic neon cluster. The dip in the curves of Fig. 2 for the hydrides clusters indicates a dynamical segregation of protons and heavy ions.

As a consequence of the segregation we expect a much lower charging of heavy ions as compared to the pristine cluster. This is indeed the case as can be seen in Fig. 3. For low intensities most carbon atoms remain neutral in the pristine as well as in the hydride cluster. This changes drastically for intermediate intensities of about 10^{18}W/cm^2, where the fraction of neutral carbon atoms surviving the light pulse illumination is small in the pristine cluster. In the hydride cluster, one the other hand, about 80% neutral heavy atoms result from recombination with the cold electrons after proton segregation in the surface layer which has been fully charged due to due to efficient field ionization. For higher intensities, we expect the proton segregation to cease (see Fig. 2) and as a consequence similar charge spectra for the pristine and the hydride cluster. This is indeed true with respect to a vanishing yield of neutral atoms. The form of the charge distribution is still somewhat different.

We have identified the effect of proton ejection also in large molecules such as lysozyme. If and how this carries over to nanocrystals of proteins is subject of ongoing studies.

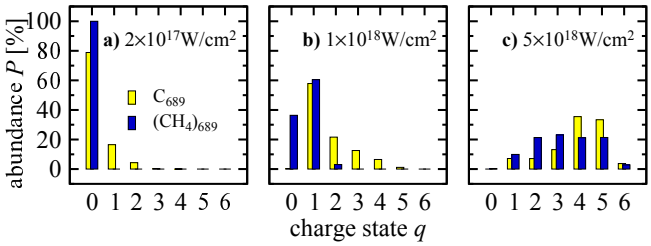

Figure 3: Charge-state distribution for carbon ions C^{q+} from $(CH_4)_{689}$ and C_{689} for various intensities I indicated in the respective panel.

What clearly emerges from Fig. 2 is the sensitivity of the proton segregation and consequently the charge distribution of the heavy ions on the intensity. All experimental spectra are integrated over intensity due to unavoidable laser focus averaging. Figure 3 demonstrates that significantly lower charging of the carbon ions remains a signature for proton segregation even under laser focus averaging and occurs only for peak intensities where proton segregation is operative.

[1] A. Midkaberize, U. Saalmann, and J. M. Rost, Phys. Rev. Lett. **102**, 128102 (2009); S. R. Krishnan et al., Phys. Rev. Lett. **107**, 173402 (2011).

[2] P-F. di Cintio, U. Saalmann, and J. M. Rost Phys. Rev. Lett. **11**, 123401 (2013).

2.8 Hierarchy of stochastic pure states for open quantum system dynamics

D. SUESS, G. RITSCHEL, W. T. STRUNZ, A. EISFELD

The treatment of the dynamics of realistic open quantum systems still poses both conceptual and computational challenges. These arise from non-Markovian behavior due to a structured environment or strong system-environment interactions. Severe assumptions, like weak-coupling or Markov approximation, are often made for practical reasons. However, they fail for many systems of interest. Non-Markovian systems are far more challenging and usually one tries to tackle them with path integral approaches or hierarchical equations of motion for the system's *reduced density matrix*.

We follow a different strategy and derive a hierarchy of stochastic differential equations for pure states in the system Hilbert space (quantum trajectories). From this *hierarchy of pure states* (HOPS) the exact reduced density operator is obtained as an ensemble average [1]. Quantum trajectories are well established in the Markov case, where single realizations describe continuously measured open quantum systems or serve as models for spontaneous wave function collapse. The generalization to the non-Markovian regime proves challenging and is an active field of research.

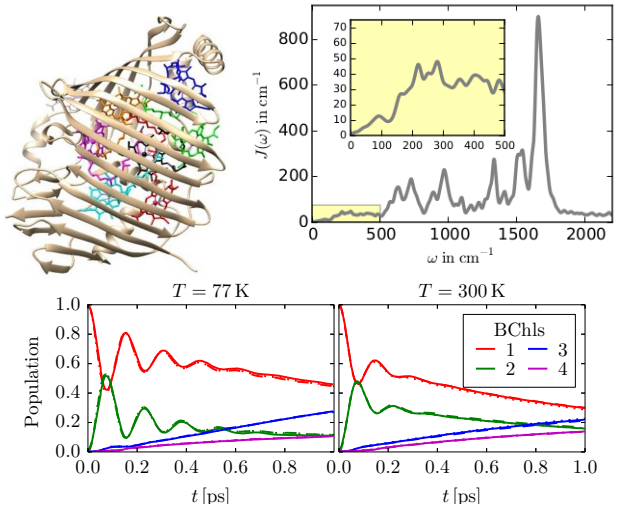

Figure 1: Coupling of excitonic and nuclear degrees of freedom plays an important role in many chemical and biological processes. For example the efficient exciation energy transfer in photosynthesis depends strongly on the coupling of electronic transition of the (bacterio)chlorophyll molecules to internal vibrations and that of the surrounding protein. Top, left: the Fenna-Matthews-Olsen complex of green sulfur bacteria with sketch of the protein scaffold and the bacteriochlorophyls (BChl). Top, right: the spectral density of a single BChl, when one takes as system part its ground and excited electronic state. Bottom: Transfer of electronic excitation energy. Dotted line, HOPS first order; dashed line, HOPS second order. For comparison also the result of a high order HEOM calculation (Ref. [3]) is shown as solid line.

The Open Quantum System: Let us consider a system linearly coupled to a bath of harmonic oscillators. The Hamiltonian is a sum

$$H_{\rm tot} = H \otimes 1 + 1 \otimes H_{\rm B} + H_{\rm int} \tag{1}$$

of the system Hamiltonian H, the bath Hamiltonian $H_{\rm B} = \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda$ and the interaction Hamiltonian

$$H_{\rm int} = \sum_\lambda (g_\lambda^* L \otimes a_\lambda^\dagger + g_\lambda L^\dagger \otimes a_\lambda). \tag{2}$$

Here, L is an operator in the system's Hilbert space and $a_\lambda^\dagger$ the creation operator of bath mode λ. The interaction strength between system and that mode is quantified by the complex number g_λ. Let us emphasize that the form of Eq. (2) does not imply a rotating wave approximation. In many important cases one has in fact $L = L^\dagger$. It is convenient to encode the frequency dependence of the interaction strength by the so called spectral density $J(\omega) = \sum_j |g_j|^2 \delta(\omega - \omega_j)$. The latter is related to the bath correlation function $\alpha(\tau)$ by

$$\alpha(\tau) = \int_0^\infty d\omega\, J(\omega) \Big(\coth\big(\frac{\omega}{2T}\big) \cos(\omega\tau) - i \sin(\omega\tau) \Big) \tag{3}$$

where T is the temperature. In Fig. 1 we show an example of the type of spectral density we are interested in. Note the spiky structure that leads to complicated non-Markovian behavior.

Non-Markovian Quantum State Diffusion: For now let us consider initial conditions $|\Psi_0\rangle = |\psi_0\rangle \otimes |\vec{0}\rangle$, where $|\vec{0}\rangle$ is the vacuum state for all a_λ in the bath Hilbert space (zero temperature). We are interested only in the dynamics in the system Hilbert space and in particular the reduced density matrix obtained by tracing over the bath degrees of freedom. Using a coherent state representation of the bath degrees of freedom, the reduced density matrix can be obtained from an ensemble average over trajectories of (non-normalized) pure states $|\psi_t(z^*)\rangle$ in the system Hilbert space via

$$\rho_t = \mathbb{E}\big\{ |\psi_t(z^*)\rangle\langle\psi_t(z^*)| \big\}, \tag{4}$$

where $z = z_t$ is a complex Gaussian stochastic process with mean $\mathbb{E}\big[z_t\big] = 0$ and correlations $\mathbb{E}\big[z_t z_s\big] = 0$ and $\mathbb{E}\big[z(t) z^*(s)\big] = \alpha(t-s)$. The time evolution of the states $|\psi_t(z^*)\rangle$ is determined [2] by

$$\partial_t \psi_t = -{\rm i} H \psi_t + L z_t^* \psi_t - L^\dagger \int_0^t {\rm d}s\, \alpha(t-s) \frac{\delta \psi_t}{\delta z_s^*} \tag{5}$$

with initial conditions $\psi_{t=0} = \psi_0$.

While Eq. (4) with (5) determine the reduced density operator exactly, in general it is unclear how to solve Eq. (5) due to the functional derivative $\frac{\delta \psi_t}{\delta z_s^*}$.

Hierarchy of pure states (HOPS): First Eq. (5) is written as

$$\partial_t \psi_t = -\mathrm{i}H\psi_t + Lz_t^*\psi_t - L^\dagger \psi_t^{(1)}, \tag{6}$$

with the auxiliary pure state $\psi_t^{(1)} := \int_0^t \mathrm{d}s\, \alpha(t-s)\frac{\delta\psi_t}{\delta z_s^*}$. We now construct a hierarchy of equations by first considering the time derivative of $\psi_t^{(1)}$. In order to illustrate the derivation of the hierarchy of equations most clearly, we consider a bath-correlation function of the form

$$\alpha(\tau) = g\, \exp[-w\tau]\ (\tau \geq 0) \tag{7}$$

with $w = \gamma + \mathrm{i}\Omega$. The derivation can easily be extended to sums of such exponentials, which are well suited to approximately describe a large class of spectral densities and also finite temperature [4]. For such an exponential correlation function one obtains

$$\partial_t \psi_t^{(1)} = (-\mathrm{i}H - w + Lz_t^*)\,\psi_t^{(1)} + \alpha(0)L\psi_t^{(0)} - L^\dagger\psi_t^{(2)},$$

with $\psi_t^{(k)} := \int_0^t \mathrm{d}s\, \alpha(t-s)\frac{\delta}{\delta z_s^*}\psi_t^{(k-1)}$. By considering the time-derivatives of $\psi_t^{(k)}$ one gets coupled stochastic equations for an infinite hierarchy of pure states

$$\begin{aligned}\partial_t \psi_t^{(k)} &= (-\mathrm{i}H - kw + Lz_t^*)\,\psi_t^{(k)} \\ &\quad + k\alpha(0)L\psi_t^{(k-1)} - L^\dagger\psi_t^{(k+1)},\end{aligned} \tag{8}$$

with $\psi_{t=0}^{(0)} = \psi_0$ and $\psi_{t=0}^{(k)} = 0$ for $k > 0$. Solving the infinite system Eq. (8) is equivalent to solving Eq. (5), with $\psi_t = \psi_t^{(k=0)}$.

Truncation: In order to transform Eq. (8) into a practical scheme, we truncate the hierarchy at some suitable $\mathcal{K}$ large enough. We found that in particular $\psi_t^{(\mathcal{K}+1)} \approx \frac{\alpha(0)}{w}L\psi_t^{(\mathcal{K})}$ is a good "terminator". We remark that the use of this particular terminator is not essential.

Non-linear evolution equation: For fundamental issues related to continuous measurement or spontaneous collapse, a theory for normalized pure states is much preferred. Moreover, the Monte-Carlo determination of the density operator according to Eq. (4) converges much faster if the contributions of individual realizations $\psi_t(z^*)$ are of the same order of magnitude (importance sampling). Remarkably, it is possible, using a Grisanov transformation, to obtain a normalizable hierarchy of evolution equations (which are now non-linear). In Fig. 2 this superior numerical behavior of the non-linear equation is demonstrated for the case of the spin-boson model.

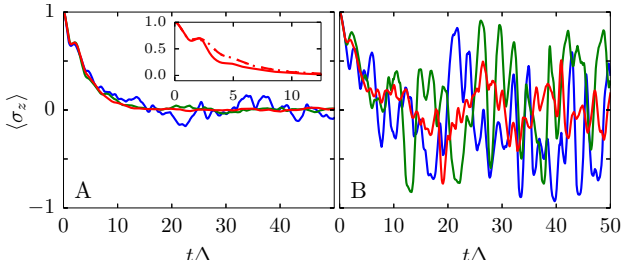

Figure 2: Dynamics of the spin-boson model. (A) Non-linear equation, (B) linear equation. In both cases $\Delta = 1$, $\epsilon = 0$ and the parameters of the spectral density are given by $g = 2$ and $w = 0.5 + 2\mathrm{i}$. The blue, green, and red lines represent 100, 1000, and 10000 realizations, respectively. The order of the hierarchy is $\mathcal{K} = 8$. The inset in A shows the convergence (for 10000 realizations) with respect to the order of the hierarchy. Dotted, dashed, and solid line are orders one, two and four respectively.

Finite temperature: The case $T > 0$ can be mapped to the zero temperature case using the *thermofield method* [5]. Remarkably, a system with self-adjoint coupling operator (i.e. $L = L^\dagger$) admits a description in terms of the non-Markovian quantum state diffusion equation (5) where now the stochastic process has correlations according to Eq. (3), which we expand as a sum of exponentials [4,7].

Applications: As an application of our formalism we considered excitation energy transfer and absorption of molecular aggregates, like the light-harvesting pigment protein complex shown in Fig. 1. In this figure (bottom) we also show the calculated transfer dynamics along this complex for different orders of HOPS and compare to the results of Ref. [3]. A detailed analysis [6] revealed that the numerical effort of HOPS is much superior compared to density matrix approaches as e.g. that of Ref. [3]. Furthermore, we could show that for the calculation of linear optical spectra one single deterministic trajectory is sufficient [5].

Outlook: Currently we are working on the extension of the method to time dependent Hamiltonians with the aim to treat the interaction of molecules with electromagnetic femtosecond pulses, which then will allow us to calculate multidimensional spectroscopy signals using stochastic wavefunctions in a similar spirit as [8] but for complex, structured environments.

[1] D. Suess, A. Eisfeld, W. T. Strunz; Phys. Rev. Lett. **113** (2014) 150403.

[2] L. Diósi, N. Gisin, W. T. Strunz; Phys. Rev. A **58** (1998) 1699.

[3] A. Ishizaki, G. R. Fleming; J. Chem. Phys. **130** (2009) 234111

[4] G. Ritschel, A. Eisfeld; J. Chem. Phys. **141** (2014) 094101.

[5] G. Ritschel, D. Suess, S. Möbius, W. T. Strunz, A. Eisfeld; J. Chem. Phys **142** (2015) 034115.

[6] D. Suess, W. T. Strunz, A. Eisfeld; J. Stat. Phys. **159** (2015) 1408.

[7] D. W. Schönleber, A. Croy, A. Eisfeld; Phys. Rev. A **91** (2015) 052108.

[8] J. Albert, M. Falge, M. Kess, J.G. Wehner, P-P. Zhang, A. Eisfeld, and V. Engel; J. Chem. Phys. **142** (2015) 212440.

2.9 Quantum transport simulations using Rydberg atoms

DAVID W. SCHÖNLEBER, MICHAEL GENKIN, SEBASTIAN WÜSTER, ALEXANDER EISFELD

Excitation transport through dipole-dipole interactions plays a prominent role in diverse physical settings, including photosynthesis, exciton transport through quantum-dot arrays, and molecular aggregates. Of crucial importance is the competition between the fundamentally coherent transport mechanism and the coupling to the environment. Often, clean studies of excitation transport are impeded by, for example, the large number of degrees of freedom in these systems, strongly coupled vibrational modes and the unknown geometry. Ultracold atoms prepared in highly-excited Rydberg states exhibit similar dipolar state-changing interactions, but are considerably simpler to study because of their relative ease to control using lasers.

Here, we show that an array of ultracold Rydberg atoms embedded in a laser driven background gas can serve as an artificial molecular aggregate for simulating exciton dynamics and energy transport with a controlled environment. Spatial disorder and decoherence introduced by the interaction with the background gas atoms can be controlled by the laser parameters. The degree of decoherence is traced back to information gained on the excitation location by the background gas acting as a probe, which provides an experimentally accessible model system for studying the effects of quantum measurement on the dynamics of a many-body quantum system.

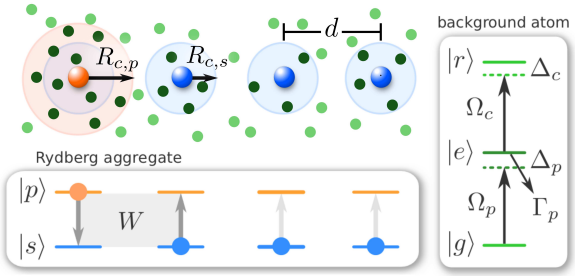

Figure 1: Sketch of an embedded Rydberg aggregate. An assembly of several Rydberg impurities in a state $|s\rangle$ (large blue) and one in a state $|p\rangle$ (large orange) are linearly arranged with spacing d in background atomic gas (shades of green). These background atoms are then addressed with an EIT scheme (right), providing detection signals within radii $R_{\mathrm{c,s/p}}$ around each impurity.

Scheme and model: Consider a chain of N Rydberg atoms with mean spacing d forming the aggregate sketched in Fig. 1. Such an arrangement can be created e.g. by exciting Rydberg states from a trapped ultracold atomic gas using tightly focused laser beams. To study transport, initially, $N-1$ atoms are prepared in the state $|s\rangle = |\nu s\rangle$ with principal quantum number ν and angular-momentum $l = 0$, while a single atom is excited to the state $|p\rangle = |\nu p\rangle$, with angular-momentum $l = 1$. This $|p\rangle$ excitation can then migrate through the aggregate via resonant dipole-dipole interactions. In addition, the aggregate is immersed in a gas of M atoms initially prepared in the electronic ground-state $|g\rangle$. These atoms are coupled by two laser fields from $|g\rangle$ via a short lived intermediate state $|e\rangle$ (spontaneous decay rate Γ_p) to a third Rydberg level, $|r\rangle = |\nu' s\rangle$.

This system is governed by the many-body Lindblad master equation for the density matrix $\hat{\rho}$ ($h = 1$)

$$\dot{\hat{\rho}} = -i[\hat{H}, \hat{\rho}] + \sum_{\alpha} \mathcal{L}_{\hat{L}_\alpha}[\hat{\rho}]. \qquad (1)$$

The Hamiltonian consists of three parts: $\hat{H} = \hat{H}_{\mathrm{agg}} + \hat{H}_{\mathrm{EIT}} + \hat{H}_{\mathrm{int}}$ describing the evolution of the aggregate, the background gas of three-level atoms, and the Rydberg-Rydberg interactions. The super-operator $\mathcal{L}_{\hat{L}_\alpha}[\hat{\rho}]$ describes spontaneous decay of the background atom α from level $|e\rangle$, thus $\mathcal{L}_{\hat{O}}[\hat{\rho}] = \hat{O}\hat{\rho}\hat{O}^\dagger - (\hat{O}^\dagger\hat{O}\hat{\rho} + \hat{\rho}\hat{O}^\dagger\hat{O})/2$ and the decay operators are $\hat{L}_\alpha = \sqrt{\Gamma_p}\hat{\sigma}^{(\alpha)}_{ge}$, with $\hat{\sigma}^{(\alpha)}_{kk'} = [|k\rangle\langle k'|]_\alpha$ acting on atom α only.

The aggregate atoms are labeled by Latin indices such as n and m. Restricted to the Hilbert space with a single excitation we can write

$$\hat{H}_{\mathrm{agg}} = \sum_{n\neq m} W_{nm}\hat{\sigma}^{(n)}_{sp}\hat{\sigma}^{(m)}_{ps} = \sum_{n\neq m} W_{nm}|\pi_n\rangle\langle\pi_m|, \qquad (2)$$

where $|\pi_n\rangle = |ss..p..ss\rangle$ (all impurity atoms in $|s\rangle$ except the n'th, which is in $|p\rangle$) and $W_{nm} = C_3/|r_n - r_m|^3$. Here C_3 is the dipole-dipole interaction strength and r_n are the positions of the aggregate atoms.

The Hamiltonian for the background gas in the rotating wave approximation reads $\hat{H}_{\mathrm{EIT}} = \sum_\alpha \big[(\Omega_p/2\,\hat{\sigma}^{(\alpha)}_{eg} + \Omega_c/2\,\hat{\sigma}^{(\alpha)}_{re} + \mathrm{H.c.}) - \Delta_p\hat{\sigma}^{(\alpha)}_{ee} - (\Delta_p+\Delta_c)\hat{\sigma}^{(\alpha)}_{rr}\big]$, where $\Omega_{p,c}$ and $\Delta_{p,c}$ are the probe and coupling Rabi frequencies and detunings, respectively. Typically $\Omega_p \ll \Omega_c$ and $\Delta_p + \Delta_c = 0$ which corresponds to conditions of electromagnetically induced transparency (EIT).

Background gas atoms interact among themselves and with the aggregate through van-der-Waals (vdW) interactions, which, for simplicity, are assumed to be isotropic. To use the background gas as a probe for the state of the aggregate it is necessary that the interactions are state dependent. Choosing the states $|s\rangle = |43s\rangle$, $|p\rangle = |43p\rangle$, and $|r\rangle = |38s\rangle$ in ^{87}Rb, we obtain $V^{(rs)}_{\alpha n} = C_{6,rs}/|r_\alpha - r_n|^6$ and $V^{(rp)}_{\alpha n} = C_{4,rp}/|r_\alpha - r_n|^4$, respectively, with $V^{(rp)} \gg V^{(rs)}$ due to a nearly resonant process, $43p + 38s \leftrightarrow 41d + 38p$. Among each other, the background atoms interact via $V^{(rr)}_{\alpha\beta} = C_{6,rr}/|r_\alpha - r_\beta|^6$.

Excitation detection: On resonance ($\Delta_p = \Delta_c = 0$), the steady state of a background gas atom has no

population in the intermediate state $|e\rangle$. Hence, no light is scattered by absorption and re-emission by this state, thus rendering the background gas transparent for the probe beam described by Ω_p (EIT effect). However, close to the aggregate, interactions $V_{\alpha n}^{(rs/p)} > \Omega_c^2/(2\Gamma_p)$ shift the energy level of the Rydberg $|r\rangle$ state of the background atom, breaking the resonance condition and thereby destroying the transparency. This creates an absorption shadow around each aggregate atom. Owing to the state-dependent interactions, the size of the absorption shadow around an aggregate atom depends on its state, sketched by blue (orange) circles in Fig. 1. The location of the p-excitation can be inferred from the different shadow sizes corresponding to $R_{\mathrm{c,s}} = (2C_{6,rs}\Gamma_p/\Omega_c^2)^{1/6}$ and $R_{\mathrm{c,p}} = (2C_{4,rp}\Gamma_p/\Omega_c^2)^{1/4}$, for s and p states, respectively. We demonstrate this with simulations of the full master equation for an aggregate with $N = 3$ probed by two randomly distributed pairs of background atoms. Taking the difference in optical response between an aggregate with a p excitation present and the corresponding aggregate without p excitation, we obtain an absorption signal which is due to the exciton dynamics only. The color-coded absorption signal displayed in Fig. 2 shows that the absorption of the background gas is directly linked to the probability distribution of the exciton population p_n (green lines).

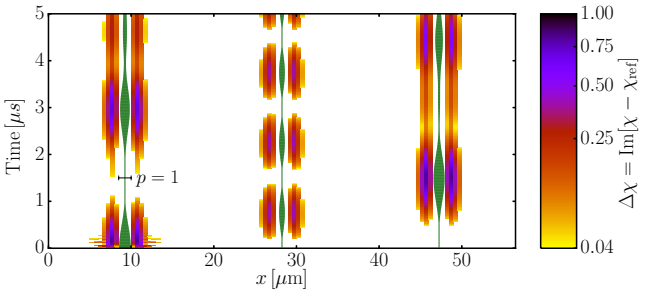

Figure 2: Link between absorption signature and excitation transport. We show the difference in optical response between dynamic and empty aggregate during transport. Green lines indicate the location of aggregate atoms r_n and their thickness the population p_n.

Measurement induced decoherence: The degree of decoherence present in this system is intimately linked to the action of the background gas acting as a real-time probe of the aggregate. That is, gaining information on the exciton location induces decoherence on the exciton dynamics. Consider the setup of Fig. 3(a). Here, the background atoms are placed in the vicinity (distance δ) of the aggregate atoms, such that transparency of the probe beam is destroyed irrespective of the state of the aggregate atom. Hence, no information can be gained on the exciton location, and the exciton dynamics proceeds coherently. Increasing the distance δ between the background gas atoms and the aggregate atoms [Fig. 3(b)], a background atom absorbs only if the adjacent aggregate atom is in the p state, thereby allowing inference of the exciton location. The corresponding exciton dynamics suffers strong decoherence as the background gas constantly measures and thus decoheres the exciton dynamics.

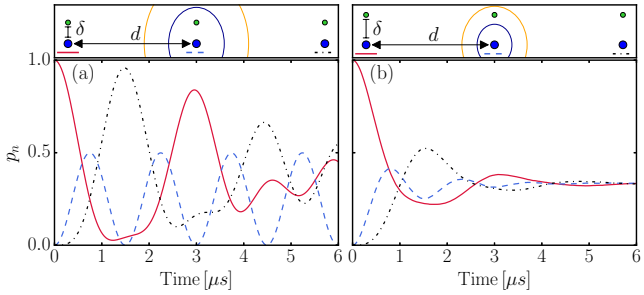

Figure 3: Exciton transport in a continuously monitored embedded Rydberg aggregate. Geometries are shown in the top panels. (a) Site occupations p_n for $n = 1, 2, 3$ (solid red, dashed blue, dot-dashed black) in a non-decohering case, $\Omega_p = 1.3$ MHz, $\Omega_c = 30$ MHz, $d = 19\mu$m, $\delta \sim 0.6\mu$m. (b) The same for a strongly decohering case with $\delta = 1.5\mu$m.

Conclusions: We have demonstrated that Rydberg atoms can be used as quantum simulators to study excitonic transport. For large exciton numbers, such investigations would be quite demanding using numerical simulations. Decoherence of the aggregate arises through continuous monitoring of the location of the excitation, providing a hands-on example of measurement induced decoherence of a quantum state [1]. Additionally, the interactions between the aggregate and the background gas can be exploited to introduce disorder.

Further applications of this system could be monitoring and decoherence of adiabatic excitation transport involving motional degrees of freedom of Rydberg atoms, as investigated in further publications of this research area [2–5].

[1] D. W. Schönleber, A. Eisfeld, M. Genkin, S. Whitlock, S. Wüster, Phys. Rev. Lett. **114** 123005 (2015).

[2] H. Zoubi, A. Eisfeld, S. Wüster, Phys. Rev. A **89** 053426 (2014).

[3] M. Genkin, S. Wüster, S. Möbius, A. Eisfeld, J.-M. Rost, J. Phys. B **47** 095003 (2014).

[4] S. Wüster, S. Möbius, M. Genkin, A. Eisfeld, J.-M. Rost, Phys. Rev. A **88** 063644 (2013).

[5] S. Möbius, M. Genkin, A. Eisfeld S. Wüster, J.-M. Rost (2013), Phys. Rev. A **87** 051602(R) (2013).

2.10 Strong optical nonlinearities from weak particle interactions in a cavity

ROBERT JOHNE, THOMAS POHL

Introduction The realization of strong interactions between single light quanta is a long-standing goal of great importance for scientific and technological applications [1]. Since photons propagate freely in vacuum, such optical nonlinearities can only be mediated via interactions with matter. Single quantum systems, such as (artificial) atoms, can provide a highly nonlinear response owing to their discrete anharmonic level structure and the associated saturation of light absorption. However, turning this feature into few-photon interactions requires very strong light-matter coupling that is typically achieved by strong confinement of light, for example in optical cavities [2,3].

Without strong mode confinement, efficient mapping of photons onto matter excitations is still possible in large ensembles due to the collectively enhanced coupling of light to many identical quantum systems. While the presence of many particles diminishes the intrinsic nonlinearity of a single scatterer, strong state-dependent interactions between the material constituents can provide additional optical nonlinearities [4]. Utilising the exaggerated properties of high-lying Rydberg state excitations in cold atomic gases, the great potential of such particle-particle interactions for few-photon operations [5] has been demonstrated in a number of recent experiments [6].

Here, we describe an approach to controllable few-photon nonlinearities that combines strong light-matter coupling and long-range particle interactions based on cold ion crystals in optical cavities. Laser-cooled ions rank amongst the most advanced platforms for quantum simulation [7] tasks, where state-selective optical forces are used to induce state-dependent interactions [8,9] mediated by collective phonon modes of the crystal. While the achievable interactions are orders of magnitude smaller than the aforementioned Rydberg atom interactions, they can still provide a powerful resource for quantum nonlinear optics, as we show below.

The setting We consider a crystalline arrangement of N ions embedded in an optical cavity, as illustrated in Fig.1a. Each ion possesses a Λ-type level structure composed of three internal states, $|a\rangle$, $|b\rangle$ and $|c\rangle$ (see Fig.1b). The $|b\rangle \to |c\rangle$ transition is driven by a classical control laser with Rabi frequency Ω_c while the transition between $|a\rangle$ and $|c\rangle$ couples near resonantly to the cavity with a coupling strength g_i for each ion. The cavity and control-field frequencies are chosen such that one obtains a resonant two-photon transition between the two stable ground states $|a\rangle$ and $|b\rangle$ and a corresponding single-photon detuning Δ from the excited

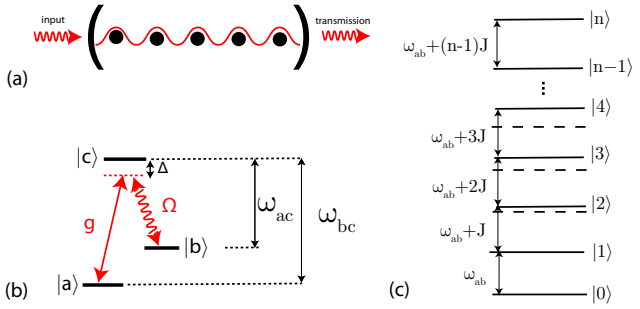

Figure 1: (a) A linear ion chain in a cavity; (b) Relevant level structure of the ions and (c) anharmonic energy spectrum of the spin states induced by the spin-spin interaction.

state $|c\rangle$. Within the rotating wave approximation and after adiabatically eliminating the excited state in the limit of large Δ, the Hamiltonian of the ion-cavity interaction can be written as

$$H = \sum_{i=1}^{N} \frac{g_i^2}{\Delta} \hat{a}^\dagger \hat{a} \hat{\sigma}_{aa}^{(i)} + \frac{\Omega^2}{\Delta} \sum_{i=1}^{N} \hat{\sigma}_{bb}^{(i)} - i \sum_i \frac{g_i \Omega}{\Delta} (\hat{\sigma}_{ab}^{(i)} \hat{a}^\dagger + \text{h.c.}) + \Omega_{in}(\hat{a} + \hat{a}^\dagger), \quad (1)$$

where the operator $\hat{a}^\dagger$ creates a cavity photon and the operators $\hat{\sigma}_{\alpha\beta}^{(i)} = |\alpha\rangle_i\langle\beta|$ denotes the ionic transition and projection operators.

Losses are described by associated Lindblad operators $\hat{L}_A[\hat{\rho}] = (2\hat{A}\hat{\rho}\hat{A}^\dagger - \hat{A}^\dagger\hat{A}\hat{\rho} - \hat{\rho}\hat{A}^\dagger\hat{A})$ for the density matrix $\hat{\rho}$ of the ion-cavity system. Accounting for all relevant loss processes the total Lindblad operator can be written as

$$\mathcal{L}[\hat{\rho}] = \kappa \hat{L}_a + \sum_i \left[\gamma_{ba} \hat{L}_{\sigma_{ba}^{(i)}} + \gamma_{ab} \hat{L}_{a\sigma_{ab}^{(i)}} \right] . \quad (2)$$

The rates $\gamma_{ab} = \gamma_{cb} g^2/\Delta^2$ and $\gamma_{ba} = \gamma_{ca}\Omega^2/\Delta^2$ describe incoherent transitions between states $|a\rangle$ and $|b\rangle$ due to spontaneous decay of the excited state $|c\rangle$ with γ_{ca} and γ_{cb} to the ground states $|a\rangle$ and $|b\rangle$, respectively. Both of these transitions can be strongly suppressed by choosing a large single-photon detuning Δ. The first term accounts for photon losses with a cavity decay rate κ.

We define the ground state of the system $|0\rangle$ as the state, where all ions are in $|a\rangle$. A long-range Ising interaction $J = J_0/N$ with an effective spin-spin Hamiltonian $H_s = J\sum_{i>j}^{N} \sigma_{bb}^{(i)}\sigma_{bb}^{(j)}$, leads to an anharmonic ladder of Dicke states $|n\rangle$ with frequencies

$$\omega_n = n\omega_{ab} + \frac{n(n-1)}{2} J, \quad (3)$$

as illustrated in Fig.1c.

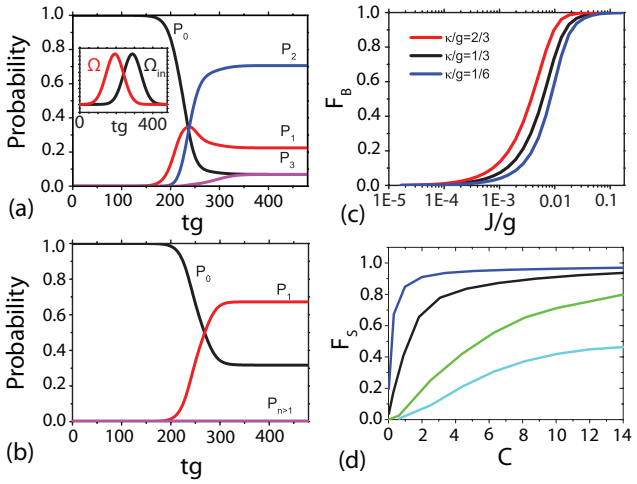

Figure 2: Interaction blockade: (a) Spin excitation probabilities P_i during the storage process with $J = 0$ and $\kappa/g = 1/3$. The inset shows the counter intuitive pulse sequence. (b) Spin excitation probabilities with $J/g = 0.01$ and $\kappa/g = 1/3$. (c) Blockade fidelity F_B versus spin-spin interaction constant J for various cavity loss rates $\kappa/g = \{2/3, 1/3, 1/6\}$ (red, black, blue) and a pulse length $Tg = 65$ (d)Storage fidelity for various input pulse Rabi frequencies $\Omega_{in}/\Omega = \{0.05, 0.1, 0.3, 1\}$ (light blue, green, black, blue) versus the cooperativity C. The other parameters are $\Delta = 10g$ and $\Omega = g$.

Single-photon generation In order to map the probe light onto ionic spin wave excitations, we consider a pulse sequence as shown in Fig.2a. By numerically solving the Master equation we obtain the probabilities $P_i(t)$ to find n ions in state $|b\rangle$.

Without spin-spin interaction ($J = 0$) an input pulse containing more than one photon flips more than one spin in the ion chain (N=3) as shown in Fig.2a. The situation changes by including the spin-spin interaction: using the same pulse sequence, only a single ion can be flipped Fig.2b and all higher excitations are blocked due to the anharmonic ladder of excited states. Thus, the ion-ion interaction induces a single photon nonlinearity with collectively enhanced light-matter coupling.

The quality of the nonlinear response can be characterised by a blockade fidelity depending on the probabilities including the spin-spin interaction $P_n^{(J)}$ and without ($P_n^{(J=0)}$) defined as

$$F_B = 1 - \frac{\sum_{n>1} P_n^{(J)}}{\sum_{n>1} P_n^{(J=0)}}. \qquad (4)$$

F_b is shown verus J and for various loss rates in Fig.2c. Remarkably above a certain critical interaction strength J the blockade is not affected by the cavity loss in striking difference to the typical photon blockade based on a Jaynes-Cummings nonlinearity, where the anharmonicity needs to exceed the cavity loss rate. This is even more surprising since in the present case the interaction J is the smallest energy scale in the system, orders of magnitude below κ, g, Ω_{in} and Ω. For typical experimental parameters, a small J of a few hundred kHz is sufficient for a full blockade.

The efficient mapping of a single photon out of a coherent pulse into the atomic ensemble is the second figure of merit for the proposed system. The storage fidelity is defined as $F_S = P_1$ after the pulse sequence assuming that the blockade fidelity is equal to one. The obtained numerically optimized storage fidelities versus the cooperativity $C = \frac{N\bar{g}^2}{\gamma\kappa}$, where $\bar{g} = 1/N \sum_i^N g_i$ for various input pulse intensities are shown in Fig.2d. For all input intensities the storage fidelity improves for increasing cooperativity. However, the maximum storage fidelity for large cooperativies saturates at different values related to the mean photon number of the incoming pulse. While F_s saturates below one for strongly attenuated input pulses, for large mean photon numbers the maximum storage fidelity approaches unity. In addition, the storage fidelity can be improved by placing many ions in the cavity due to the collectively enhanced light-matter coupling.

Summary and Conclusions We demonstrated that the synthetic spin interactions between laser-dressed ions can be used to control light on the single-photon level, despite being far smaller than typical light-matter coupling strengths and the photon-loss rate of the cavity. This permits enhanced light-matter coupling by working with ionic ensembles, while maintaining high optical nonlinearities mediated by ionic interactions. The proposed setting opens the door to a range of applications from nonclassical light generation to photonic quantum logic, and appears feasible with current experimental technology [10]

[1] D. E. Chang, V. Vuletić and M. D. Lukin, Nature Phot. **8** (2014) 685.

[2] C.-Y. Jin, R. Johne, M. Y. Swinkels, T. B. Hoang, L. Midolo, P. J. van Veldhoven and A. Fiore, Nature Nanotech. **9**, (2014) 886.

[3] F. Pagliano, Y. Cho, T. Xia, F. van Otten, R. Johne and A. Fiore, Nature Comm. **5** (2014) 5786.

[4] A. V. Gorshkov *et al.*, Phys. Rev. Lett. **107** (2011) 133602.

[5] A. V. Gorshkov, R. Nath and T. Pohl, Phys. Rev. Lett. **110** (2013) 153601.

[6] T. Peyronel, O. Firstenberg, Q.-Y. Liang, S. Hofferberth, A. V. Gorshkov, T. Pohl, M. D. Lukin and V. Vuletić, Nature **488** (2012) 57.

[7] R. Blatt and C. Roos, Nature Phys. **8** (2012) 277.

[8] D. Porras and J. Cirac, Phys. Rev. Lett. **92** (2004) 207901.

[9] K. Kim, M.-S. Chang, R. Islam, S. Korenblit, L.-M. Duan and C. Monroe, Phys. Rev. Lett. **103** (2009) 120502.

[10] B. Casabone, K. Friebe, B. Brandstätter, K. Schüppert, R. Blatt and T. E. Northup, Phys. Rev. Lett. **114** (2015) 023602.

2.11 Single-photon routing in interacting atomic ensembles

CALLUM MURRAY, THOMAS POHL

Introduction Rooted in our elementary understanding of light lies the notion that photons in vacuum do not interact with one another. Nevertheless, the implications that such interactions would have for both fundamental and applied science would be profound, and have ushered a new era of research into nonlinear optics at the ultimate quantum level, over the past years. It has recently emerged that the coherent coupling of photons to strongly interacting atomic Rydberg states provides high promise in this regard, with the central idea being to mediate photon interactions via the long ranged interactions between the matter constituents. Here we present a new approach to synthetic photon interactions which, in contrast to current strategies, enables high-fidelity photon processing, from dispersive quantum phase gates to dissipative all-optical transistors.

The basic idea The light matter coupling is based on so-called electromagnetically transparency (EIT) [1]. It emerges from a resonant two-photon coupling between two stable atomic states of a dense gas, and permits near lossless light propagation and complete coherent mapping between photons and matter excitations. The simplest protocol for realizing photonic interactions is achieved by first performing such a mapping to prepare a delocalised collective Rydberg excitation [2], after which a secondary gate photon is made to propagate through it. The stored spinwave then establishes a volume of influence in which the strong interactions preclude any further Rydberg excitation, effectively exposing a local two level medium for the propagating photon [3]. For an off-resonant single photon coupling, the stored spinwave then predominantly imprints a dispersive phase shift on the gate photon, whilst in the resonant regime it causes strong absorption. The usefulness of both effects for photon processing depends on the optical depth, OD_b, of the interaction volume.

In the off-resonant regime a high-fidelity gate operation typically requires such large values of OD_b (Fig.2) that are difficult to achieve in experiments and lead to additional decoherence effects [4]. On the other hand, the interaction-induced absorption in the resonant case can find use as an all-optical transistor in which a single control photon can extinguish a large number of gate photons [3, 5], as demonstrated in recent experiments [4, 6, 7]. Yet, its utility for performing quantum operations is limited. While a true quantum transistor entangles the state of the spinwave with that of the output field, dissipative interactions cause projective measurements of the spinwave state and, thus, yield a classical photon switch. Moreover, the scattered light provides spatial information on the stored spinwave [5], resulting in strong decoherence that prevents its subsequent read-out.

A new approach to Rydberg quantum optics The root of these problems lies in the fact that the optical nonlinearities in this conventional setting are reliant on the *breaking* of EIT conditions, which is inevitably accompanied by dissipation, ill-suited to coherent quantum processing. To address this shortcoming, we consider a new approach towards photonic quantum logic based on the interaction-induced reflection of light. Our scheme leverages on the *modification* of EIT conditions, rather than breaking them, to a yield a highly coherent optical nonlinearity.

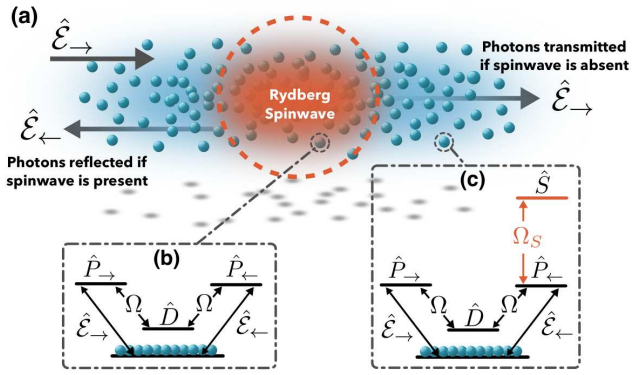

Figure 1: (a) Photon routing is achieved by reflecting photons off of a stored Rydberg spinwave stored in a cold atomic gas. Panel (c) shows the level scheme of the ensemble atoms for vanishing Rydberg interactions, and (b) shows how this is modified within the interaction volume of a stored spinwave due to strong van der Waals interactions between the propagating Rydberg state $\hat{S}$ and the stored Rydberg excitation. Describing this system in the Heisenberg picture, $\hat{P}_{\rightleftarrows}$ are polarisation coherences, $\hat{D}$ and $\hat{S}$ are ground state and Rydberg spinwave coherences respectively and Ω and Ω_S are classical fields coupling these various modes.

The underlying idea is to enable the coherent backscattering of a photon in the mode $\hat{\mathcal{E}}^\dagger_\rightarrow$ into a reverse propagating mode $\hat{\mathcal{E}}^\dagger_\leftarrow$ conditionally on the presence of a stored Rydberg spinwave. The schematic of this setting, along with the proposed level structure, is shown in Fig. 1. The two quantum light fields couple the atomic ground state to two low-lying states, whose collective excitations in the gas are described by the Bosonic operators $\hat{P}_\rightarrow$ and $\hat{P}_\leftarrow$. These in turn are coupled by a classical field (Ω) to another hyperfine ground state ($\hat{D}$), forming a double-Λ system shown in Fig. 1b. Finally $\hat{P}_\leftarrow$ is coupled to a high-lying Rydberg state ($\hat{S}$),

such that the effectiveness of this coupling can be modified by the strong van der Waals interaction of $\hat{S}$ with the spinwave.

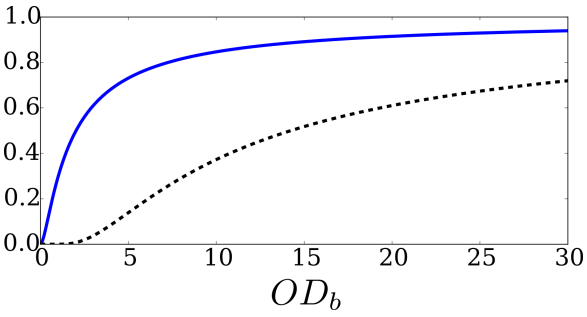

Figure 2: The fidelity of reflection (solid line) as compared to the fidelity of a dispersive $\pi-$phase gate based on conventional Rydberg EIT (dashed line) as a function of the optical depth of the medium per blockade radius.

Rydberg spinwave absent – In the absence of a stored spinwave, photons propagate through the medium unimpeded. The mechanism behind this transmission can be understood in terms of the following simple argument. Under strong driving of the Rydberg transition (Fig.2c), the two-level subsystem formed by $\hat{S}$ and $\hat{P}_{\leftarrow}$ splits into a doublet of light shifted states. As it transpires, the counter-propagating fields $\hat{\mathcal{E}}_{\rightarrow}$ and $\hat{\mathcal{E}}_{\leftarrow}$ then exactly decouple as a direct manifestation of destructive interference between excitation pathways involving the two light shifted states. Consequently, the photon mode $\hat{\mathcal{E}}^{\dagger}_{\rightarrow}$ forms a dark state polariton $\hat{\Psi}_0$ involving $\hat{D}$ that is transmitted through the medium with high fidelity.

Rydberg spinwave present – In the presence of the stored spin wave its interaction with $\hat{S}$ suppresses this effect, leading to the coherent generation of photons in the mode $\hat{\mathcal{E}}^{\dagger}_{\leftarrow}$. Importantly, the proposed coupling scheme still promotes a dark state polariton $\hat{\Psi}_1$, now involving $\hat{D}$ as well as $\hat{\mathcal{E}}_{\rightarrow}$ and $\hat{\mathcal{E}}_{\leftarrow}$. Most crucially though, the motion of this polariton is governed by a quadratic dispersion, akin to that of a stationary massive particle. This lack of linear dispersion prevents photons from traversing the interaction region, and ultimately results in their coherent backscattering via the intermediate formation of the stationary mode $\hat{\Psi}_1$. This setting, hence, realizes an effective repulsive interaction between the spinwave and incoming photons, and thereby permits routing of multi-photon states with very low loss.

By avoiding the immediate processing of photons within the medium (either dispersively or dissipatively), the developed single-photon router forms a universal building block for photonic quantum logic. The fidelity of such operations is ultimately given by the efficiency of reflection. As shown in Fig.2, its performance significantly supersedes that of the dispersive phase gate described above.

Moreover, the coherent nature of the conditional reflection has a much more favourable back-action on the state of the stored spinwave (Fig.3), as the effect of scattering-induced decoherence is strongly suppressed. It can, therefore, function as an all-optical quantum transistor in an experimentally attainable parameter regime.

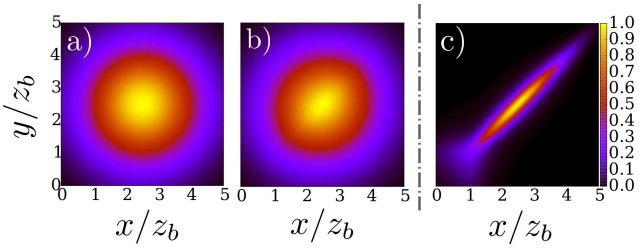

Figure 3: (a) Initial density matrix of a stored spinwave with a Gaussian spatial profile. Following the coherent reflection of a single photon, the final state of the spinwave remains largely unchanged, as shown by the final density matrix in b). This contrasts with the effect of dissipative nonlinearities associated with conventional Rydberg EIT that result in strong decoherence of the spinwave, as shown in (c).

Conclusion and outlook In conclusion, we have devised a new approach to quantum optical nonlinearities in strongly interacting Rydberg gases that is based on the interaction-induced reflection of light to serve as a universal building block for all-optical quantum information processing. While we have focussed here on the simple situation of a single spinwave and a single photon, the implications of the discovered mechanism extend beyond that of quantum computing. For example, the resulting repulsive photon-shield may lead to strong coherent two-photon scattering and suggests interesting many-body physics of photons to be explored in the future.

[1] M. Fleischhauer, A. Imamoglu and J. P. Marangos, Rev. Mod. Phys. **77** (2005) 633.

[2] Y. O. Dudin and A. Kuzmich, Science **336** (2012) 887.

[3] A. V. Gorshkov *et al.*, Phys. Rev. Lett. **107** (2011) 133602.

[4] S. Baur, D. Tiarks, G. Rempe and S. Dürr Phys. Rev. Lett. **112** (2014) 073901.

[5] A. V. Gorshkov, R. Nath and T. Pohl, Phys. Rev. Lett. **110** (2013) 153601.

[6] T. Peyronel, O. Firstenberg, Q.-Y. Liang, S. Hofferberth, A. V. Gorshkov, T. Pohl, M. D. Lukin and V. Vuletić, Nature **488** (2012) 57.

[7] H. Gorniaczyk, C. Tresp, J. Schmidt, H. Fedder and S. Hofferberth, Phys. Rev. Lett. **113** (2014) 053601.

2.12 Characterization of attosecond pulses by inner-shell hole dynamics

JHIH-AN YOU, JAN MARCUS DAHLSTRÖM, NINA ROHRINGER

The development of attosecond light sources allows for pump-probe measurements of correlated electron dynamics, such as hole dynamics and autoionization processes, in atoms, molecules and solids. To provide an accurate time-zero in these experiments and to completely characterize the pulses in the time domain are long-standing challenges in attosecond physics. The streak-camera method [1,2] is a powerful tool for characterization of isolated XUV attosecond pulses by analyzing photoelectrons by a phase-locked IR laser field. However, in this kind of scheme based on above-threshold ionization (ATI), the IR field coupling with the ionic potential induces some additional phase shifts (giving rise to a response or delay of "time zero" in a pump-probe measurement), imprinted on the photoelectron spectrum, that affect the accuracy of the attosecond pulse characterization [3–5]. In the small kinetic energy region of wavepackets, this response time can be considerable, reaching hundreds of attoseconds. To overcome this obstacle, we investigate an alternative method which we refer to as STRIDER (Stimulation of Transitions in the Remaining Ion for Detuned Electron Release) [6].

In STRIDER, we spectrally shear the photoelectrons using two coherent XUV fields that stimulate hole dynamics in the residual ion, following photoionization with the XUV attosecond pulse, as shown in Fig. 1 (a). The pump pulse $E_1(t)$ is broadband with central frequency ω_1 and unknown spectral phase $\phi_1(\omega)$ (or group delay $d\phi_1/d\omega$):

$$E_1(t) = \frac{1}{2\pi}\int d\omega |\tilde{E}_1(\omega)| e^{i[\phi_1(\omega)-\omega t]}. \qquad (1)$$

The goal of the STRIDER method is to reconstruct the unknown spectral phase of the attosecond pulse. The probe fields

$$\tilde{E}_{2/3}(\omega) = |E_0| \exp[i\phi_{2/3}]\delta(\omega - \omega_{2/3}) \qquad (2)$$

with frequencies $\omega_{2/3}$ are symmetrically red and blue detuned by $\delta\omega$ from the hole transition in order to introduce spectral shearing of the photoelectrons to lower and higher kinetic energies, respectively. Due to the interference of the two pathways brought by two probe fields, shown in Fig. 1 (a), the signal of the photoelectron spectra with an inner shell hole modulates with the relative phase between two probe pulses. It is important to note that we consider photoelectron spectra from particular ionic channels and assume that the state of the ion is measured in coincidence with the photoelectron. Our theoretical calculations are performed within 1D time-dependent configuration interaction singles (TDCIS) for the wavepacket propagation [7] and the time-dependent surface flux (t-SURFF) method for calculating the photoelectron spectra [8]. Here, we take the long lived 2s–2p transition of neon atom (26.9 eV) as an example. Fig. 1 (b) and (c) show the photoelectron spectra with outer (2p) and inner (2s) hole in the residual ion. The two narrow peaks (2,3) in Fig. 1 (b) are due to the absorption of the pair of probe fields with photon energy $\omega_{2/3} = 26.9 \pm 1$ eV by the outer-valence electron and the broad peaks (1,1′) are due to the absorption of the XUV attosecond pulse with central energy $\omega_1 = 68$ eV. Other peaks $(2, 3, \mathrm{S}+, \mathrm{S}-, \mathrm{P}^2, \mathrm{P}^{2\prime}, \mathrm{P}^3)$ are due to high-order interactions. In the following analysis, we only focus on the peak (S+), that originates from the pathway of photoionization from the 2p orbital by the XUV attosecond pulse, followed by absorption of a probe photon that induces a transfer of the hole to the 2s orbital.

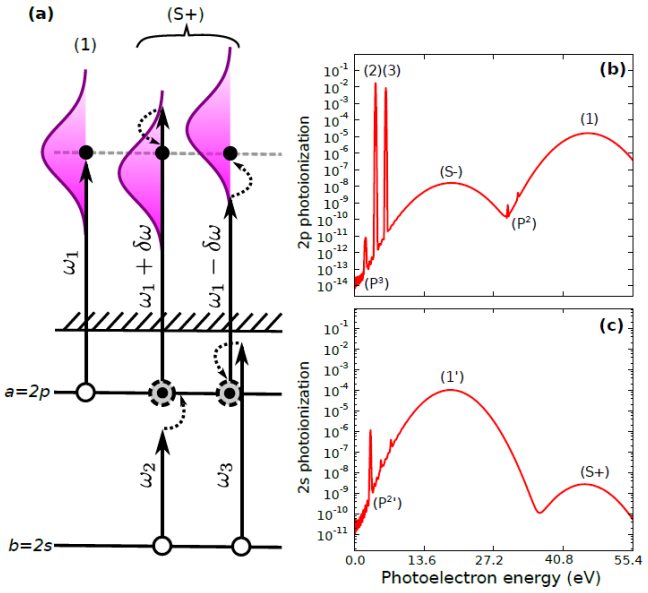

Figure 1: **Overview of STRIDER scheme:** (a) Photon diagram for: (1) Replica of attosecond pulse from outer valence, $a = 2p$; and (S+) spectrally sheared replicas by stimulated hole transitions leading to a hole in the inner valence, $b = 2s$. (b) Outer-valence photoelectron spectrum. (c) Inner-valence photoelectron spectrum.

The photoelectron spectra with an inner shell (2s) hole in the residual ion as a function of the kinetic energy and the relative phase $\phi_{23} = \phi_2 - \phi_3$ of the probe pulses is shown in Fig. 2 for (a) a Fourier limited pulse, $\phi_1(\omega) = 0$; (b, c) a quadratic phase dependence $\phi_1(\omega) = \alpha(\omega - \omega_1)^2$ with $\alpha = 10$ and 100; and (d) a cubic phase dependence $\phi_1(\omega) = \beta(\omega - \omega_1)^3$ with $\beta = 100$. To reveal the probe-phase dependent modulation, the spectra are normalized along the vertical

axis by their maximal value (Fig. 2 (e)-(h)). The evolution of the maximum for at a given kinetic energy is represented by a dashed line and follows the equation $\phi_{23} = 2\delta\omega\tau_1^{\mathrm{GD}}(\omega) + \text{constant}$. The group delay τ_1^{GD} can therefore be directly extracted by fitting the dashed line by the equation. We get the retrieved parameters $\alpha = 0.01$, 9.95, 99.4 and $\beta = 99.1$, in excellent agreement with the actual values.

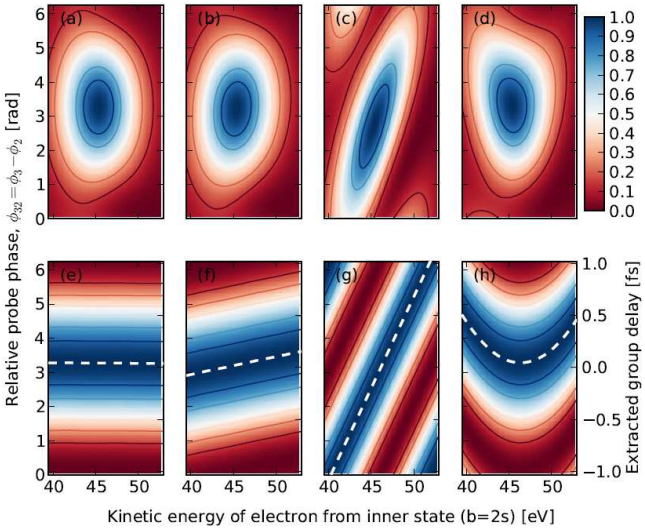

Figure 2: **Delay-dependent modulations of the (S+) peak.** (a)-(d) normalized photoelectron peak [see (S+) in Fig. 1 (d)] as a function of the phase difference between probe fields for (a) unchirped pulse; (b, c) increasing linear chirp; and (d) quadratic chirp. (e)-(h) same as (a)-(d) but with normalization along the vertical axis to reveal the modulation over delay at each kinetic energy. The dashed white curve shows the sub-femtosecond group delay of the pump pulse with extracted (actual) phase parameters $\alpha = 0.01(0)$, $9.95(10)$, $99.4(100)$ and $\beta = 99.1(100)$.

To assess the accuracy of the STRIDER method for real 3D systems, we estimate the response time by lowest-order many-body perturbation theory in 3D [5, 9]. If the model is restricted to stimulated hole transition, as shown in Fig. 3 (c), the response time is independent on the kinetic energy shown by the dashed line in Fig. 3 (a). However, when the ATI processes shown in Fig. 3 (d) are included, the response time exhibits a linear drift on both final partial waves shown by circles and diamonds, respectively. The detection of an electron with momentum along the laser polarization axis exhibits a linear drift of 0.634 as/eV (black line). The short response time is explained by the low ATI yield, which is 2-3 orders of magnitude smaller than that of stimulates hole transition as shown in Fig. 3 (b).

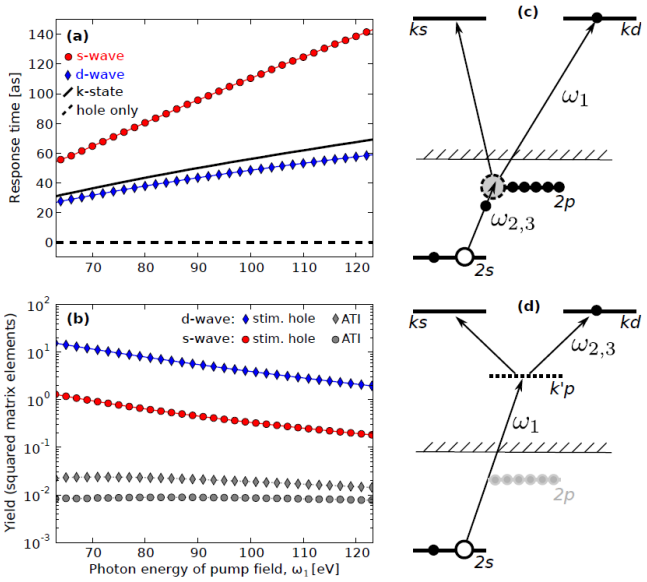

Figure 3: **Attosecond response time of STRIDER for neon atoms:** (a) Response time for photoelectron ejection along the polarization of the XUV field (black curve) from neon atoms calculated using lowest-order perturbation theory. The response time on the partial d and s waves are shown for comparison by diamonds and circles, respectively. (b) Yield (squared two-photon matrix elements) for stimulated hole transitions (red and blue) and ATI process (grey), where d and s waves are labeled by diamonds and circles, respectively. (c) Photon diagram for stimulated hole transition, $2p \to 2s$, after ejection of outer electron, $2p \to ks/d$. (d) Photon diagram for ATI process from the inner state, $2s \to k'p \to ks/d$. The probe field detuning is $\delta\omega = 1eV$.

In conclusion, we propose a new all XUV probe scheme – STRIDER – for characterization of attosecond pulses based on induced hole dynamics by two weak XUV phase-controlled, narrow-band probe fields. The method could find application at intense table-top XUV systems and new seeded x-ray free-electron lasers sources, to accurately determine the spectral phases of attosecond pulses. Compared to other methods, the reconstruction algorithm is straightforward. The response time of the scheme is small but needs correction for ATI contributions, if high accuracy of the spectral phase is requested. The proposed method can be extended to attosecond pulse trains. In this case, the demanding requirement of coincidence detection can be lifted which renders the method more experimentally feasible.

[1] J. Itatani, F. Quéré, G. L. Yudin, M. Y. Ivanov, F. Krausz, P. B. Corkum, Phys. Rev. Lett. **88** (2002) 173903.

[2] M. Michael, S. Gilbertson, S. D. Khan, Z. Chang, Opt. Express **18** (2010) 13006.

[3] M. Schultze et al.,Science **328** (2010) 1658.

[4] K. Klünder et al., Phys. Rev. Lett. **106** (2011) 143002.

[5] J. M. Dahlström, A. L´Huillier, A. Maquet, J. Phys. B At. Mol. Opt. Phys. A **45** (2012) 183001.

[6] J. You, N. Rohringer, J. M. Dahlström, submitted. (2015).

[7] N. Rohringer, A. Gordon, R. Santra, Phys. Rev. A **74** (2006) 43420.

[8] L. Tao, A. Scrinzi, New J. Phys. **14** (2012) 013021.

[9] J. M. Dahlström, E. Lindroth, J. Phys. B At. Mol. Opt. Phys. A **47** (2014) 124012.

High-brightness EUV laser in Xenon pumped by a soft x-ray free-electron laser

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Introduction X-ray free-electron lasers (XFELs) are the first short-wavelength x-ray sources that allow the study of nonlinear light-matter interaction in the x-ray spectral domain [2], with prospects of transferring coherent nonlinear optical pump-probe spectroscopy to shorter wavelengths. Stimulated x-ray emission and stimulated x-ray Raman scattering are the fundamental building blocks of these nonlinear pump-probe techniques and our group could successfully demonstrate these processes in Neon [3, 4] at an emission wavelength of 1.5 nm. A recent effort of our group is to extend stimulated emission processes to both shorter [5] and longer wavelengths, to explore the full spectrum of current day XFEL sources. Here, we report on amplified spontaneous extreme ultra-violet (EUV) emission following optical inner-shell pumping of Xenon gas with high-intensity femtosecond (fs) pulses of the FLASH free-electron laser in Hamburg.

Xenon, with a giant resonant-like structure of the photoionization cross-section of its 4d electronic shell at around 93 eV photon energy, was among the first targets on the quest for nonlinear x-ray matter interaction. At FLASH, this lead to the production of charge states up to 21^+ [6] by nonlinear sequential multiple ionization. Consequently, the FEL interaction leads to saturable absorption (bleaching) of transitions in neutral and highly charged Xenon ions and a rapidly-evolving plasma far from thermodynamical equilibrium. Here, we address the role of radiative decay of such a highly-excited and transient plasma.

Short-wavelength amplified spontaneous emission at 108.9 nm wavelength in Xenon following inner-shell ionization was first demonstrated in 1986 [7]. In that experiment, a plasma-based broad-band soft x-ray source of nanosecond duration was used to ionize the 4d shell in Xenon. The 4d hole decays by the Auger effect, resulting in different two-hole configurations in the n=5 shell of Xe^{2+}. The different final ionic channels result in a population inversion within the n=5 shell, that leads to lasing at a transition of 108.9 nm. The situation with presently available high-intensity FEL sources of fs duration is quite different. The high photon fluxes and consequently ionization rates of the 4d shell result in a sizable population inversion of 4d versus 5p electronic shell. Therefore, is it possible to amplify spontaneous emission on this transition, knowing that it only lives transiently on a fs timescale due to subsequent Auger decay? Can the original lasing emission in Xe^{2+} at 108.9 nm be quenched by subsequent photoionization of the 4d shell of Xe^{2+}? Or conversely, can this quenching lead to ultrashort pulses at 108.0 nm by ionization gating? Can lasing lines be observed in higher charge states?

Experimental results In our experiment, 100-fs pulses of the FLASH FEL were focused into a 3 mm long gas cell filled with Xenon at pressures ranging from 5 to 100 mbar. We chose two different photon energies for ionizing the Xenon target: 72.5 eV, i.e. just above the 4d ionization threshold of Xenon and below the 4d ionization threshold of Xe^{2+}, and 92 eV, around the peak of the giant 4d resonance, allowing for sequential multi-ionization up to high charge states in Xe. A high-resolution spectrometer ($\lambda/\Delta\lambda \approx 10^4$) was set-up in forward propagation direction of the FEL beam to observe both the transmitted FEL spectrum and the created line-radiation on a single-shot basis.

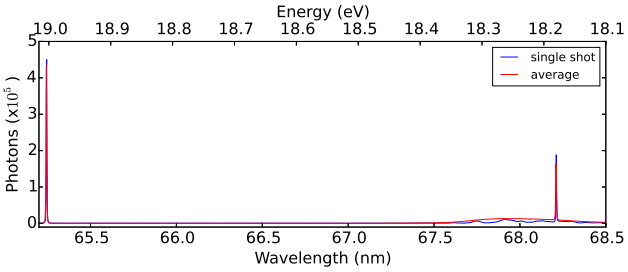

Figure 1: Single shot and averaged spectra obtained with 80 μJ pulse of 72.5 eV photon energy. We can observe the SASE in 4th diffraction order and two lasing transitions of Xenon.

For both FEL photon-energy choices, we identified 3 lasing emission lines of transitions within the n=5 shell of Xenon: at (65.35 ± 0.1) nm, at (68.29 ± 0.1) nm and at (108.9 ± 1.4) nm. The first two lines could be simultaneously observed on the detector for a fixed grating position (see Fig. 1), which significantly improved the wavelength determination: although their absolute wavelengths have ± 0.1 nm accuracy, the wavelengths difference is known within 0.05 nm, according to the accuracy of our calibration. Coincidentally, for an FEL photon energy of 72.5 eV, the line observed at 68.29 nm superimposes with the 4^{th} diffraction order of the SASE FEL emission. Fig.1 shows a single-shot spectrum and an average of the two emission lines along with the FEL spectrum. Despite our good spectrometer resolution, identifying the transition of the 65.35 and 68.29 nm line emission is difficult. We infer the charge states from the following considerations. The observation of the same three lines at different pump-photon energies is striking. At 72 eV, the production of charge states beyond Xe^{2+} is quenched by 4d inner-shell ionization [8], while highly charged ions are expected at 92 eV. This means that the observed emission lines of 65.35 and 68.29 nm most probably result from a single photo-ionization of

the 4d shell in Xenon. Due to correlation effects (shake-off, shake-up, double-Auger decay) ionization of the 4d shell can results in charge states larger than Xe^{2+}. We therefore restrict our transition level identification to charge states below Xe^{5+}, which however still results in a large number of possible transitions listed in the NIST database [9] between 65.2 and 68.4 nm. Constraining the wavelength difference between the two transitions to the observed (2.95 ± 0.05) nm further limits the choice of transitions(Table 2).

		Configurations	
Species	λ (nm)	Lower level	Upper level
Xe^{3+}	65.3695	$5s^25p^3\ ^2D^*_{5/2}$	$5s^25p^2(^3P)6s\ ^4P_{5/2}$
Xe^{2+}	68.2563	$5s^25p^4\ ^3P_0$	$5s^25p^3(^2D^*)5d\ ^3P^*_1$
Xe^{4+}	68.2573	$5s^25p^2\ ^3P_2$	$5s^25p(^2P^*)5d\ ^3F^*_3$
Xe^{2+}	68.2926	$5s^25p^4\ ^1D_2$	$5s5p^5\ ^1P^*_1$
Xe^{3+}	65.4765	$5s^25p^3\ ^2D^*_{3/2}$	$5s5p^4\ ^2P_{3/2}$
Xe^{2+}	68.2926	$5s^25p^4\ ^1D_2$	$5s5p^5\ ^1P^*_1$
Xe^{3+}	68.3180	$5s^25p^3\ ^2D^*_{3/2}$	$5s^25p^2(3P)5d\ ^4P_{5/2}$
Xe^{4+}	68.3866	$5s^25p^2\ ^3P_1$	$5s5p^3\ ^3S^*_1$
Xe^{2+}	108.8954	$5s^25p^3(^2D^*)5d\ ^1P^*_1$	$5p^6\ ^1S_0$

Table 1: Best candidates for spectral lines from NIST database that have wavelengths within the error of measurement. Each line at 65 nm can be matched with three lines at 68 nm.

Exponential amplification of the three emission lines was demonstrated by measuring the emission signal as a function of the incoming FEL energy, as can be seen in Fig. 2 for the line-emission at 65.35 nm. Varying the incoming FEl pulse-energy by a factor of three results in an increase of the emission signal by more than 4 orders of magnitude. Saturation of the lasing signal is clearly observed in both photon energy cases, with an onset occuring at around 55 μJ for 72.5 eV and 30 μJ for 92 eV photon energy. We did not observe any variation of the emission line width of the emission lines as a function of pressure or pulse energy. The bandwidth of the transitions are only a few meV, limited by the resolution of our spectrometer setup, suggesting that the corresponding radiative lifetimes are much longer than the FEL pulse duration. The lower limit of the lifetime for the 65.35 nm and 68.29 nm emission is 350 fs, and 750 fs for the 108.9 nm emission. Unlike in the case of the inner-shell photoionization laser in Neon [3], the stimulated emission in Xenon is not due to a transient population inversion in the photoionized plasma, but happens long after the passage of the FEL pulse through the target. It is therefore a last relaxation step, following cascades of photoionization and Auger-decay.

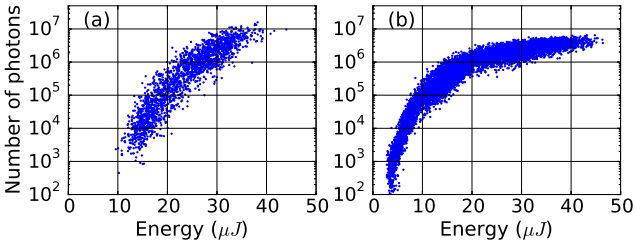

Figure 2: Intensity as a function of FEL incoming energy for the 65.35 nm lasing line with a) 72.5 eV and b) 92 eV photon energy

Conclusions Multiple-ionization following exposure of Xenon gas with tightly focused FEL pulses of ∼100 fs duration tuned above the 4d-ionization threshold in Xenon results in amplified spontaneous emission. Despite the high intensity, lasing emanates from relatively low charge states $\leq Xe^{4+}$ that are long-lived, created by one-photon ionization of the 4d shell and subsequent Auger-cascades. Ionization quenching of the lasing emission that would result in a line-broadening of the emission lines was not observed, suggesting that multiple-ionization of the Xenon target cannot be maintained over the whole length of the dense Xenon target. Due to the relatively small transition dipole moments, transient lasing between the 5p and 4d shell in Xe^+ is not observed, despite the large transient population inversion created in the target. In an upcoming experiment, collective radiative emission of Xenon clusters at solid densities will be studied, with a realm of potentially new effects and emission features.

[1] This work was performed in collaboration with: *Max Planck Institut für Kernphysik*: S. Bernitt, M. Blessenohl, H. Bekker, S. Dobrodey, J. R. Crespo Lopez-Urrutia, *Deutsches Elektronen-SYnchrotron*: C. Bomme, B. Erk, Z. Yin, D. Rolles, *Imperial College London*: A. Sanchez-Gonzalez, *Kassel Univ.*: P. Schmidt, A. Knie, A. Ehresmann, *Kansas State Univ.*: A. Rudenko

[2] N. Rohringer, Physik Journal **14** (5) (2015) 31. Nichtlineare Optik mit Röntgenlicht

[3] N. Rohringer et al., Nature **481** (2012) 488.

[4] C. Weninger et al., Phys. Rev. Lett. **111** (2013) 233902.

[5] U. Bergman, V. Yachandra, N. Rohringer et al., Stimulated X-ray emission in transition metal complexes, LCLS experiment LG89, July 9-13, 2015

[6] A. A. Sorokin, S. V. Bobashev, T. Feigl, K. Tiedtke, H. Wabnitz, and M. Richter, Phys. Rev. Lett. **99** (2007) 213002.

[7] H. C. Kapteyn, R. W. Lee and R. W. Falcone, Phys. Rev. Lett. **57** (1986) 2939.

[8] P. Andersen, T. Andersen, F. Folkmann, V. K. Ivanov, H. Kjeldsen and J. B. West, J. Phys. B **34** (2001) 2009.

[9] Kramida, A., Ralchenko, Yu., Reader, J. and NIST ASD Team (2014). NIST Atomic Spectra Database (version 5.2).

2.13 Autocatalytic droplets: A theory of centrosome assembly

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Centrosomes organize cell division Centrosomes are spherical protein assemblies in cells that are essential for cell division [1]. During cell division, a mitotic spindle forms, which segregates the duplicated chromosomes into the two daughter cells. The spindle is organized with the help of two centrosomes located at the spindle poles. A centrosome consist of centrioles which nucleate the assembly of a surrounding amorphous pericentriolar material (PCM). While the structure of centrioles has been long known [2], little is known about the structure and dynamics of the PCM.

We propose that the centrosome is a liquid-like droplet that assembles in an autocatalytic process. Our theoretical study of centrosome dynamics is based on a combination of phase separation physics and non-equilibrium chemical reactions. The basic idea is that the centrosome is formed by material that is initially dissolved in the cytoplasm as form A that can be converted to droplet material B, see Fig. 1. We study centrosome nucleation and growth in comparison with quantitative experiments.

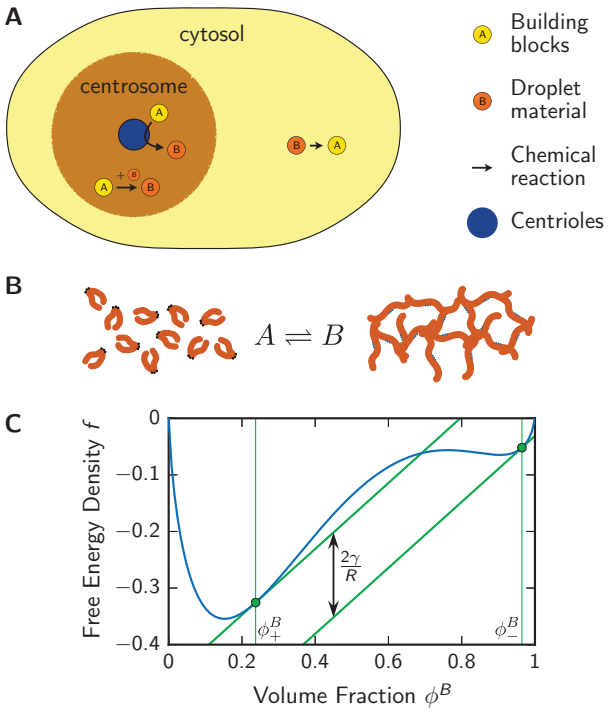

Figure 1: (A) Representation of a centrosome consisting of centrioles (blue) surrounded by a dense phase (orange) of droplet material (PCM). (B) Chemical transitions between soluble building blocks A and droplet material B control the droplet formation. (C) Schematic free energy density (blue line) as a function of the volume fraction ϕ^B of the droplet material. The Maxwell construction (green) determines the equilibrium volume fractions ϕ_-^B and ϕ_+^B, respectively inside and outside the interface with surface tension γ and curvature R^{-1}.

Physical description of centrosomes as active droplets Phase separation of the droplet material B from the cytoplasm leads to droplets bounded by sharp interfaces. We use an effective droplet description, where the interface is characterized by concentration jumps. The concentrations that coexist inside and outside of the interface follow from the local thermodynamics by a Maxwell construction, see Fig. 1C. This condition is equivalent to the condition of equal chemical potentials inside and outside the droplet interface. Furthermore, the pressure difference across the interface obeys a Laplace law.

We have shown that the chemical conversion between droplet material B and soluble building blocks A is described by the chemical reactions [3]

$$A + B \xrightarrow{k} 2B \tag{1}$$

$$B \xrightarrow{k_{BA}} A\,. \tag{2}$$

The reaction (1) describes the autocatalytic production of droplet material, while the first-order reaction (2) accounts for the turnover of droplet material to soluble building blocks. The autocatalytic reaction implies that droplets grow in an autocatalytic process and promote their own growth. Such autocatalytic droplets need a preexisting droplet to grow and spontaneous nucleation is thus strongly suppressed. In the case of centrosomes, this nucleator is the centriole. In order to nucleate centrosomes, the centrioles possess an enzymatic activity to catalyze the reaction $A \to B$ on their surface. We call this property centriole activity. Centrosome nucleation is therefore a chemical droplet nucleation process.

We introduce the volume fractions ϕ^A and ϕ^B of centrosome material in forms A and B, respectively. Inside and outside of a droplet, they obey the reaction-diffusion equations

$$\partial_t \phi^A = D_A \nabla^2 \phi^A - k\phi^A\phi^B + k_{BA}\phi^B \tag{3a}$$

$$\partial_t \phi^B = D_B \nabla^2 \phi^B + k\phi^A\phi^B - k_{BA}\phi^B\,, \tag{3b}$$

where D_A and D_B are the diffusivities of the components A and B. The chemical reactions given in Eqs. (1)–(2) are captured by the reaction terms. The diffusive flux $j^B = -D_B\nabla\phi^B$ of droplet material drives droplet growth. The dynamics of the droplet radius R can be described by

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \frac{j_-^B - j_+^B}{\phi_-^B - \phi_+^B}\,, \tag{4}$$

where ϕ_-^B and ϕ_+^B denote the volume fractions at the interface inside and outside of the droplet and j_-^B and j_+^B are the associated diffusion fluxes.

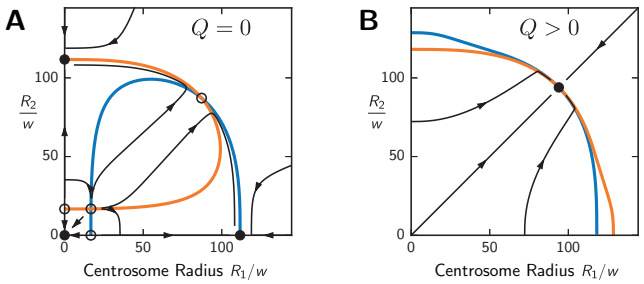

Figure 2: Behavior of two autocatalytic droplets as a function of their radii R_1 and R_2 normalized by the interface width w. The black arrows indicate the temporal evolution of the radii. The blue and orange lines are the nullclines, which indicate where the growth rate of droplets 1 and 2 vanish, respectively. Their intersections are stable (discs) or unstable fixed points (open circles). (A) Ostwald ripening for passive centrioles ($Q = 0$). (B) Suppression of Ostwald ripening for active centrioles (sufficiently large Q).

Centrosomes are thus chemically active droplets that are governed by a combination of the physics of phase separation, diffusion, and chemical reactions.

Active nucleation Centrosomes are nucleated by the catalytic activity of the centrioles, which leads to a small initial amount of droplet material on their surface. This catalytic activity must be strong enough to overcome the destabilizing effects of surface tension. Similar to classical droplets, chemically active droplets only grow if they exceed a critical size. In addition, the autocatalytic nature of growth further suppresses spontaneous nucleation. Using chemically active centrioles, the cell can therefore precisely control the number of formed centrosomes and suppress the nucleation of further droplets.

Autocatalytic growth After nucleation, centrosome growth is dominated by the autocatalytic reaction. Larger droplets thus accumulate more material per unit time and grow faster. Growth continuous until the surrounding cytosol is depleted of building blocks. The droplet eventually reaches a stationary state in which the production of droplet material is balanced by the back-conversion to soluble building blocks. This explains the sigmoidal growth curves that have been observed in experiments [4].

Suppression of Ostwald ripening Classical droplets undergo Ostwald ripening, which implies that two droplets of equal size are unstable and one grows at the expense of the other. We have shown that chemical reactions can suppress Ostwald ripening and that two active droplets of equal size can be stable [5]. Fig. 2 shows the dynamics of two autocatalytic droplets.

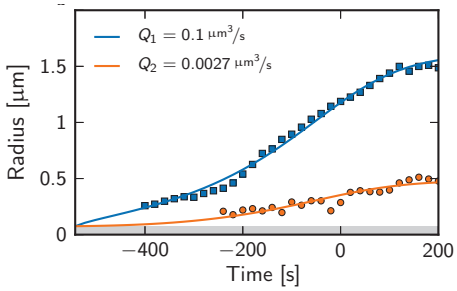

Figure 3: Centrosome radius in the theory (lines) compared to experimental data (dots) from a perturbation experiment with unequal centrioles. In the theory, we account for this by an unequal catalytic activity Q_1 and Q_2 at the centrioles.

In the absence of a catalytic core, two equal-sized droplets are unstable (A). However, this state is stable for sufficiently strong catalytic activity (B). Because of this suppression of Ostwald ripening two centrosomes of equal size can be stable in a cell.

Test of the theory by experiments Our theory accounts for the observed sigmoidal growth curve of centrosomes and the observation that centrosome volume scales with cell volume. Perturbation experiments in which centrosome number or cell size are altered can also be explained by our theory. A particularly interesting experiment is a perturbation where the centrioles of the two centrosomes are unequal. In this case, growth curves differ and the two centrosomes have very different sizes. We can account for this particular growth process in our theory by introducing different centriole activities for the two centrosomes, see Fig. 3. In this case, two centrosomes of different size can coexist in a stationary state.

Conclusions We propose a theory of centrosomes, which can account for their nucleation, growth kinetics, and steady states. Centrosomes are chemically active droplets that are nucleated by catalytically active centrioles. Their size is determined by the amount of building blocks provided by the cell and therefore the total volume of all centrosomes in a cell scales with cell volume. Our theory provides an example for the spatial organization of cells by phase separation. Centrosomes are membrane-less organelles that organize chemical reactions in space. There is a growing number of such liquid-like organelles currently being identified, which may be examples of active droplets governed by similar principles.

[1] M. Bornens, Science **335** 422 (2012).

[2] P. Gönczy, Nat Rev Mol Cell Biol **13** 425 (2012) .

[3] D. Zwicker, M. Decker, S. Jaensch, A. A. Hyman, F. Jülicher, Proc. Natl. Acad. Sci. USA **111** E2636 (2014).

[4] M. Decker, S. Jaensch, A. Pozniakovsky, A. Zinke, K. F. O'Connell, W. Zachariae, E. Myers, A. A. Hyman, Curr. Biol. **21** 1259 (2011).

[5] D. Zwicker, A. A. Hyman, F. Jülicher, in preparation.

2.14 Wave physics in vertebrate segmentation

DAVID J. JÖRG, FRANK JÜLICHER

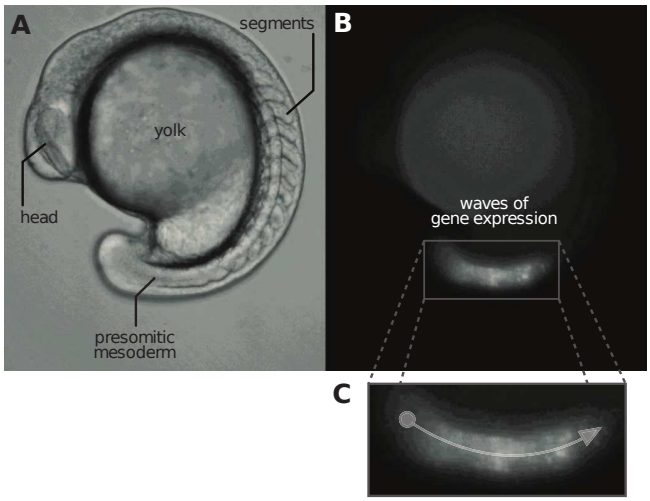

Figure 1: Precursors of vertebrate segments in a developing fish embryo [2]. New segments form sequentially from genetic waves generated in the unsegmented tissue (presomitic mesoderm). **A.** Bright-field microscopy image showing the embryo in a lateral view, clearly displaying the segmented body plan. **B.** The same embryo as in (A) in a fluorescent channel highlighting in a snapshot the wave pattern of oscillating gene expression. **C.** Waves are characterized by the one-dimensional intensity profile along a curved coordinate axis.

Vertebrate segmentation. In all vertebrate animals, including humans, the segmentation of the body plan proceeds during embryonic development in a process called *somitogenesis* [1]. During somitogenesis, the elongating body axis segments rhythmically and sequentially into *somites*, the precursors of vertebrae and ribs. Failure of proper segmentation, caused for instance by mutations, can give rise to birth defects such as congenital scoliosis. Somites are formed in characteristic time intervals from an unsegmented progenitor tissue, the *presomitic mesoderm* (Fig. 1). Segmentation is controlled by a pattern forming system based on coupled cellular oscillations in gene product concentrations. Coordinated oscillations across the segmenting tissue generate waves that travel from the posterior tip to the anterior end (Fig. 2). These wave patterns have been shown to occur in various vertebrates such as zebrafish, chick, mouse, frog, and snake [1]. Segment formation occurs upon arrival of a wave at the anterior end of the oscillating tissue, with one formed segment corresponding to each completed oscillation cycle at the anterior end. Segmentation is a highly dynamic process: in parallel with segment formation, the body axis elongates while at the same time the oscillating tissue shortens as cells leave the presomitic mesoderm at the anterior end to form somites.

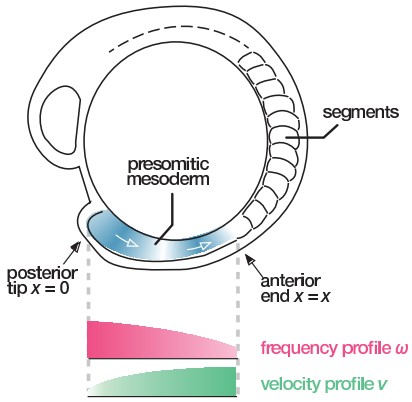

Figure 2: Schematic depiction of a zebrafish embryo during somitogenesis exhibiting wave patterns of gene expresssion (blue), together with the spatial profiles of intrinsic frequencies (red) and cell flow velocities (green).

Our ultimate aim is to understand the process of vertebrate segmentation from the single-cell level to the collective behavior of the multicellular system that constitutes the tissue-level patterning system. The question we address here is which principles determine the time intervals between the formation of successive segments. In close collaboration with the group of Andrew C. Oates, we have shown that this period of segmentation results from the collective behavior of many oscillating cells and is determined by wave dynamics in a dynamic background.

Segmentation as a patterning process. We quantified the spatiotemporal oscillation patterns in a transgenic zebrafish line, in which the oscillating gene *Her1* was fluorescently tagged (Fig. 1B). We used a wavelet transform to determine the spatiotemporal phase $\phi(x,t)$. This clearly revealed the motion of waves through the tissue and enabled quantitative analysis of the wave patterns [2] (Fig. 3A).

Continuum theory of oscillatory wave patterns. To understand the dynamics of these wave patterns and the physics underlying the segmentation rate, we developed a minimal continuum theory of vertebrate segmentation based on coupled phase oscillators in a dynamic medium that takes into account local growth and shortening of the oscillating tissue. Oscillations are described by their local phase $\phi(x,t)$. The dynamic equation for ϕ is given by [3–5]

$$\partial_t \phi + v\partial_x \phi = \omega + \frac{\varepsilon}{2}\partial_x^2 \phi \qquad (1)$$

Here, $\omega(x)$ is a spatial profile of intrinsic frequencies of the oscillators, $v(x)$ is the cell velocity, and ε is the coupling strength.

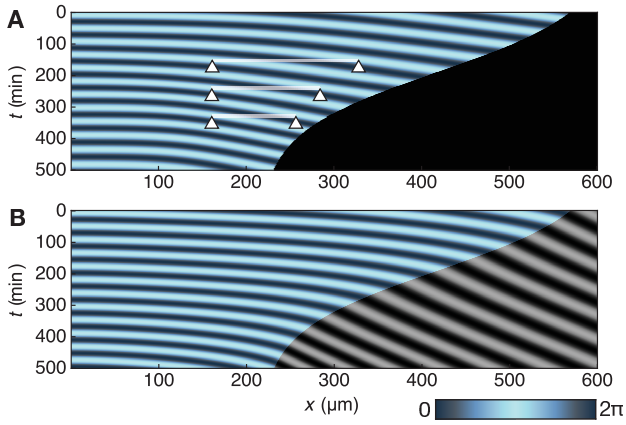

Figure 3: Wave patterns of gene expression. **A.** Experimentally determined average phase patterns in zebrafish embryos. Modified from Ref. [2]. **B.** Theoretical phase patterns obtained as a solution to Eq. (1) [5].

We consider a spatial profile of intrinsic frequencies ω corresponding to a gradual slowdown of the oscillations across the oscillating tissue and a position-dependent cell velocity field v (Fig. 2). In zebrafish, the oscillating tissue substantially shortens during segmentation (Fig. 3A). We determine the parameters of our theory such that it captures the dynamics of the wave patterns observed in experiments on developing zebrafish embryos (compare Figs. 3A and B). We find that the wave patterns completely determine the timing of morphological segmentation and the length of formed segments (Fig. 4). Our analysis revealed that the anterior end of the oscillating tissue moves into the waves, giving rise to a Doppler effect. This Doppler effect contributes to the rate of morphological segmentation. In addition, the wavelength of the wave pattern changes over time which additionally modulates the segmentation rate (white arrows in Fig. 3A).

Timing of segmentation. In our theory, the segmentation rate and the frequency of genetic oscillations are related by [5]

$$\Omega_{\mathrm{S}} \simeq (1+\bar{v}/v_0)(1-\Delta)\Omega_{\mathrm{P}} \qquad (2)$$

where Ω_{P} is the frequency at $x = 0$, $\bar{v} = |\mathrm{d}\bar{x}/\mathrm{d}t|$ is the shortening speed of the oscillating tissue, v_0 is the cell velocity at the anterior end, and $\Delta = \bar{v}(v_0\omega_0)^{-1}\int_0^1 \omega(\xi)(1+\bar{v}\xi/v_0)^{-2}\,\mathrm{d}\xi$ with $\Delta > 0$. In Eq. (2), the term $1+\bar{v}/v_0$ describes a Doppler effect. Here $\bar{v}$ corresponds to the speed of the moving observer (the anterior end) and v_0 is the speed of wave propagation.

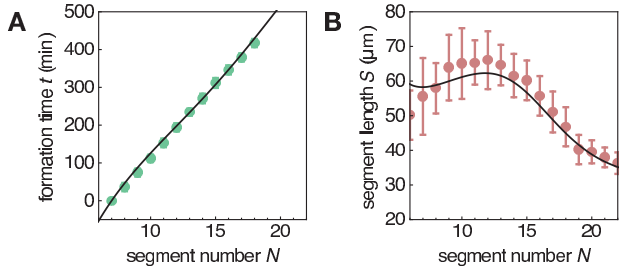

Figure 4: Dynamics of segmentation. **A.** Formation time t of segment number N determined in experiments (green) and from the theory (black). Formation time $t = 0$ corresponds to the formation of segment $N = 7$. Experimental data points are averages over 18 embryos. **B.** Segment length S at time of segment formation determined in experiments (red) and from the theory (black). Experimental data points are averages over 10 embryos.

In addition to the Doppler effect, a factor $1-\Delta$ appears that describes the frequency change due to the dynamically changing wavelength. This factor presents a contribution that opposes the Doppler effect, consistent with experimental observations [2]. The Doppler effect and this dynamic wavelength effect can be illustrated by considering a plane wave with frequency ω and wavenumber k, $u(x,t) = \mathrm{e}^{\mathrm{i}\omega t+\mathrm{i}kx}$. A Doppler effect is experienced by an observer moving with speed v relative to the wave. The observed frequency differs from the wave frequency by kv as

$$u(x_0+vt,t) = \mathrm{e}^{\mathrm{i}(\omega+kv)t+\mathrm{i}kx}\,. \qquad (3)$$

A dynamic wavelength effect is caused by a time-dependent wave number, $k(t) = k_0 + k_1 t$, leading to a position-dependent frequency,

$$u(x,t) = \mathrm{e}^{\mathrm{i}(\omega+k_1 x)t+\mathrm{i}kx}\,. \qquad (4)$$

A dynamic wavelength effect may also occur in other systems such as gases ionized by laser pulses [6].

Summary. Vertebrate segmentation is controlled by a complex pattern forming system that involves waves of gene expression sweeping through the segmenting tissue. We have shown that the changing tissue length introduces wave phenomena that can be discussed in the context of classical wave physics. This is in particular the Doppler effect but also the unconventional dynamic change of the wavelength that both contribute to determine the timing of segment formation. Our theory is able to quantitatively capture the features of the occurring wave patterns, the timing of segment formation, and the length of formed segments.

[1] A. C. Oates, L. G. Morelli, S. Ares, Development **639** (2012) 625–639.

[2] D. Soroldoni, D. J. Jörg, L. G. Morelli, D. L. Richmond, J. Schindelin, F. Jülicher, A. C. Oates, Science **345** (2014) 222–225.

[3] L. G. Morelli., S. Ares, L. Herrgen, C. Schröter, F. Jülicher, A. C. Oates, HFSP J. **3** (2009) 55–66.

[4] S. Ares, L. G. Morelli., D. J. Jörg, A. C. Oates, F. Jülicher, Phys. Rev. Lett. **108** (2012) 204101.

[5] D. J. Jörg, L. G. Morelli, D. Soroldoni, A. C. Oates, F. Jülicher, New J. Phys. **17** (2015) 093042.

[6] A. Couairon, A. Mysyrowicz, Phys. Rep. **441** (2007), 47–189
L. Berge, S. Skupin, R. Nuter, J. Kasparian, J.-P. Wolf, Rep. Prog. Phys. **70** (2007), 1633–1713

2.15 Force transmission in adhesion-independent cell migration

ANNA ERZBERGER, GUILLAUME SALBREUX

The mechanisms driving cell migration during processes such as development, inflammation and cancer are diverse. In the last 10-20 years, numerous studies have been conducted on cells migrating on flat surfaces. In these conditions, cell locomotion relies on extending cellular protrusions such as lamellipodia, and forming strong attachment points with the substrate [1]. The traction stresses involved have been measured to be in the range of several kPa, with single focal adhesions transmitting forces of several nN [2]. However, in complex environments such as live tissue, cells exhibit motile behaviour, which is independent of specific adhesions [3]. A mechanical understanding of such adhesion-independent movement types is lacking. Common characteristics observed in different cell types are bleb formation, actomyosin accumulation in the rear, and dependence on myosin ll. Our goal is to understand the physics of adhesion-independent cell migration in confinement. We use continuum mechanics to describe the mesoscopic behavior of the involved cytoskeletal materials, and compare our predictions to quantitative measurements combining live imaging and microfluidics. Experiments were performed on a suspended blebbing subline of rat cancer cells (Walker cells), which are unable to migrate on flat substrates but move effectively in confinement and do not form specific substrate adhesions [4]. When placed in microchannels, the cells display a well defined, static morphology while migrating, featuring a blebbing leading edge, a cylindrical cell body and a uropod-like tail (Fig 1A). Fluorescence microscopy reveals that both filamentous actin (F-Actin) and myosin II are enriched at the cell cortex and display a distinct concentration gradient increasing towards the cell rear (Fig 1A). Furthermore, the cells exhibit a steady cortical flow towards the cell rear during migration. Laser ablations of the cortex in migrating Walker cells revealed that cortical contractility at the cell rear is essential for migration: disruption of the cortical actin network at the rear of the cell body strongly decreases cell velocity, while movement remains unaffected by ablation in the cell front [4]. We developed a theoretical description of Walker cell migration, describing the actin cortex as a thin layer of active, viscous fluid (Fig 1B). Correspondingly, the tension $t^i{}_j$ in the cortex is a sum of a viscous part, proportional to the gradient of flow, and an active part, reflecting internal contractile tension:

$$t^i{}_j = \eta_s \left[v^i{}_j - \frac{1}{2} v^k{}_k \delta^i{}_j \right] + \eta_b v^k{}_k \delta^i{}_j + \zeta(c) \delta^i{}_j, \qquad (1)$$

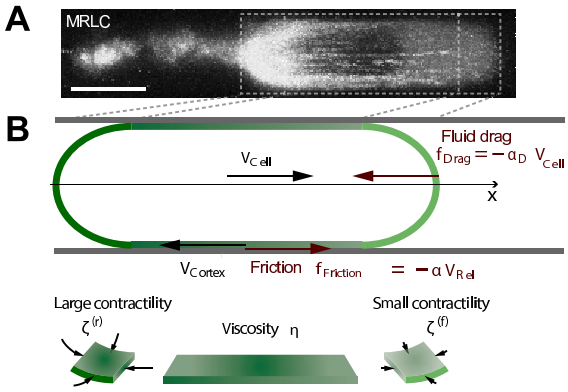

Figure 1: Theoretical description of adhesion-independent cell migration. **A**. Time-average (3min) maximum intensity projection of a migrating cell expressing fluorescently labelled myosin II (MRLC). On timescales exceeding the bleb life cycle, the cell shape is stationary. **B**. Schematic and parameters of the theoretical description of adhesion-independent cell migration. The cell cortex is represented by an axisymmetric surface with viscosity η, subjected to contractile active tension ζ, $[V_{\mathrm{Rel}} = V_{\mathrm{Cell}} + V_{\mathrm{Cortex}}]$.

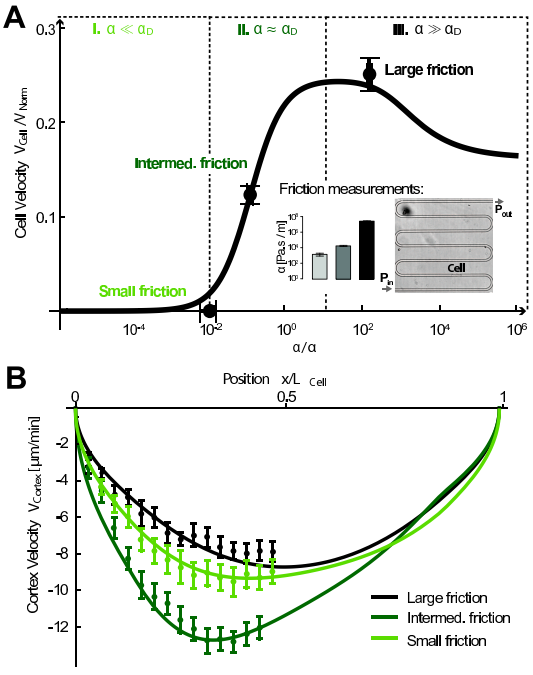

Figure 2: Role of substrate friction for Walker cell migration. **A**. Cell velocity as a function of friction (dots: experimental data (error: s.e.m.), solid line: fitted theoretical curve). Normalization, $V_{\mathrm{Norm}} = L(\zeta^{(\mathrm{r})} - \zeta^{(\mathrm{f})})/\eta$. Measurement of friction coefficients (inset). The cell-substrate friction coefficient was measured for three different channel coatings (BSA, F127 and BSA/F127-mixture) by applying a pressure to the channel entry and measuring the velocity of non-polarized cells (error bars represents s.e.m.). **B**. Cortical flow profiles in different friction conditions quantified using particle image velocimetry (PIV). Dots: experimental data; lines: fitted theoretical curves calculated for measured myosin gradients.

where η_s and η_b are the shear and bulk viscosities, and $v^i{}_j$ is the strain rate tensor. The active tension $\zeta(c)$ is generated by myosin II motor proteins and assumed to be proportional to their concentration c in the cortical layer. The polarised myosin distribution observed in cell migration thus translates into a gradient of active tension, which drives material flows within the actomyosin cortex, and deformations of the cell surface. We assume that the cell shape is confined to a cylinder in the region where it is in contact with the microchannel walls, and that the rear and front pole regions are free to take the shape satisfying force balance (Fig. 1B). Furthermore, we assume that cortical flows in the region in contact with the channel are resisted by a tangential friction force density, proportional to the velocity of the flow relative to the channel wall. A friction coefficient α characterizes this proportionality relation

$$f_{\mathrm{friction}} = -\alpha(V_{\mathrm{cortex}} + V_{\mathrm{cell}}). \qquad (2)$$

Additionally, an external force arises from the motion of the fluid medium present in the microchannel, which must flow around or through the cell, or be pushed forward as the cell moves. This is taken into account by introducing a fluid drag coefficient α_D

$$f_{\mathrm{drag}} = -\alpha_D V_{\mathrm{cell}}. \qquad (3)$$

We solve the resulting equations analytically, obtaining expressions for the cell shape, cell velocity and the cortical flow profile as a function of the mechanical parameters. We identify two separate effects enabling non-adhesive cell movement in confinement, both relying on a gradient of myosin II activity along the cell: (i) retrograde flow, which is resisted by a friction force, where the cell is in contact with the channel walls, pushing the cell forward, and (ii) contraction of the cell rear and expansion of the front, resulting in net movement of the cell. Both effects enable cell movement only if the friction between the cortex and the confining walls is sufficiently large. A threshold friction can be identified, above which cortical flows produce sufficient thrust to overcome the drag force resisting cell motion (Fig 2). To verify these predictions, we developed a microfluidic system to modify and measure friction in the microchannels. We generated three different friction environments by modifying the microchannel surface coatings, and measured the achieved friction coefficients by applying different pressures at the channel entry and measuring the resulting cell velocity (Fig 2A, inset). We proceeded to perform a detailed quantification of the myosin II distribution and of the cortical flow fields in the three different conditions and fitted these data with the theoretical flow curves (Fig 2B), thereby extracting the remaining unknown mechanical parameters of cell movement. The model equations could be fitted very accurately using a single set of three parameters (the cortex viscosity, the active tension drop along the cell, and the fluid drag coefficient) to all data from migration experiments in three different friction regimes [4]. Finally, we calculated the stresses exerted by Walker cells on the substrate during migration, and found that the local axial stresses did not exceed 1 Pa (Fig 3), and are thus considerably smaller than stresses exerted by adhesive cells, which have been measured ranging from tens to thousands of Pa (i.e. see [5]- [6]). Additionally, we computed the dipolar moment of the force distribution (Fig 3), and found that for blebbing Walker cells, the force dipole is positive, in contrast to all previously characterized crawling cells, for which the dipolar moment of the force distribution has been shown to be negative (reviewed in [7]).

In summary, while lamellipodial cells generate large pulling forces in the cell front to move forward, friction-based migration relies on weak thrust generated in the rear part of the cell. Consequences of these differences for elastic cell-cell interactions during crawling cell movement remain to be investigated.

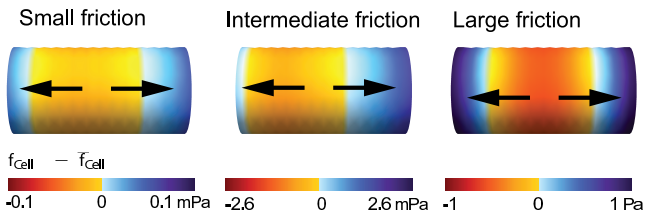

Figure 3: Distribution of forces (variation around the mean) exerted by migrating Walker cells on the channel wall. Cell migration direction is to the right, the force is oriented on average in the direction opposite to this motion, and the stress magnitudes are in the millipascal - pascal range, considerably smaller than stresses reported for cellular movement involving focal adhesions. Cells exert a positive, extensile force dipole on their surrounding environment (large friction $7.7\ 10^{-17}$N.m, intermed. $2.5\ 10^{-18}$ N.m and small $4.4\ 10^{-20}$ N.m).

[1] J. T. Parsons, A. R. Horwitz, M. A. Schwartz, Nat. Rev. Mol. Cell Biol. **11** (2010) 633-643.

[2] N. Q. Balaban, et al., Nat. Cell Biol. **3** (2001) 466-472.

[3] T. Laemmermann, et al., Nature **453** (2008) 51.

[4] M. Bergert, A. Erzberger, R. Desai, I. Aspalter, A. Oates, G. Charras, G. Salbreux, E. Paluch, Nat. Cell Biol. **17** (2015) 524-529.

[5] S. Munevar, Y. L. Wang, M. Dembo, Biophys. J. **80** (2001) 1744 - 1757.

[6] H. Tanimoto, M. Sano, Biophys. J. **106** (2014) 16 - 25.

[7] U. S. Schwarz, S. A. Safran, Rev. Mod. Phys. **85** (2013) 1327.

2.16 Mechanics of cyst formation in epithelia

SILVANUS ALT, GUILLAUME SALBREUX

Epithelial tissues are cellular monolayers which play an important role in the embryonic development and the adult lives of animals. Epithelial cells have an apicobasal polarity perpendicular to the tissue and are attached on their basal side to an extracellular matrix. Shape changes of epithelia play a crucial role in setting the organism shape, during the development and life or organisms.

The formation of cysts (Fig. 1) is an example of such a shape change. Cysts are regions of tissue which deform outside of the plane of the epithelium and are often present in human epithelial tumours [1]. We have investigated the physical mechanisms behind the formation of these structures in collaboration with the group of Anne Classen at LMU Munich. Experiments performed in the profilerating epithelium of the *Drosophila* wing disc as a model system allow to modify genetically a clone in the tissue, i.e. a group of neighbouring cells arising from division of one or several common mother cells. These experiments showed that clones for transcription factors (i) associated with cell fate specification and (ii) not normally expressed in the tissue results in their apical invagination (Fig. 1A). This suggests that juxtaposition of tissues with different fates is responsible for the formation of these anomalous epithelial structures.

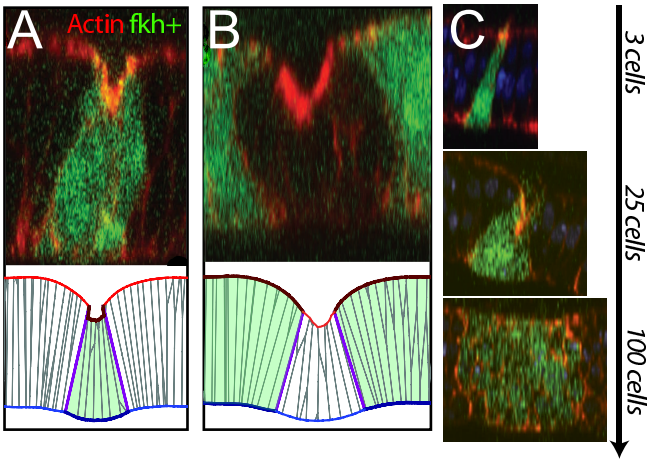

Figure 1: Cyst formation in epithelia. Mutant cells are labelled in green. A. Tissue cross-section showing indentation of a tissue clone into a cyst. B. Inverse wild-type cyst forming in a mutant tissue. C. Only clones of intermediate size form cysts.

Several experimental observations point to a possible mechanism for cyst formation: small mutant clones surrounded by wild-type cells form cysts, but small groups of wild-type cells surrounded by mutant cells also form cysts, and actin filaments within the actin cortex are recruited at the interface between mutant and wild-type cells (Fig. 1A-B). These experiments suggest that cyst formation is not a result of modified properties of cells within the cyst but results from modifications at the boundary between the cyst and the wild-type tissue. In addition, only clones of intermediate size containing between a few and 100 cells show significant out-of-plane deformations (Fig. 1C).

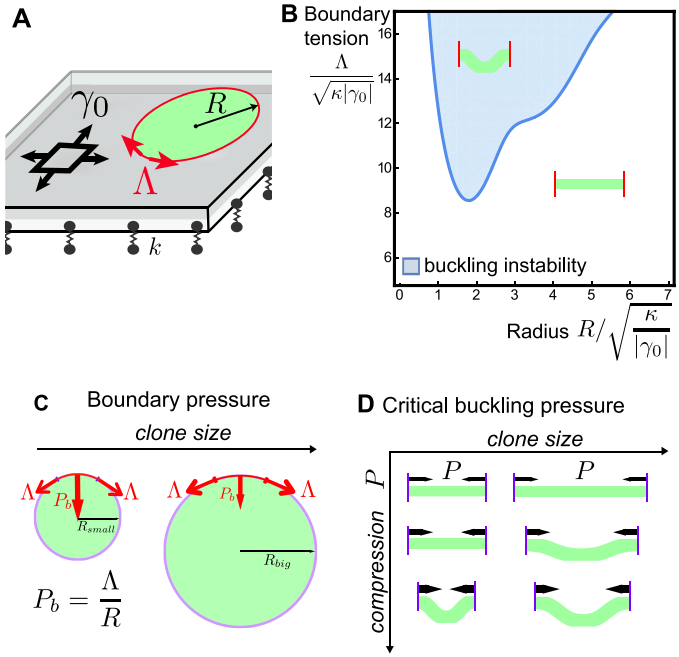

Figure 2: A. Schematic of the elastic model of cyst formation. B. Phase diagram of buckling instability of a clone. C, D. Two opposite mechanical effects results in size dependency of cyst formation.

We first reasoned that general mechanical principles may help understanding these observations. We use a generic continuum theory representing the tissue a thin elastic membrane with the effective mechanical energy (Fig. 2A)

$$W = \int dS \left[\frac{\kappa}{2} C^2 + \gamma_0 + \frac{k}{2} h^2 \right] \qquad (1)$$

with C the tissue curvature, κ a bending modulus, γ_0 the tissue surface tension, h the position of the tissue relative to a reference plane representing the basal extracellular matrix, and k an elastic modulus representing links between the tissue and the basal extracellular matrix. We assume that the formation of a clone leads to an increased line tension Λ at the boundary between the clone and the wild-type tissue. The resulting compression can then drive a buckling instability of the clone, depending on two simple physical effects: (i) the law of Laplace implies that the tissue compression in the clone is set by Λ/R with R the clone radius, such that smaller clone are under stronger compression

and are more susceptible to buckle; (ii) the resistance to buckling is higher for deformation on smaller length scale, such that smaller clones are less susceptible to buckle (Fig. 2C-D). The combination of these two opposite effects results in a phase diagram for the buckling of a clone where only clones of intermediate size buckle (Fig. 2B), in accordance with experimental observations.

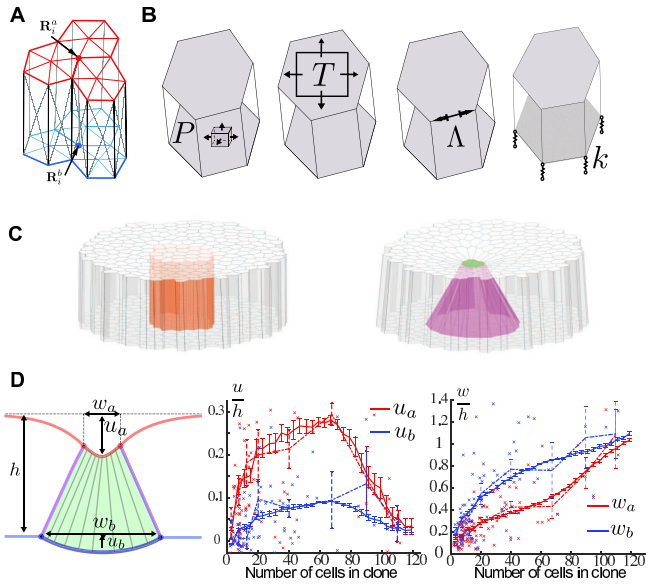

Figure 3: A. In the 3D vertex model, the tissue geometry is characterized by a set of apical and basal vertices. Planar triangles connecting the central and contour vertices define cell boundaries. B. Forces acting on a vertex are obtained by taking into accountt cell pressure. C. 3D vertex model of cyst formation. D. Quantification of cyst shape as a function of cyst size. Dotted line: experiments, continuous line: simulations.

To understand the tissue deformation quantitatively, we have developed a 3D vertex model allowing to simulate the detailed 3-dimensional cellular structure of the tissue. In the 3D vertex model, the tissue geometry is characterised by a set of apical and basal vertices (Fig. 3A). For each cell surface, an additional central vertex is introduced at the barycentre of the surface contour. Planar triangles connecting the central and contour vertices define cell boundaries. Forces acting on the vertices are obtained by introducing an effective mechanical work function W (Fig. 3B):

$$W = \sum_k T_k A_k + \sum_{i,j} \Lambda_{ij} l_{ij} - \sum_\alpha P_\alpha V_\alpha + \sum_b \frac{k}{2} z_b^2 - T_e A, \tag{2}$$

which takes into account (1) surface tensions T_k acting on cell surfaces k, both apical, basal and lateral, (2) line tensions Λ_{ij} acting on apical and basal edges connecting neighbouring vertices i and j, (3) the intracellular pressure P_α constraining the volume of the cell V_α, These forces arise from cytoskeletal structures at the cell surface that are contractile and generate tensions on the cell surface. In addition, (4) basal springs with modulus k resist the deformation of basal vertices with height z_b away from a reference plane representing the ECM, (5) external forces establish an overall tissue compressive stress T_e coupled to the tissue area A. The force f_i acting on vertex i is then obtained from differentiation of the mechanical work,

$$\mathbf{f}_i = -\frac{\partial W}{\partial \mathbf{x}_i}, \tag{3}$$

and the vertices positions are updated according to these forces.

The presence of a clone is then simulated by placing a number of cells N_c, corresponding to misspecified cells, within a cell population corresponding to wild-type cells (Fig. 3C) and then modified the line and surface tensions at the interface between misspecified and wild type cells. The resulting clone deformation is quantified by measuring the resulting maximum apical and basal indentation and the apical and basal clone width (Fig. 3D). We adjusted model parameters to account for the tissue shape before and after cyst formation. An excellent agreement with experimental measurements can be found for an increase in forces at the boundary of a factor ~ 3 compared to forces exerted in wild-type tissues (Fig. 3D). This factor is comparable to reported values of increased tensions at cellular junctions observed during normal development [2].

We have shown that a buckling instability driven by interfacial tension at the tissue boundary is responsible for cyst formation. Our conclusions are obtained by a combining a generic, continuum theory of tissue mechanics with a detailed description of three-dimensional cell shape of cells in a tissue. This approach will be useful to address the physics of other three-dimensional tissue deformations that occur during development [4].

[1] G. Bell, B. Thompson, Sem. Cell Dev. Bio., **28** (2014), 70.

[2] K. Landsberg, R. Farhadifar, J. Ranft, D. Umetsu, T. Widmann, T. Bittig, A. Said, F. Jülicher, C. Dahmann, Curr. Bio. **19** (2009), 1950.

[3] C. Bielmeier, S. Alt, V. Weichselberger, M. La Fortezza, H. Harz, F. Jülicher, G. Salbreux, A. Classen, submitted.

[4] L. Davidson, Trends in Cell Bio., **22** (2012), 82.

2.17 Clustering of *Neisseria gonorrhoeae* bacteria

WOLFRAM PÖNISCH, CHRISTOPH WEBER, VASILY ZABURDAEV

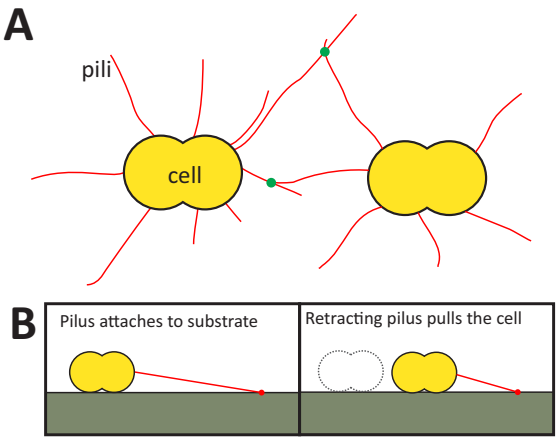

Figure 1: (A) Sketch of the diplococcus shaped *N. gonorrhoeae* bacteria with type IV pili emerging out of the cell membrane. The pili are able to bind to each other (green dots). (B) The tip of a pilus is able to attach to a substrate. The retraction of the pilus produces a pulling force acting on the cell which causes its displacement.

Pili-mediated colony formation of *N. gonorrhoeae* The bacterium *Neisseria gonorrhoeae* is the causative agent of the second most common sexually transmitted disease gonorrhea. An essential step during the infection process is the formation of microcolonies consisting of a few hundreds to a few thousands of cells. The formation of colonies is triggered by type IV pili, several μm-long and 6 nm thin semiflexible polymers that protrude out of the cell membrane [1]. The surface motility of the bacteria results exclusively from pulling forces generated by the retraction of multiple pili emerging from the cell membrane and adhering to a surface (i.e. epithelial cells) [2] (see Fig. 1). An analogous mechanism causes the aggregation of cells due to pili-pili-interactions. The molecular motor (pilT) involved in this process is one of the strongest motors known in nature and is able to produce forces that are of the order of 100 pN [3]. Pili of different cells are able to form bundles. The retraction of the pili causes attractive cell-cell-interactions that are sufficient to mediate the colony formation [4]. The characteristic cell division time (80 - 200 min. [5]) is however noticeably larger than the time scale of the assembly of colonies which starts after a few minutes. The central process that drives the agglomeration is the merging of two colonies.

Merging of *N. gonorrhoeae* microcolonies In collaboration with the lab of Nicolas Biais we analyzed the pili-mediated merging of two similarly-sized spherical microcolonies (see Fig. 2).

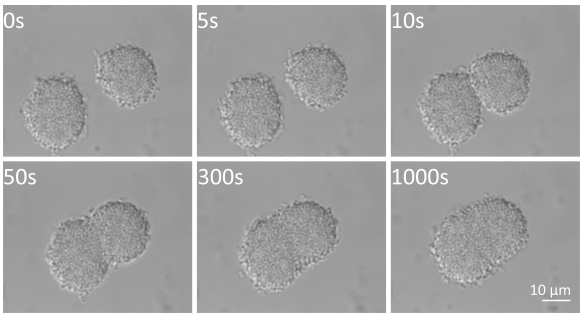

Figure 2: Merging of two equally-sized microcolonies. Each spheroid consists of roughly 4000 cells.

By fitting an ellipse to the shape of the two microcolonies and measuring its eccentricity (see Fig. 3) we are able to show that the merging can be characterized by a fast initial approach of the two colonies, which is followed by an extremely slow (multiple decades in time) relaxation to a sphere.

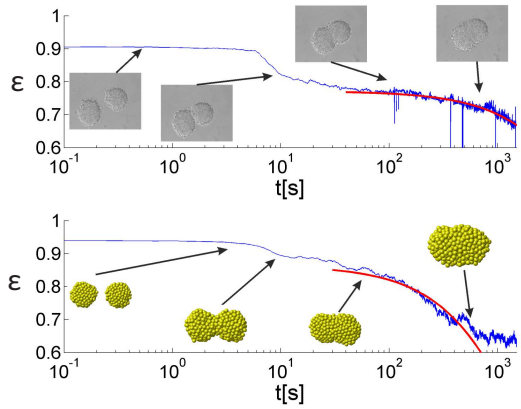

Figure 3: (Top) The binary shape of the colonies is used to compute the eccentricity ϵ of the colonies. In the beginning the two colonies are not interacting. After 10 s the two colonies attract each other and rapidly approach each other until they reach an ellipsoidal shape. The ellipsoid relaxes to a sphere with a characteristic time scale of $\sim$180 minutes. (Bottom) Eccentricity of the shape of two simulated microcolonies. The characteristic time of $\sim$30 minutes results from the fact that the initial colony size is smaller.

Model of the pili-mediated microcolony formation of *N. gonorrhoeae* We developed a particle-based simulation model to verify that the formation of microcolonies can solely be explained by pili-mediated cell-cell-interactions. Initially we used a simplified model where spherical cells attract each other via pili and repel each other due to soft excluded volume interactions. The pili are modeled as stiff rods emerging perpendicular from the cell membrane. This assumption is justified by having an average pili length of 1 μm and a persistence length of 5 μm [6]. Motivated by pili-substrate interactions the pili bind to the membrane of

neighboring cells. To incorporate pulling forces, we consider pili as hookean springs so that it is possible to compute the pulling forces of retracting pili acting on the cells. The retraction velocity v_r of the pilus is a function of the pulling force F, a process that is called stalling [7]:

$$v_r = \max\left[0, v_0 \cdot \left(1 - \frac{F}{F_p}\right)\right] \tag{1}$$

Furthermore the detachment rate of pili is a function of the force acting on the pili. Assuming that the pilus-substrate and pilus-membrane interaction points are chemical bonds, the detachment rates γ_s and γ_m are given by ($i = s, m$):

$$\gamma_i = \left[\frac{1}{t_i} \cdot \exp\left(\frac{F}{F_i}\right)\right] \tag{2}$$

This model is sufficient to reproduce qualitatively a similar behavior during the merging of microcolonies as seen during experiments (see Fig. 3).

The Layer-Bulk-Model In order to explain the fast initial approach and the slow relaxation of *N. gonorrhoeae* microcolonies during coalescence we propose the so called layer-bulk-model (see fig. 4). We assume that a colony consists of two regions:

- An inner bulk with weakly motile cells. The cells are caged and exposed to high pulling forces due to an increased number of interacting pili. The cells may even show solid-like behavior.
- An outer layer of highly motile cells. The thickness of this layer is comparable to the single cell size.

To validate this model we experimentally measured the mean square displacement (MSD) of single cells inside of a microcolony as a function of their position. We were able to show that cells inside of the bulk are strongly subdiffusive while the cells of the outer layer are more motile and weakly subdiffusive (see fig. 4).

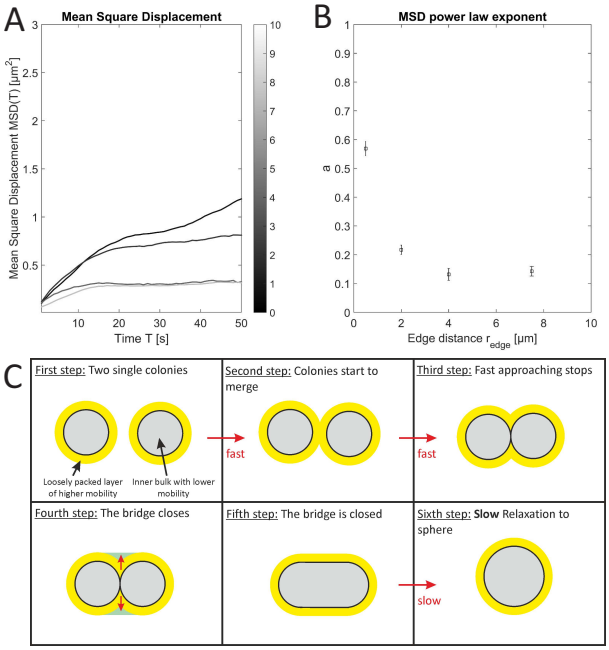

Figure 4: (A) By labeling a small fraction of cells inside of a microcolony we were able to track cells as a function of their position and compute their mean square displacment. The plots are color-coded as a function of their distance from the surface in μm, thus a black line corresponds to a surface cell while a grey line represents bulk cells. As one can see the mean square displacement is considerably larger at the surface. (B) By fitting a power law to the mean square displacements it was possible to compute the exponent which gives information about the diffusive behavior. The cells at the surface are weakly subdiffusive with an exponent around 0.6, the cells in the bulk are strongly subdiffusive with an exponent of 0.2. (C) The layer-bulk model: Two colonies attract each other due to pili-interactions until they start to collide. The fast approach will continue until the two bulk are in contact. The bridge of the colonies will close so that a ellipsoidal colony forms. This colony relaxes to a a sphere with a large characteristic time scale resulting from the bulk properties.

Perspective In this project we developed the first model that describes the pili-mediated assembly of microcolonies. We used a simplified approach to model the attractive pili-mediated interactions between cells. In the future we will consider the bundling of two individual pili and a realistic diplococcus shape of the cells. Furthermore we will apply the model to measure the MSD of individual cells as a function of their distance from the colony edge. Additionally we can apply our model to simulate and analyze the collective behavior of microcolony assembly on a substrate.

[1] L. Craig, M. Pique, J. Tainer, Nature Reviews Microbiology **2** (2004) 363-378.

[2] V. Zaburdaev, N. Biais, M. Schmiedeberg, J. Eriksson, A. Jonsson, M. Sheetz, D. Weitz, Biophysical Journal **107** (2014) 1523-1531.

[3] N. Biais, B.Ladoux, D. Higashi, M. So., M. Sheetz, PLoS Biology **6(4)** (2008) 907-913.

[4] A. Imhaus, G. Duménil, The EMBO Journal **33(16)** (2014) 1767-1783.

[5] M. Takei, Y. Yamaguchi, H. Fukuda, M. Yasuda, T. Deguchi, Journal of Clinical Microbiology **43(9)** (2005) 4321-4327.

[6] J. Skerker, H. Berg, PNAS **98(12)** (2001) 6901-6904.

[7] B. Maier, Soft Matter **9** (2013) 5667-5671.

2.18 The maternal to zygotic transition of zebrafish embryo.

JENS KARSCHAU, VASILY ZABURDAEV

Introduction DNA is the blueprint of all life on Earth and it is passed on from one cell generation to the next as an organism grows. Although each cell within an organism contains an exact copy of the DNA which originated in a single egg cell, not all of them perform the same function. This symmetry breaking is observed during early embryonic development when the cells change from a synchronous rhythm of division to an asynchronous one. For example, in zebrafish, this occurs at around the 10th division following egg fertilisation [3]. This decisive point in embryogenesis is referred to as maternal to zygotic transition; it is not only the point at which the cell cycle duration is perturbed, but is also marked by the activation of genome–transcription. Prior to the maternal to zygotic transition an embryo relies purely on the resources which the mother provided the egg with. Cells can rapidly synthesise their DNA, divide, and the embryo increases its cell number. At first those cells do not produce their own proteins by keeping DNA transcription repressed. As the number of cells (and so the total amount of DNA) increases, the number of proteins available to each cell decreases. This includes DNA-bound proteins, such as those which may repress transcription. This has lead researchers to suggest that as the repressors become diluted throughout the cells, gene–activators are able to bind and thus releases cells from genome–silencing [1] [2].

Robustness in terms of genome activation refers to the cell's capacity to buffer fluctuations driven by gene competitors, i.e. repressors and activators. We propose to analyse this robustness of the complex regulation of genome silencing and genome activation in vertebrate development. We test the hypothesis that differing concentrations of DNA-interacting proteins desynchronise an initially synchronously dividing cell population, and will investigate the consequences of competitor binding during DNA synthesis in a given cell. We first establish an activator–repressor model which explains genome activation. Activation results from a genome activator eventually winning the competition to bind with its preferred site on the DNA. In the long–term progression of the project we see many exciting extensions that will build on our model and collaboration with the Vastenhouw lab at MPI-CBG. Those points will include how cellular and nuclear geometry affect reaction rates, as well as a microscopic version of our competition model on the DNA basepair level.

The Activator-Repressor Model The traditional biological model of genome activation, which is depicted in Fig. 1(a) considers a highly abundant repressor of unknown origin [1]. At first, the repressor is present in excessive amount in the embryo, but as cells divide it binds to newly synthesised DNA. With some time, this generates a condition where there is no free repressor left in the embryo and the genome activates. It results from the DNA being free from repressors.

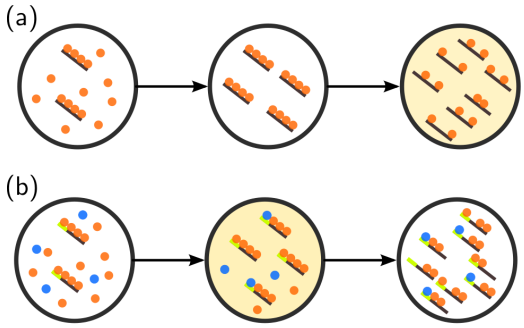

Figure 1: Models of genome activation. (a) The traditional model suggests a repressor (orange circles) of unknown origin. At the beginning it is present in excessive amounts in the embryo (large circle). As DNA (black line) is produced over time, repressors bind to it. Eventually, there is not enough repressor left to bind to all DNA and the genome activates (indicated by yellow shading). (b) Our proposed model suggests that besides a repressor, there is also an activator (blue circles). Activators only bind to their relevant sites on the DNA (green part of DNA). Similarly to the model in (a) repressors titrate out over time as the DNA amount increases. The model gives genome activation (2nd picture), which is prior to DNA unwinding (3rd picture) here.

Our collaborators in the Vastenhouw lab at the MPI-CBG recently identified nucleosomes to act as repressors in zebrafish embryos. Nucleosomes compact DNA to fit it into the nucleus, and at the same time this compaction hinders the DNA from being read. In vitro experiments performed with frog embryo extract also suggest this [2]. However, the eminent role of nucleosomes as repressors now renders the traditional model of genome activation invalid. If the traditional model were true, parts of the DNA had to unwind before genome activation can occur. This is, however, not observed in experiments.

This leads us to suggest a new revised model, and so far there does not exist any comprehensive analysis of the genome activation process. Our proposed model encompasses an activator and a repressor as shown in Fig. 1(b) and in more detail in Fig. 2(a). On one hand, activators can only bind to a few specific sites on DNA—corresponding to gene activation sites. On the other hand, repressors have uniform probability to bind anywhere on the DNA. We consider the exponential increase of DNA during the first dozen division cycles of an early embryo. The overall concentrations of

repressors and activators remain fixed, but the number available to an individual cell is halved with every division cycle.

Our model shows that initially DNA stays strongly repressed; yet as DNA replicates free repressors become sparse. This then allows for activators to bind to previously repressed sites and trigger genome activation. Whilst free repressors adsorb onto newly produced DNA substrate, the probability of an activator to eventually bind with its corresponding site increases. DNA increases exponentially, hence resulting in a sharp transition in Fig. 2(b). This is when the free nucleosome pool becomes low. Activators now have a chance to win the competition with nucleosomes and bind with most of their target sites. The fraction bound with activators is maximal and can trigger genome activation. It is only later in our model that the free nucleosome pool is fully depleted and DNA begins to unwrap.

We hypothesise that DNA unwrapping will not occur in the real biological system. Once activators bind to DNA, they will subsequently promote protein production. This will replenish the nucleosome pool to keep up with the rate of DNA production.

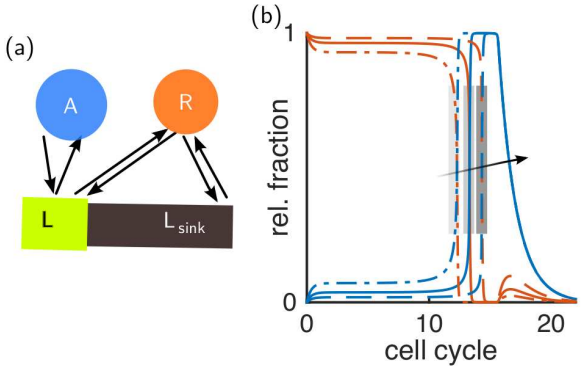

Figure 2: (a) The activator-repressor model for genome activation considers an activator (blue circle) and a repressor (orange circle) that stay in competition for DNA binding sites. Activators bind only to a particular piece of DNA: the transcription activation sites. Repressors bind to virtually anywhere along a DNA piece. (b) Variations of the initial conditions in repressor (orange line) numbers shift the sharp transition; so that activators (blue lines) eventually fully bind with their DNA sites. The grey colour code marks the point of transition as it occurs for increasing initial repressor amounts. Upon repressor addition (dotted line), genome activation occurs later compared to the zebrafish *wild–type* (solid lines) results. Depletion of the repressor (point dotted line) results in an earlier transition.

We use the model to make predictions that are in line with our experiments. A decrease in the initial number of repressors shifts the transition to genome activation to an earlier time point in Fig 2(b). If we instead start with increased repressor conditions (high levels of nucleosome forming proteins in the early embryo), we delay the onset of genome activation in Fig. 2(b). We can correlate our model predictions with preliminary experiments (data not shown) which indicate the same behaviour in the early zebrafish embryo. Transcription level measurements give insight when the DNA first becomes read. Furthermore, the Vastenhouw lab employs single molecule FISH to visualise individual mRNA transcripts (the product of DNA transcription), which in the long run will supplement our model with more data.

Conclusions The proposed model not only describes a mechanism for precise genome activation, but can also account for DNA still being compacted at the same time. The transition in our model from a repressed to an activated state is mainly driven by the amount of repressors initially present. To achieve a shift to one cell cycle earlier or later either requires halving or doubling nucleosome amounts compared to the reference *wild–type* number.

Future Directions We will advance the project via an extension of our existing simple deterministic model to a stochastic one. We will use a car–parking type model from statistical physics, where we will test the distribution of nucleosomes and activators numerically as well as calculate it analytically. Depending on the affinity for nucleosome binding a particular DNA region, the model will predict the likelihood for that particular region to become activated—a prediction which can also be tested in experiments. Ultimately, a combination of the parking model and a dynamic model of DNA replication will further our understanding of how not yet occupied DNA sites become bound by nucleosomes.

A further route of investigation is the process of nuclear import of repressors. The nucleus, which encloses the DNA, is much smaller than its surrounding cytoplasm. Nucleosome–forming proteins must be constantly pumped in to keep up with the demand from the ever growing DNA substrate. As long as this pumping rate is maximal, we can use constant binding rates. Some preliminary data, however, suggests that nuclear import slows down towards the maternal zygotic transition. At the same time the nuclear size changes disproportionally to the cytoplasmic one. This bears an excellent opportunity for us to extend the activator repressor model, and investigate effects arising from nuclear transport.

[1] J. Newport, M. Kirschner, Cell. **3** (1982) 675–686.

[2] A.A. Amodeo, D. Jukam, A.F. Straight, J.M. Skotheim, Proc. Natl. Acad. Sci., **112**(10) (2015) E1086–E1095.

[3] D.A. Kane, C.B. Kimmel, Development. **119** (1993) 447—456.

2.19 Dynamics and predictability of attention in social media

JOSÉ M. MIOTTO, EDUARDO G. ALTMANN

Introduction When social-media items are abundant, the public attention is the scarce factor for which they compete [1]. Success in such economy of attention is hard to predict and very uneven: the distribution of attention among different items typically shows heavy tails, which resemble income distributions and are an outcome of a complex dynamics, as illustrated in Fig. 1. Here we investigate how unexpected the appearance of viral items (extreme events) is [2] and we model the dynamics of attention in online systems [3], two problems with theoretical and commercial interest.

Digital records of human activity bring new perspectives to this traditional field (that goes back to the work of Pareto in the XIX century). We collected different datasets in which items compete for attention (e.g., online scientific publications and discussion groups). Here we report mainly the results in our largest dataset: 16.2 million time series of a video-sharing website (YouTube), for which X_t is the amount of views a video received in the t first days and dX_t is the amount of views received exactly on day t. The large amount of data allow us to obtain an unprecedent quantification of fluctuations around expected values, an evaluation of the accuracy of the prediction of individual items, and a mechanistic understanding of the dynamics.

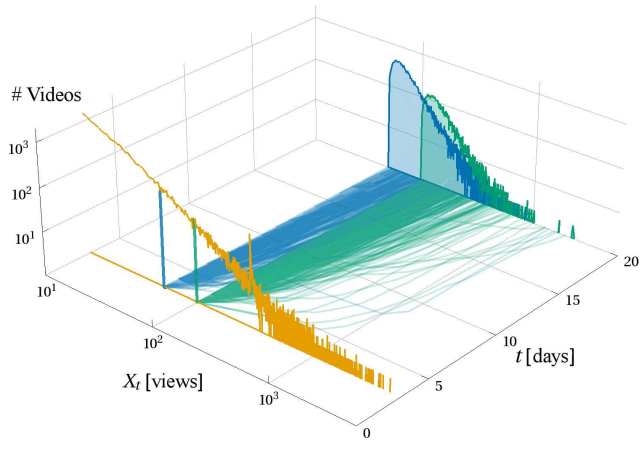

Figure 1: Evolution of videos' views. The distribution of views at day $t = 3$ after publication shows fat tails (in orange). Videos with the same number of views at early times ($X_3 = 50$ in blue and $X_3 = 100$ in green) show radically different behaviour in the future (distributions are shown at $t = 20$).

Dynamical model A natural choice to describe the evolution of attention as a dynamical system is to use a stochastic differential equation [4]

$$dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dW_t, \qquad (1)$$

where dW_t is a Wiener process (with normal distribution $\mathcal{N}(0, \sqrt{dt})$), μ is the average of new views and represents the deterministic part of the evolution, and the fluctuation term σ accounts for the size of external, sampling, and unknown effects.

We infer $\mu(X_t, t)$ and $\sigma(X_t, t)$ in Eq. (1) from empirical approximations of the distribution $P(dX_t|X_t)$. From the average of $P(dX_t|X_t)$ we obtain $\mu(X_t, t) \sim a_t X_t$ with a_t decaying in roughly one week. This linear dependence in X_t indicates the effect of proportional growth – known as Gibrat's law, rich-get-richer mechanism, Matthew effect, or preferential attachment– and is often considered an explanation for the onset of fat-tailed distributions. The estimation of $\sigma(X_t, t)$ from the second moment of $P(dX_t|X_t)$ show again a linear relation $\sigma(X_t) \propto X_t$ consistent with previous proposals in the context of Gibrat's law. However, we observe that the estimation depends on the sample size. Figure 2 shows a more detailed analysis of $P(dX_t|X_t)$ that reveals that the data is well described by a Lévy-Stable distribution and is not compatible with the expectation from Eq. (1) with a general dependence $\sigma(X_t) \propto X_t^{\beta}$.

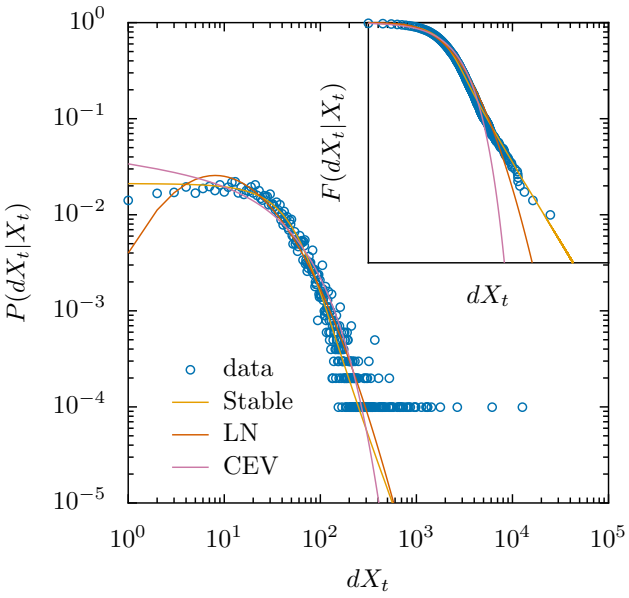

Figure 2: Distribution $P(dX_t|X_t)$ for videos with $X_{t=3} \approx 500$. Inset: complementary cumulative distribution. The three solid lines indicate the fits of the Lévy Stable (Stable), the log-normal (LN), and the distribution for the constant elasticity of variance (CEV, $\beta \neq 1$).

Based on these observations the improved model we propose for the dynamics of views is

$$dX_t = a_t X_t dt + b_t X_t dL_t, \qquad (2)$$

where the noise term dL_t has a Lévy-Stable distribution (with asymmetry parameter 1 and tail parameter α) and a_t, b_t are estimated from $P(dX_t|X_t)$ for different

X_t and t. The linearity in Eq. (2) points at an independent growth rate with respect to X_t, as Gibrat's law states, but with a different fluctuation term. In summary, the linearity of the growth models cannot be seen as responsible for the onset of fat-tailed distribution because such distributions appear already in the fluctuations of the evolution of items with identical X_t. More importantly, the inclusion of Lévy fluctuations lead to a dramatic improvement in the prediction of the most successful items, as shown below.

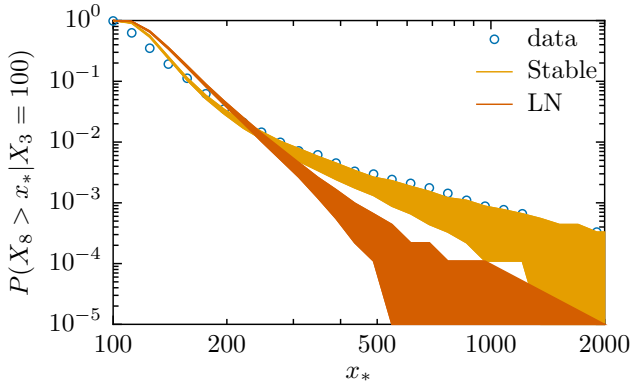

Figure 3: Probability of exceeding a threshold x_*, for videos with $X_3 = 100$, according to the time-evolved models at $t_* = 8$. The solid lines indicate the model with Lévy-Stable noise (Eq. 2, Stable) and the one with log-normal noise (Eq. 1 with linear terms, LN); the shaded areas are the 90% confidence intervals.

Prediction and predictability of extreme events. The model presented above poses a serious challenge to the predictability of views. For instance, the quality of the prediction measured as $(\hat{Y} - Y)^2$, where $\hat{Y}$ is the predicted value and Y is the actual value, becomes undefined because the Lévy-Stable distribution do not have finite variance. A solution is to consider the alternative prediction problem of whether a video will pass a certain threshold $X_{t_*} > x_*$ (which we call an event E) given the information known at time $0 \leq t < t_*$?

Our first use of this prediction problem is to compare our model – Eq. (2) – to the traditional approach – Eq. (1). For each model we compare the estimation of the probability of an extreme event with the observed number of events. Figure 3 shows that predictions based on the usual Wiener-noise model (1) systematically underestimate the number of extremely successful items landing at the tail of the distribution, while the Lévy-noise model suffers only a shift due to the neglected correlations in the videos' activity.

Our second use of the prediction problem stated above is to quantify the importance of different factors and the predictability of the system. In this case we consider the problem of issuing a binary prediction (yes/no) to the question whether a video will become an extreme event. We obtained the optimal prediction strategy of this classification problem, based on the probabilities $P(E|g)$ of an event E given that the video belongs to a group g (e.g., all videos with the same X_t or with the same topic). The quality of prediction of the optimal strategy quantifies the predictability (i.e., the potential prediction) of the system for the given problem and information, and can be estimated by computing the area under the curve in the hit×false-alarm space as [2]

$$\Pi = \sum_g \sum_{h<g} \frac{P(g)P(h)\left(P(E|h) - P(E|g)\right)}{P(E)(1 - P(E))}, \qquad (3)$$

where $P(g)$ is the probability of group g and g is ordered by decreasing $P(E|g)$, i.e., $h < g \Rightarrow P(E|h) > P(E|g)$.

Equation (3) can be applied to quantify the predictability of different problems and the relevance of different factors:

- Consider the case of predicting whether YouTube videos at $t_* = 20$ days will have more than $x_* = 1000$ views. Using the views achieved by the items after $t = 3$ days we obtain a predictability of $\Pi = 90\%$. Using the day of the week the video was published to group the items leads to $\Pi = 3\%$ against $\Pi = 31\%$ obtained using the categories of the videos. This result, which is robust against variations of x_* and t_*, shows that the category but not the day of the week is a relevant information in determining the occurrence of extreme events in YouTube.
- Consider the problem of identifying in advance the papers published in the online journal PLOS ONE that received at least 7500 views 2 years after publication (only $P(E) = 1\%$ achieve this threshold). Knowing the number of views at $t = 2$ months after publication leads to a predictability of $\Pi = 93\%$. A predictability $\Pi = 19\%$ is achieved alone by knowing the number of authors of the paper.

Our most important finding in Ref [2] – which computed the predictability Π in different cases – is that Π increases when the threshold x_* used to define extreme events $X_{t_*} > x_*$ increases. This indicates that, despite the inherently stochastic collective dynamics of users, efficient prediction is increasingly possible for the most successful items.

[1] F. Wu and B.A. Huberman, *Novelty and collective attention*, Proc Natl Acad Sci USA 104: 17599 (2007).

[2] J.M. Miotto, E.G. Altmann, *Predictability of Extreme Events in Social Media*, PLOS ONE 9, e111506 (2014).

[3] J.M. Miotto, H. Kantz, E.G. Altmann, *Stochastic dynamics of popularity in online systems*, in preparation.

[4] T. Maillart, D. Sornette, S. Spaeth, and G. Von Krogh, *Empirical tests of Zipf's law mechanisms in open source linux distribution*, Phys. Rev. Lett. 101, 218701 (2008).

2.20 Adoption of linguistic innovations

MARTIN GERLACH, EDUARDO G. ALTMANN

Summary Adoption of innovations is a classical problem in which complex-systems models have been successfully applied [1]. The recent availability of large records of written text allows for an application of these ideas to understand how *linguistic* innovations are adopted [2]. In the work reported here [3], we focus on words which compete for the same meaning and we track the relative frequency $\rho(t)$ of the (prevailing) word. Fig. 1 shows three representative examples of the data we analyze. By relating $\rho(t)$ to the fraction of adopters of an innovation we are able to compare the data to different models. Contrary to claims coming from historical linguistic, based on very limited quantitative analysis, we find that the shape of the adoption curve is not an universal S-curve. We relate the shape of the adoption curve to the strength of different factors leading to the adoption. In particular, we focus on factors that are endogenous (e.g., imitation) and exogenous (e.g., imposed conventions) to the population. Altogether, our results show how information on the adoption mechanisms can be obtained from the combination of empirical adoption curves and general models.

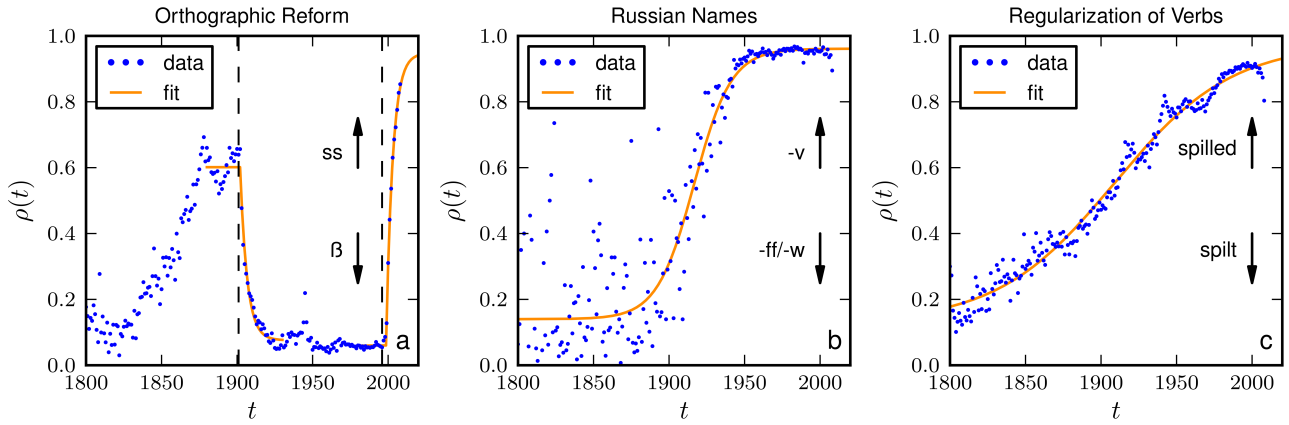

Figure 1: Examples of historical adoptions of linguistic innovations. Data: Google n-gram corpus of millions of books in German (a) and English (a,b). The solid lines are fits of the solution of Eq. (4). a: words that changed from "ss" to "ß" in the German orthographic reform of 1996. b: orthography of Russian names in the Latin alphabet (e.g., "Saratov" used to be written also as "Saratoff" or "Saratow"). c: past form of the verb spill.

Theoretical framework Consider that $i = 1 \dots N \to \infty$ identical agents (**assumption 1**) adopt an innovation. We are mainly interested in $\rho(t) = N(t)/N$, the fraction of adopters at time t, which we assume to monotonically increase $\rho(0) \approx 0$ to $\rho(\infty) = 1$. We also assume that agents after adopting the innovation do not change back (**assumption 2**).

The class of models we study within our framework considers agents characterized by a binary variable $s = \{0, 1\}$ connected to each other in a social network . We focus on models with a monotone dynamics, which are defined by the probability $F_{k,m}$ of switching from 0 to 1 given that the agent has k neighbors and m neighbors in state 1. Two well studied cases are:

$$\text{Bass model: } F_{k,m} = a + b\frac{m}{k}, \tag{1}$$

$$\text{Threshold model: } F_{k,m} = \begin{cases} a, & m/k > 1-b \\ 1, & m/k \leq 1-b \end{cases}, \tag{2}$$

for which the parameters a (b) controls the strength of exogenous (endogenous) factors.

Importance of factors Our first contribution is to propose a measure that quantifies, a the population level, the importance of different factors in the adoption. The idea is to count the fraction of agents that adopted the innovation because of a given factor. Let $g_i(t) = \sum_j g_i^j(t)$ the probability of adoption for agent i at time t and $g_i^j(t)$ be the strength of a factor j acting on i, e.g. endogenous or exogenous to the population. If t_i^* denotes the time when agent i adopts the innovation, $g_i^j(t_i^*)$ is a natural quantification of the contribution of factor j to the change of agent i. We define the normalized quantification of the change in the whole population due to factor j as an average over all agents

$$G^j = \frac{1}{N}\sum_{i=1}^{N} \frac{g_i^j(t_i^*)}{g_i(t_i^*)}. \tag{3}$$

Here we are interested in estimating the strength of exogenous factors, denoted by G.

Solution in Simple models The simplest model within the framework above considers an homogenous population and the Bass model (1). In this case the model correspond to a simple population dynamics equation

$$\frac{d\rho(t)}{dt} = (a + b\rho(t))(1 - \rho(t)). \tag{4}$$

This model can be solved analytically and $\rho(t)$ recovers in limiting cases a symmetric S-curve (for $a = 0$) and an exponential relaxation (for $b = 0$). The strength of exogenous factors is

$$G = \frac{a}{b} \log_e(\frac{a+b}{a}). \tag{5}$$

It reveals that the case $a = b$, which suggests equal contribution of the factors in the Bass model, leads to a $G = \log_e 2 \approx 0.69 > 0.5$ (exogenous factor prevails).

In the general case of complex networks, we use the framework of approximate master equations [4], which describes the stochastic binary dynamics in a random network with an arbitrary degree distribution P_k. The strength of exogenous factors (3) is given by

$$G = \sum_k P_k \sum_{m=0}^{k} \int_0^\infty s_{k,m} F_{k,0} \mathrm{d}t, \tag{6}$$

where $s_{k,m} = s_{k,m}(t)$ is the fraction of agents of the k, m class in state 0.

Estimation in surrogate data In order to test the feasibility of estimating G from time series $\rho(t)$, we generated different surrogate data by simulating different adoption processes – Eqs. (1) and (2) with different a, b– in scale-free networks. For each simulation we computed the true G – from Eq. (6) – and the adoption curve $\rho(t)$. We then tested three different estimations of G based on $\rho(t)$: (i) a comparison between the fits of symmetric S-curve and exponential; (ii) Eq. (5) with a, b obtained from the fit of the solution of Eq. (4); and (iii) a non-parametric estimation of $(d\rho/dt)/(1-\rho)$. The main idea behind all these methods – supported by the different models – is that cases for which exogenous factors are present lead to steeper starts and less symmetric adoption curves $\rho(t)$. The comparison with the surrogate and real data reveal the range of validity and sensitivity of the methods to noise. In the surrogate data, method (iii) provided the best solution. For the (noisy) real data, method (ii) is best suited and was used.

Estimation in data The results of the estimation of G in different time series are shown in Fig. 2. The case of words affected by the German orthographic reform show a stronger presence of exogenous factors, consistent with the interpretation of the (exogenous) role of language academies in language change. The romanization of Russian names indicates a prevalence of endogenous factors, consistent with historical records. The regularization of English verbs shows a much richer behavior. Besides some unresolved cases (e.g. the verb cleave), the general tendency is for a predominance of endogenous factors (e.g. the verbs spill and light), with some exceptions (e.g. the verb wake).

These results confirm that the shape of the adoption S-curve is not universal and show that within our framework we can obtain information on the underlying adoption mechanism.

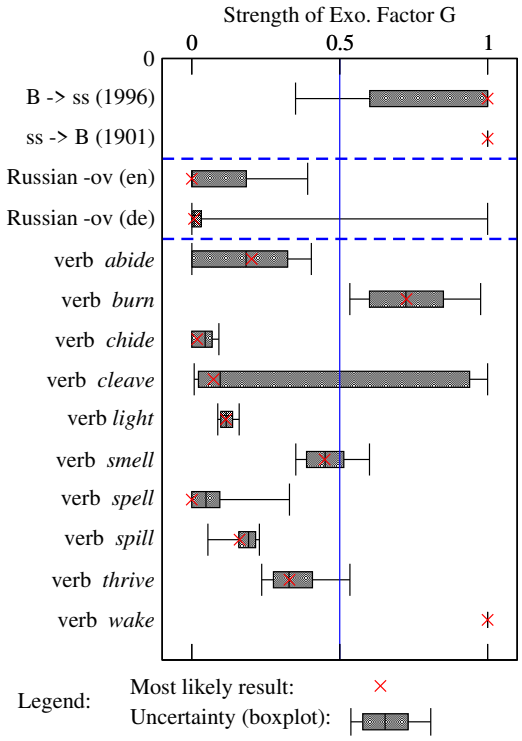

Figure 2: Estimation of the strength of exogenous factors in the adoption of different linguistic innovations. Uncertainties were computed using bootstrapping.

[1] E. Rogers, *Diffusion of innovations*, New York, NY: Simon and Schuster (2010).

[2] R. Blythe R and W. Croft, *S-curves and the mechanisms of propagation in language change*, Language 88, 269 (2012).

[3] F. Ghanbarnejad, M. Gerlach, J. M. Miotto, and E. G. Altmann, *Extracting information from S-curves of language change*, J. R. Soc. Interface 11, 201410144 (2014).

[4] J. Gleeson, *Binary-state dynamics on complex networks: pair approximation and beyond*, Phys. Rev. X 3, 021004 (2013).

2.21 Predicting and preventing extreme events in spatially extended systems: A case study

STEPHAN BIALONSKI, HOLGER KANTZ

Introduction. The dynamics of many spatially extended systems can show extreme events, ranging from thunderstorms and earthquakes to harmful algal blooms and epileptic seizures. Although extreme events occur rarely in many natural systems, they represent strong and recurrent deviations from the regular dynamical behavior and can severely affect human life. The prediction of such events does not only mean to forecast *when* an event happens, but also *where* it occurs and *how it propagates* through space. Predicting such events is highly desirable but is a non-trivial challenge given the rareness of events and our incomplete knowledge about the exact equations of motion which underlie the dynamics of many complex systems.

Our proof of principle for a solution to this problem [1] adopts the concept of local embedding spaces [2]. Hence, we predict the future locally in space, and by parallel update, we gain a future time slice of the whole system. Repeating this iteratively, we obtain forecasts with a larger lead time. We mimic the typical situation in field studies where the exact equations of motions are usually unknown and only some but not all degrees of freedom of the system are observed. We demonstrate our approach in a test case where extreme events occur in an excitable, spatially extended, reaction–diffusion-type dynamics. Based on our predictions, we are able to prevent events before they occur via tiny and spatiotemporally localized perturbations.

Test case. Inspired by previous work [3] we consider a network of coupled Fitzhugh–Nagumo units with fine-tuned parameters so that it exhibits extreme events in the form of rare large amplitude excitations starting seemingly randomly somewhere in the network, propagating in a systematic way and being extinguished when hitting the system's boundaries. The local units at the lattice sites consist of a voltage-like variable x_i and a recovery variable y_i,

$$\dot{x}_i = x_i(a - x_i)(x_i - 1) - y_i + k\sum_{j=1}^{N} A_{ij}(x_j - x_i),$$

$$\dot{y}_i = b_i x_i - c y_i,$$

where the binary adjacency matrix A determines the coupling to other units. The coupling strength was set to $k = 0.0128$, while the remaining parameters were set to $a = -0.03$, $c = 0.02$. Parameter heterogeneity is introduced by $b_i = 0.006 + 0.002((i-1) \mod 5)$. Our $N = 100$ units are coupled in a chain-like way,

$$A_{ij} = A_{ji} = \begin{cases} 1 & \text{for} \quad 0 < |i-j| \leq 5, \\ 0 & \text{otherwise.} \end{cases}$$

When performing predictions we assume that we do not know the equations of motion and that we can only observe the voltage-like variables $x_i, i \in \{1, \ldots, 100\}$ as shown in panel (a) of figure 1. Most of the time, low-amplitude oscillations can be observed (here visible for $t < 250$) but now and then, an excitation emerges and propagates through the network topology until it gets extinct ($250 < t < 420$).

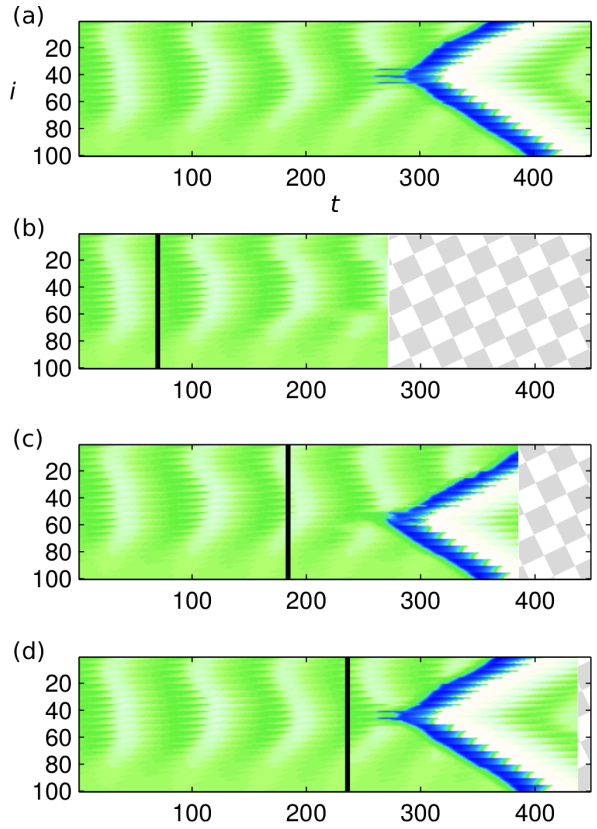

Figure 1: (a) Temporal evolution of the voltage-like variables x_i for all units before and during an exemplary extreme event. (b)–(d) Iterative predictions start at different points in time (indicated by black vertical lines) and consist of 200 iterative steps. The checkerboard patterns mark regions for which no predictions were made. Values of x_i range from -0.35 (white) to 0.95 (blue).

Data-driven predictions. All known prediction methods implicitly or explicitly rely on the Lorenz method of analogues [4]: Because of the smoothness of the right hand side of the ODE, similar states in the past have similar futures. To predict the future state of a given deterministic system, one searches in the vicinity of the current state for a state in the past which is close in state space. The future of this neighboring state can serve as the prediction.

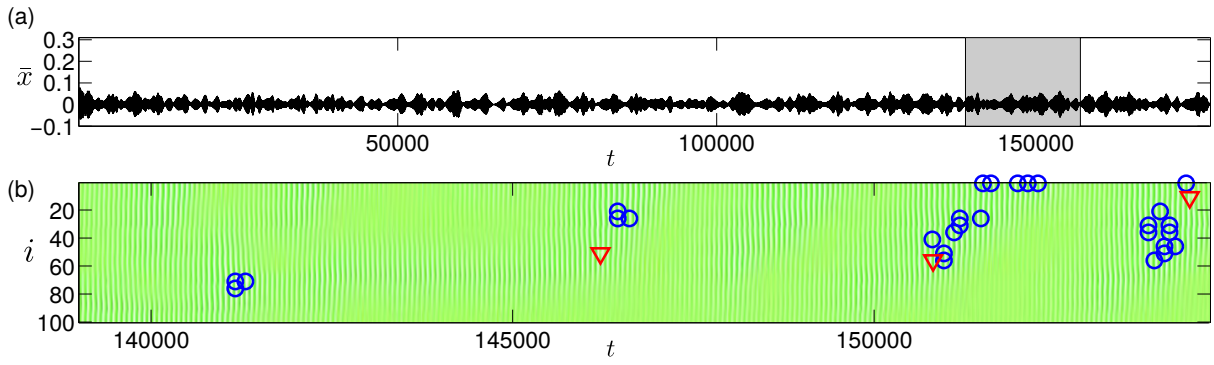

Figure 2: (a) Temporal evolution of the mean value $\bar{x}$ of the voltage like variables of all units for a control experiment. $\bar{x}$ never crossed the value 0.1 which indicates that extreme events were successfully prevented and thus did not occur. (b) Temporal evolutions of x_i for an exemplary segment of panel (a) (marked gray). Blue circles and red triangles indicate points in space and time at which the occurrence of an extreme event was correctly (blue dots) or erroneously (red triangles) predicted and prevented by small, spatiotemporally localized perturbations. Each perturbation was realized by adding the value 0.1 to the recovery variable of the unit predicted to be involved in an onset.

However, as in realistic prediction tasks, we do not observe the full state vector. Takens' celebrated delay embedding theorem [5] offers a way to reconstruct the unobserved components implicitly. It states that under quite general conditions an embedding space can be constructed that inherits all deterministic properties of the unknown dynamics. Typical constructions of embedding spaces rely on a single time series only and use consecutive samples in time to construct embedding vectors. This approach was successfully applied for predicting the dynamics of low-dimensional systems, but it has to fail for high dimensional dynamics due to what is called the curse of dimensionality.

When distributed sensors record the evolution of many degrees of freedom at different points in space a reconstruction of local states [2] can be employed. The key idea is that in a spatially extended system, where different degrees of freedom refer to different locations in space, the immediate future of a site is mainly determined by the dynamics of the site itself as well as of its nearest neighbors. This can be thought of as a consequence of the finite speed with which information propagates through the system. For each unit i, we define a local embedding space E_i and populate it with vectors s_i^t whose components include not only delayed values of x_i but also values of the topological neighbors of i. We define the vector s_i^t of unit i at time t as

$$\mathbf{s}_i^t = \Big(x_{i-m_{si}^*}^t, \ldots, x_i^t, \ldots, x_{i+m_{si}^\dagger}^t, \ldots \\ x_{i-m_{si}^*}^{t-m_t}, \ldots, x_i^{t-m_t}, \ldots, x_{i+m_{si}^\dagger}^{t-m_t}\Big),$$

with

$$m_{si}^* = m_s - \Theta(m_s - i)(m_s - i + 1)$$
$$m_{si}^\dagger = m_s - \Theta(m_s - (N - i))(m_s - (N - i)),$$

where x_i^t denotes the value of the voltage-like variable x of unit i at time t, Θ denotes the Heaviside function, m_t and m_s denote the number of delayed values and the maximum number of spatial neighbors, respectively. The definitions of m_{si}^* and $m_{si}^\dagger$ ensure that, for units close to the boundaries of the chain-like topology, only available spatial neighbors to the left and right side of unit i are considered. Values of the free parameters $(m_s, m_t) = (2, 2)$ were determined by a parameter scan in which we identified the pair of parameters that led to the best predictions (as quantified by the mean squared error between predicted and original dynamics) for an exemplary time series of our model. Local embedding spaces of all units were populated with vectors constructed from the multivariate time series (training set) of length $T = 10^5$ which contained 13 different extreme events.

Results. Results presented in panels (b)-(d) of figure 1 indicate that our approach allows us not only to predict low-amplitude oscillations very well (panel (b)) but also to forecast the beginning, propagation, and extinction of an extreme event (panels (c) and (d)) based on the time series of a subset of observables only. We observed the spatiotemporal onsets of extreme events to become better predictable the closer they are in time. In a control experiment (cf. figure 2), we successfully prevented extreme events completely in this system by applying tiny perturbations aimed at exactly these units which we predicted to be involved in onsets of extreme events.

[1] S. Bialonski, G. Ansmann, and H. Kantz. *submitted*, 2015.

[2] U. Parlitz and C. Merkwirth. *Phys. Rev. Lett.*, 84:1890–1893, 2000.

[3] G. Ansmann, R. Rajat, K. Lehnertz, and U. Feudel. *Phys. Rev. E*, 88:052911, 2013.

[4] E. N. Lorenz. *J. Atmos. Sci.*, 26:636–646, 1969.

[5] F. Takens. In D. A. Rand and L.-S. Young, editors, Volume 898 of *Lecture Notes in Mathematics*, pages 366–381. Springer-Verlag, Berlin, 1981; T. Sauer, J. Yorke, and M. Casdagli. *J. Stat. Phys.*, 65:579–616, 1991.

2.22 Analytical results for a numerical tool: the detrended fluctuation analysis

MARC HÖLL, HOLGER KANTZ

Long lasting memory is an important phenomenon found in many dynamical systems, such as in biology, hydrology, climate, and finance. These so-called long range correlated - or dependent - processes are characterized by a diverging autocorrelation time or by a spectral density with a singularity at the origin. This reflects a strong dependence between the present and the past: the system "forgets" its initial condition extremely slowly. Moreover, since the correlation time is infinite, it cannot be used to define a characteristic time scale of the system. Asymptotically, the autocorrelation function (ACF) follows a power law

$$C(s) = \frac{\langle (x_t - \mu)(x_{t+s} - \mu) \rangle}{\langle (x_t - \mu)^2 \rangle} \sim s^{-\gamma} \qquad (1)$$

with the ensemble mean $\langle x_t \rangle = \mu \ \forall t$ (weak stationarity) and the correlation exponent $0 < \gamma < 1$. This behaviour has interesting implications for time series analysis where many results used for short range correlated processes are no longer meaningful.

First evidence of this phenomenon was found by Hurst studying time series data of river flows [1]. His empirical results were in contrast to (short range correlated) theoretical models. This discrepancy is called Hurst effect. There are two possible explanations for time series exhibiting the Hurst effect. The first is that the process has long memory as described above. In [2] Mandelbrot was the first to propose a stationary model with this feature called fractional Gaussian noise (FGN). Another possible explanation for the Hurst effect is that a process with short memory has additional non-stationarities caused by external effects. This was first investigated by [3].

Many processes in nature are non-stationary. Therefore one is interested in distinguishing reliably between long memory and non-stationarities. One of the most important and widely used methods claiming to solve this problem is the detrended fluctuation analysis (DFA) introduced by Peng et al. [4]. The DFA is based on the random walk theory and the provided fluctuation function $F(s)$ is related to the ACF, see detailed description in [5]. In words, one first adds up the observed signal thereby creating a kind of random walk. This walk is cut into disjoint time windows of length s. On every window, one determines the "trend" by fitting a polynomial of kth order to this path, and calculates the squared distance between the path and the fitting polynomial. The average of this distance as a function of s (averaged over all time windows contained in the data set) is called the fluctuation function $F(s)$, and the order k of the detrending polynomial gives the name DFA(k). The goal of this procedure is to remove artefacts from a superimposed trend, which might modify the scaling behaviour in s of these fluctuations. The exponent α of the asymptotic behaviour

$$F(s) \sim s^{\alpha} \qquad (2)$$

is connected to γ through $\alpha = 1 - \gamma/2$ for long memory processes and it is $\alpha = 1/2$ for short memory processes. Although the DFA is so popular and stated as the best choice for unknown processes [6] there is - beside [7] analyzing FGN - no systematic analytical investigation on it. This is particularly unsatisfying since there are empirical observations of failures of the DFA on model processes, e.g., [8].

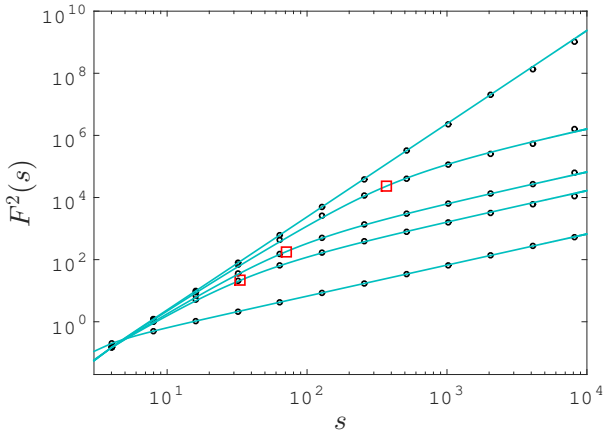

Figure 1: Analytical fluctuation functions (solid lines) of the white noise, the AR(1) process with $s_c = 4.5, 9.5$ and 49.5 and the random walk (from bottom to top) and their empirical fluctuation functions directly obtained from DFA (circles) where we averaged over 30 realisations of the process. The red squares show the crossover s_x from (3) for each AR(1) process.

In order to understand the findings of [8] we calculate analytically the fluctuation function for DFA(1) of the first order autoregressive process AR(1) with characteristic correlation time s_c in [9]. We use the fact that $F(s)$ can be written as sum of normally distributed random numbers and derive an analytical expression for it. The most important result of this work is that this process exhibits a crossover between a region with $\alpha > 1/2$ and the expected value $\alpha = 1/2$ at

$$s_\times = c_1 \frac{e^{1/s_c}}{e^{2/s_c} - 1} \qquad (3)$$

with $c_1 = 15$, see Fig.1. The value of α on small temporal scales s is limited by $3/2$, which is the correct scaling if $a = 1$, which is the limit when the signal itself becomes a Brownian path. This violation of scaling on small scales has a fundamental implication for real data sets. In order to be able to observe the correct scaling

behaviour, one must be able to analyze $F(s)$ on time windows larger than $s_\times$, and in order to perform reasonable statistical estimates, one needs about 50 different windows. Hence, a save determination of the correct scaling with $\alpha = 1/2$ is only possible, if the time series length is at least $N > 50 s_x \approx 250 s_c$, which is much more than it would be needed to savely observe the exponential decay of the autocorrelation function. Therefore, as we have shown, DFA is a very data consuming method, and a lack of data generates wrong results. The reason for this is the detrending itself: The trend function in a window of size s is a function of all time series elements inside this window. Hence, by detrending, a kind of dependence is introduced into the data, whose effect only vanishes for really large s.

In a next step, we systematically investigate stationary processes in [10] in general. We find that the fluctuation function of a stationary process x is

$$F^2(s) = \langle x^2 \rangle \left(W(s) + \sum_{r=1}^{s-1} C(r) L_r(s) \right) \qquad (4)$$

where $W(s)$ and $L_r(s)$ are calculable functions of r and s, depending on the detrending order k of DFA. The data properties enter through the autocorrelation function $C(r)$. This explicit relationship between the fluctuation function and the autocorrelation function can be used to calculate $F(s)$ for particular examples which can be useful in applications, as will be discussed next.

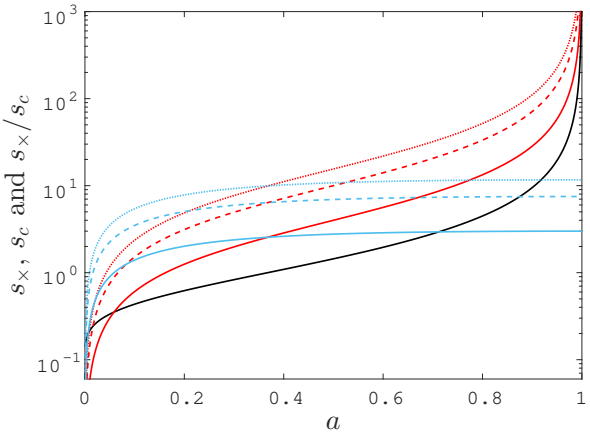

Figure 2: The crossover times $s_\times$ (red curves) for different detrending orders k in comparison to the autocorrelation time $s_c = -1/\ln a$ (black curve) as a function of the parameter a for an AR(1) process, as well as their ratios. Detrending orders are $k = 0$ (solid), $k = 1$ (dashed), and $k = 2$ (dotted).

As shown in our manuscript [10], Eq.(4) allows us to obtain the scaling behaviour of $F(s)$ for short and long memory processes based on the autocorrelation function alone. As expected, one can thereby prove that the fluctuation function of short memory processes asymptotically increases indeed like $s^{1/2}$. But there is always a crossover $s_\times$ for every short memory process with characteristic correlation time s_c. So we could generalise the result in (3) where c_1 has to be replaced by c_k with the detrending order k. The first three values are $c_0 = 6$, $c_1 = 15$ and $c_2 = 70/3$. The crossover is larger the higher the detrending order of the DFA is. This is a problem when we have to deal with complicated trends and confirms that indeed the detrending is responsible for the violation of scaling. The relationship between the crossover scale $s_\times$ and the correlation time s_c is illustrated in Fig.2 for an AR(1) process.

The positive finding of our analysis is that we can show that for truely long memory processes with correlation parameter γ there is no crossover, i.e., the relationship between F and the ACF described in (2) holds for all s. We also calculate the fluctuation function for ARFIMA processes [11], which are long range correlated processes modeling fractional Gaussian noises.

As said, the idea of DFA is to remove non-stationarities which would otherwise lead to wrong estimates of the decay of correlations. Therefore, we also analyze how well this works. We investigate the influence of processes with additive trends on otherwise short range correlated data [10]. Formula (4) can easily be extended to these issues which again might be interesting for applications. Our current understanding shows that the DFA can handle continuous trends or at least they are recognizable, which was already found numerically in [12].

However, with non-continuous trends the DFA seems to have problems. As simplest example we study short memory process with an additive constant trend μ_1 which changes at a break point to the value μ_2. Such sudden changes are, e.g., seen in heart rate data, when the physical activity of a proband changes. For some parameter domains the DFA erroneously detects long memory. As a next step we will analyze this problem in detail and illustrate it with real data.

[1] H.E. Hurst, Transactions of the American Society of Civil Engineers **116**, 770 (1951)

[2] B.B. Mandelbrot, J.W. van Ness, SIAM Review **10**, 422 (1968)

[3] R.N. Bhattacharya, V.K. Gupta, E. Waymire, Journal of Applied Probability **20**, 649 (1983)

[4] C.K. Peng, S.V. Buldyrev, S. Havlin, M. Simons, H.E. Stanley, A.L. Goldberger, Phys. Rev. E **49**, 1685 (1994)

[5] J.W. Kantelhardt, E. Koscielny-Bunde, H.H.A. Rego, S. Havlin, A. Bunde, Physica A **295**, 441 (2001)

[6] A. Bashan, R. Bartsch, J.W. Kantelhardt, S. Havlin, Physica A **387**, 5080 (2008)

[7] M.S. Taqqu, V. Teverovsky, W. Willinger, Fractals **3**, 785 (1995).

[8] D. Maraun, H.W. Rust, J. Timmer, Nonlinear Processes in Geophysics **11**, 495 (2004)

[9] M. Höll, H. Kantz, European Physical Journal B **88**, 126 (2015)

[10] M. Höll, H. Kantz, manuscript in preparation

[11] C.W.J. Granger, Journal of Econometrics **14**, 227 (1980)

[12] K. Hu, P.C. Ivanov, Z. Chen, P. Carpena, H.E. Stanley, Physical Review E **64**, 011114 (2001)

2.23 The distribution of work performed on a NIS junction - a test of the Crooks-Tasaki fluctuation relation

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Non-equilibrium statistical physics has been a topic of growing interest. This interest has been fuelled not only by the fundamental role that out-of-equilibrium fluctuations play in bringing about thermodynamic equilibrium, but also by an increased interest in understanding systems, in particular quantum systems, displaying far-from-equilibrium dynamics. A central role in our understanding of many-body systems out of equilibrium is played by fluctuation relations like the Jarzynski equality [2] that relates free energy changes to the work performed on a system, without the need of an explicit knowledge of the associated entropy changes. It later was realized that the Jarzynski equality is a direct consequence of the Crooks-Tasaki fluctuation relation [3,4]. Despite their theoretical significance, a direct experimental verification of such fluctuation relations is difficult in quantum systems. Here, we report on a proposal for an experiment that permits the measurement of the work performed an a metal-insulator-superconductor (NIS) junction, which, as it is explicitly shown, will allow for a direct experimental test of the Crooks-Tasaki relation [1, 5]. Unlike other proposed tests of the Crooks-Tasaki fluctuation relations, ours has the advantage that the released heat scales with the contact area between the superconducting and normal metal films that constitute the junction, a quantity that is easily controllable in an experiment, which makes our proposal amenable to experimental verification.

The work probability distribution, $P_\beta(W,\tau)$, is defined, for a class of work protocols where the system is decoupled from the thermal bath during the application of the protocol (see below), of duration τ, as [4]

$$P_\beta(W,\tau) = \frac{1}{\mathcal{Z}(\beta)}\sum_{m,n} e^{-\beta E_m^0} \mid \langle n,\tau|\widehat{U}(\tau,0)|m,0\rangle \mid^2 \times \delta(W-E_n^\tau+E_m^0)\,, \quad (1)$$

where $|m,0\rangle$ are the eigenstates of the system's Hamiltonian at the beginning of the protocol, $\widehat{H}(0)$ and E_m^0 are the corresponding eigenvalues, and where $|n,\tau\rangle$ are the eigenstates of the system's Hamiltonian at the end of the protocol, $\widehat{H}(\tau)$ with E_n^τ being the corresponding eigenvalues, with $\beta = 1/(k_B T)$ and $\mathcal{Z}(\beta) = Tr(e^{-\beta\widehat{H}(0)})$. The operator $\widehat{U}(\tau,0)$ is the time-evolution operator of the system during the protocol, i.e. in the interval $[0,\tau]$, which can be written as a time-ordered exponential of

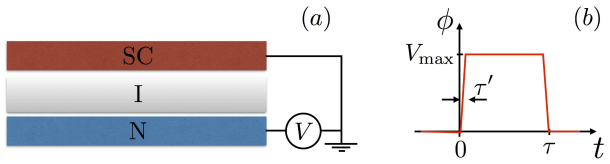

Figure 1: (a) schematic of a normal metal-insulator-superconductor (NIS) junction. (b) The voltage vs. time protocol considered in this work.

the full Hamiltonian of the system. The NIS junction is composed of a normal-metal film, a thin insulating layer and a superconducting film (see figure 1(a)). Such a junction can be described by an Hamiltonian consisting of three terms: a Fermi-gas describing the normal-metal film, a BCS superconductor describing the superconducting film and a tunnelling Hamiltonian coupling the two, which gives rise to induced superconductivity in the normal-metal film through the proximity effect. We use the Hamiltonian $\widehat{H}(t) = \widehat{H}_n(t) + \widehat{H}_s + \widehat{X}$. The operator $\widehat{H}_n(t) = \sum_{\mathbf{k},\sigma}(\xi_{\mathbf{k}}^n - e\,\phi(t))\,\widehat{c}^\dagger_{n\mathbf{k}\sigma}\widehat{c}_{n\mathbf{k}\sigma}$ is a free-fermion Hamiltonian describing the normal-metal, with $\phi(t)$ being the voltage difference across the junction, whose value changes in time. The operator

$$\widehat{H}_s = \sum_{\mathbf{k},\sigma}\xi_{\mathbf{k}}^s\,\widehat{c}^\dagger_{s\mathbf{k}\sigma}\widehat{c}_{s\mathbf{k}\sigma} + \sum_{\mathbf{k}}\left(\Delta_{\mathbf{k}}\widehat{c}^\dagger_{s\mathbf{k}\uparrow}\widehat{c}^\dagger_{s-\mathbf{k}\downarrow} + \overline{\Delta}_{\mathbf{k}}\widehat{c}_{s-\mathbf{k}\downarrow}\widehat{c}_{s\mathbf{k}\uparrow}\right)$$

is the Hamiltonian describing a BCS superconductor with pairing function $\Delta_{\mathbf{k}}$. $\widehat{X} = \sum_{\mathbf{k},\sigma} t^\sigma(\vec{k})\left(\widehat{c}^\dagger_{s\mathbf{k}\sigma}\widehat{c}_{n\mathbf{k}\sigma} + \widehat{c}^\dagger_{n\,-\mathbf{k}\,-\sigma}\widehat{c}_{s\,-\mathbf{k}\,-\sigma}\right)$ represents the tunnelling process across the junction, whose matrix elements are considered to be invariant under time-reversal and small compared to $\Delta_{\mathbf{k}}$.

The work characteristic-function of the NIS junction is the Fourier transform of equation (1), and is given by

$$\mathcal{G}_\beta(\upsilon,\tau) = Tr\left[\widehat{U}^\dagger(\tau,0)\,e^{i\widehat{H}(\tau)\upsilon}\,\widehat{U}(\tau,0)\,e^{-i\widehat{H}(0)\upsilon}\,\widehat{\rho}(\beta)\right],$$

where $\widehat{\rho}(\beta) = e^{-\beta\widehat{H}(0)}/\mathcal{Z}(\beta)$ is the density matrix of the junction before the application of the protocol. We consider the NIS to be initially ($t < 0$) in equilibrium with an heat bath at temperature T and that the voltage ϕ across the junction is zero. Such voltage is changed from 0 to a finite value $V_{\max}$ and returned to zero within

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a finite time-interval starting at $t = 0$ and ending at $t = \tau$. During such an interval the junction is decoupled from the heat bath. Also, $\phi(t)$ varies smoothly within a time-interval $\tau' \ll \tau$ and is returned to zero at the end of the protocol within the same time frame (see figure 1(b)).

One obtains for the logarithm of the NIS work characteristic-function, which is the generating function of the connected work-moments, the result

$$\mathcal{W}_\beta(\upsilon,\tau) \equiv \ln \mathcal{G}_\beta(\upsilon,\tau) = \sum_{\mathbf{k}} \ln \left\{ (1-p_{\mathbf{k}}) + p_{\mathbf{k}} \cdot \frac{\cosh\left[(\beta + 2i\upsilon)\sqrt{|\Delta^n_{\mathbf{k}}|^2 + (\tilde{\xi}^n_{\mathbf{k}})^2}\right]}{\cosh\left(\beta\sqrt{|\Delta^n_{\mathbf{k}}|^2 + (\tilde{\xi}^n_{\mathbf{k}})^2}\right)} \right\} \quad (2)$$

with $p_{\mathbf{k}} = \frac{|\Delta^n_{\mathbf{k}}|^2 (eV_{\max})^2}{(|\Delta^n_{\mathbf{k}}|^2 + (\tilde{\xi}^n_{\mathbf{k}})^2)(|\Delta^n_{\mathbf{k}}|^2 + (\tilde{\xi}^n_{\mathbf{k}} - eV_{\max})^2)} \times \sin^2\left(\frac{\tau}{\hbar}\sqrt{|\Delta^n_{\mathbf{k}}|^2 + (\tilde{\xi}^n_{\mathbf{k}} - eV_{\max})^2}\right)$.

The average work dissipated per atom in the normal-metal film, $\bar{w}$, is

$$\bar{w} = \frac{2(eV_{\max})^2}{\mathcal{N}_{at}} \sum_{\mathbf{k}} \tanh\left(\beta\sqrt{|\Delta^n_{\mathbf{k}}|^2 + (\tilde{\xi}^n_{\mathbf{k}})^2}\right) \times \frac{|\Delta^n_{\mathbf{k}}|^2 \sin^2\left(\frac{\tau}{\hbar}\sqrt{|\Delta^n_{\mathbf{k}}|^2 + (\tilde{\xi}^n_{\mathbf{k}} - eV_{\max})^2}\right)}{\sqrt{|\Delta^n_{\mathbf{k}}|^2 + (\tilde{\xi}^n_{\mathbf{k}})^2}(|\Delta^n_{\mathbf{k}}|^2 + (\tilde{\xi}^n_{\mathbf{k}} - eV_{\max})^2)} \quad (3)$$

where $\mathcal{N}_{at}$ is the total number of atoms in the normal-metal film.

The full characterisation of the work fluctuations requires the determination of the work probability distribution. Writing the probability distribution in terms of the logarithm of the characteristic function, as defined in Eq. (2), one has

$$P_\beta(W,\tau) = \int_{-\infty}^{+\infty} \frac{d\upsilon}{2\pi} e^{-iW\upsilon + \mathcal{W}_\beta(\upsilon,\tau)} . \quad (4)$$

Since W is an extensive quantity, *i.e.* it is proportional to $\mathcal{N}_{\text{at}}$, the integral can be computed using a saddle-point approximation. One obtains

$$w = \int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi\, \rho(\xi)\partial_x S(\xi,x) , \quad (5)$$

where $w = W/\mathcal{N}_{at}$ is the work per atom of the sample and $S(\xi,x)$ is given by $S(\xi,x) =$

$$\ln\left\{(1-p(\xi)) + p(\xi)\cdot\frac{\cosh\left[(\beta+2x)\sqrt{|\Delta^n(\xi)|^2+\xi^2}\right]}{\cosh\left[\beta\sqrt{|\Delta^n(\xi)|^2+\xi^2}\right]}\right\},$$

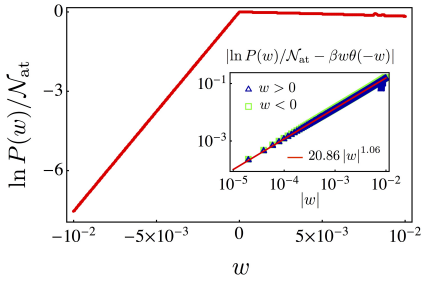

Figure 2: Logarithm of the work per atom distribution for a $AlMn/AlO_2/Al$ junction at $T = 1\,K$.

Numerically solving Eq. (5) for a set of values of w (with the same assumptions as in the two calculations previously performed) and substituting its solution in Eq. (4), one obtains the result plotted in figure 2 for the logarithm of $P_\beta(W,\tau)$, divided by $\mathcal{N}_{at}$. This calculation indicates that the work probability distribution is a stretched exponential for both positive and negative W. In the inset, the exponent associated with such a stretched exponential is determined for positive W (blue triangles).

Our primary motivation for this study was the analysis of the validity of the Crooks-Tasaki relation in an experimentally relevant setting. The measurement of the released heat is carried out at constant temperature by coupling the system to an external probe that absorbs a quantity of heat $\Delta Q = W$ isothermally. If the absorption occurs reversibly, it corresponds to an increase of entropy of the probe equal to $\Delta S = \Delta Q/T$. The probe will increase in volume as result of the heat absorbed, the variation of volume being given by $\Delta V = \kappa_T \Delta S/\alpha$ where κ_T is the isothermal compressibility of the probe and α its thermal expansion coefficient. Therefore, the relative variation of the volume of the probe is given by $\Delta V/V = W/(\gamma n c_v T)$, where $\gamma = \frac{\alpha v_m}{c_v k_T}$ is the Grüneisen parameter of the material that constitutes the probe, v_m its molar volume, n is the number of moles of material contained in the probe, and c_v the material's molar heat capacity. The measurement of the relative variation of the probe's volume $\Delta V/V$ thus gives direct experimental access to the work produced during the prescribed protocol [1]. Based on the setup of Ref. [6] and assuming that the film itself will act as the probe, we can estimate $\Delta V/V$. For aluminium, $\gamma \approx 2.1$ and $c_v \approx 1.5\,mJ\,mol^{-1}\,K^{-1}$. If we use $\langle W\rangle_\beta \approx 5\,\mu J/g$, we obtain a relative deviation $\Delta V/V \approx 0.01$, on average, which should be measurable using, e.g. capacitive methods.

[1] J. E. Santos, P. Ribeiro & S. Kirchner, arXiv:1506.02905 (2015) and submitted.

[2] C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997).

[3] G. E. Crooks, J. Stat. Phys. **90**, 1481 (1998).

[4] H. Tasaki, cond-mat/0009244v2 p. unpublished (2000).

[5] G. E. Crooks, J. Stat. Mech.: Theor. Exp. **2008**, P10023 (2008).

[6] P. J. Lowell, G. C. ONeil, J. M. Underwood, and J. N. Ullom, App. Phys. Lett. **102**, 082601 (2013).

2.24 Modeling ultrafast shadowgraphy in laser-plasma interaction experiments

EVANGELOS SIMINOS, STEFAN SKUPIN

The interaction of intense laser pulses with plasmas can lead to the excitation of nonlinear structures in the plasma, such as wakes, solitons, shocks and filaments. The time evolution of such structures is highly nontrivial and a lot of effort has been invested in developing theoretical tools and experimental diagnostics to investigate it. In a typical Laser-wakefield accelerator (LWFA) setup a relativistically intense laser pulse (the 'pump' pulse) excites an electron plasma wave (the 'wake') which propagates with a phase velocity v_p equal to the pump pulse group velocity $v_g \simeq c$ through the plasma. Ambient electrons can be trapped and accelerated in the field of the wake, producing quasi-monoenergetic electron beams [1]. Stable operation of such accelerators requires a thorough understanding of nonlinear laser-plasma interaction processes motivating the development of novel diagnostics. The characteristic length scale of the wake is the plasma wavelength λ_p. Therefore, optical probing of such a wake with a transversely propagating probe pulse requires a probe pulse duration: $c\,\tau_{\rm pr} \ll \lambda_p$. Typically this corresponds to a duration of few laser cycles $\tau_L = 2\pi/\omega_L$, where ω_L the frequency of the probe pulse. Recently, pump-probe experiments utilized probe pulses of few femtosecond duration to obtain the first direct shadowgraphic images of a wake propagating in an underdense plasma [2,3].

Conventional shadowgraphy can be analyzed using geometrical optics and formulated as an inverse problem: for a given shadowgraphic image local gradients in index of refraction can be determined, see, e.g., Ref. [4]. In ultrafast shadowgraphy of laser induced wakes this is not in general straightforward. The effect of longitudinal motion of the wake as the probe pulse traverses, the presence of strong magnetic fields as well as relativistic effects are not negligible and need to be taken into account. At the same time diffraction effects can be significant when the probe pulse wavelength $\lambda_{\rm pr}$ is comparable to the plasma skin depth λ_s which is the characteristic length scale of density gradients in the plasma. For parameters used in recent experiments [3] this is often the case and the effect of diffraction has to be accounted for.

In this report the shadowgraphic image formation process is analyzed through the use of three-dimensional particle-in-cell (PIC) simulations of the full pump-probe setup. Propagation of the pump pulse through the plasma is simulated and at different delays a probe pulse propagating transversely to the pump is launched. After the probe traverses the wake, postprocessing in Fourier space allows to take into account the effect of a typical imaging setup in shadowgraphic image formation. Synthetic shadowgrams generated using this methodology turned out to be crucial for the correct interpretation of experimental measurments [3].

We performed simulations of LWFA with the PIC code EPOCH with parameters similar to the ones used in recent experiments that utilized ultrafast shadowgraphy to study injection in LWFA [3]. We consider a plasma of density $n_0 = 1.7 \times 10^{19}\,\mathrm{cm}^{-3}$. A pump laser pulse propagating along the x direction with an intensity FWHM duration of 36 fs was focused to a spot size of $18.84\,\mu$m. The pump pulse maximum intensity (in vacuum) was $I_0 = 2.5 \times 10^{18}\,\mathrm{W/cm}^2$. Probe propagation along the y-direction has been also fully simulated in 3D with EPOCH. Probe pulse parameters were similar to the ones in recent experiments [3]: central wavelength $\lambda_{\rm pr} = 0.75\,\mu$m, bandwidth limited duration of $\tau_{BL} = 4.4$ fs (intensity FWHM) and a negative linear chirp that increased duration to $\tau_{\rm pr} = 12$ fs and maximum intensity $I_{\rm pr} = 8.6 \times 10^{14}\,\mathrm{W/cm}^2$. We allowed the probe pulse to propagate past the wake structure, until its center reached approximately $y_B = -20\mu$m. In Fig. 1(a-c) we track the evolution of the envelope of the probe electric field as it crosses the wake. Fig. 1(b-c) indicates that modulations in the intensity of the probe pulse occur as the latter interacts with density gradients in the wake. The highest intensity modulations occur at the front of the bubble (the first period of the wakefield) where the pump drives the wake.

Once the probe pulse reaches y_B there are no substantial density perturbations in the plasma and therefore any local phase differences induced by the wake have been imprinted to the probe pulse. However, if we simply try to reconstruct a shadowgram by recording the time-integrated intensity passing through the plane y_B, as shown Fig. 1(d), there are two problems with the image we obtain. In the front of the wake there is strong scattering of pump light which is of much higher intensity than the probe intensity. This scattered light is not present in the experimental shadowgrams [2, 3]. As we will see the reason for this is that the aperture of the imaging system eliminates most of the side-scattered light. Moreover, the wake structure appears blurred in Fig. 1(d). The reason for this is strong diffraction, since the length scale for density gradients ($\lambda_s = 1.3\,\mu$m here) is comparable to the wavelength of the probe pulse ($\lambda_{\rm pr} = 0.75\mu$m). Thus, in order to be able to compare PIC simulation results to experimental shadowgrams, we have to take into account the influence of a typical imaging system in shadowgram formation.

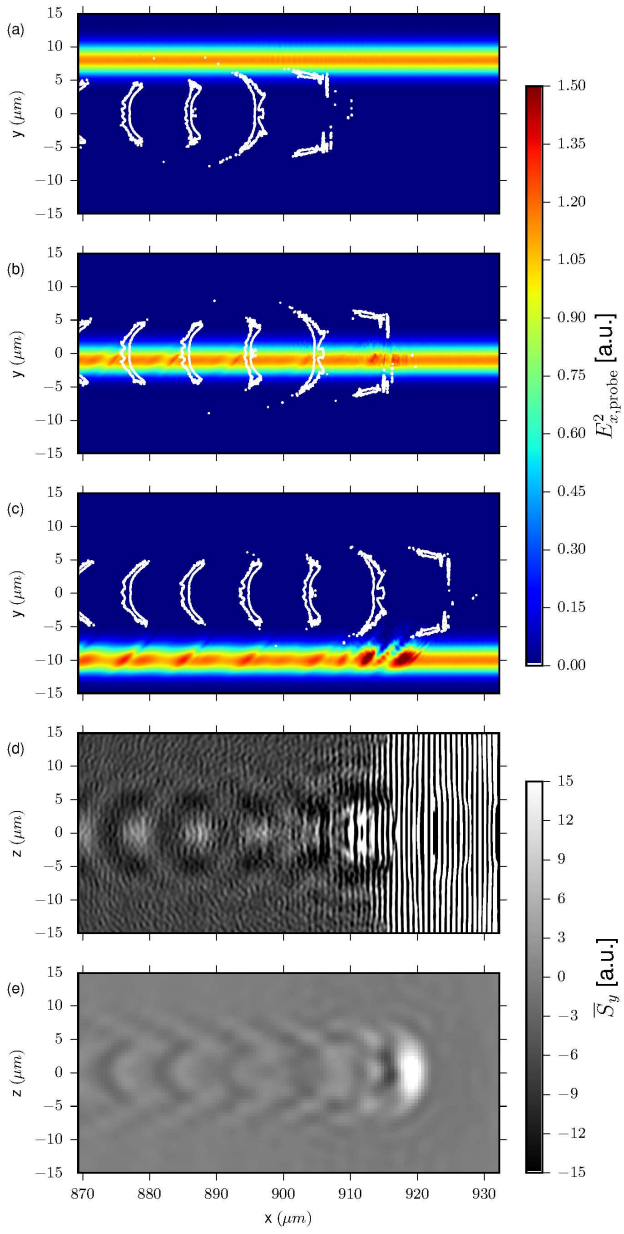

Figure 1: Probe pulse propagation past the wake. Panels (a)-(c): Three snapshots from the PIC simulation showing the probe electric field amplitude E_x^{probe} and contours of the plasma density corresponding to $n = 2\,n_0$. (d) Image obtained by recording the time-integrated Poynting flux $\langle S_y \rangle$ passing trough the plane $y = -20\,\mu$m (e) Time-integrated Poynting flux $\langle S_y \rangle$ after adjusting for focusing optics, assuming the object plane is at $y_o = 0$.

In order to reconstruct shadowgrams from our PIC simulation results, we will use two major simplifications. Firstly, the transverse size of the simulation box in our PIC simulations is limited to a couple of tens of microns, and it is not possible to directly account for the optical imaging. However, this is not really neccessary anyway, because once the probe pulse has propagated through the plasma wake, all information related to the laser-plasma interaction process are already imprinted in its wavefronts. Thus, we will assume that the probe pulse propagates further on in vacuum, and neglect the influence of any low density plasma and/or gas which may be present between the main interaction region and the imaging system.

By doing so, we can resort to much more efficient spectral pulse propagation methods. Secondly, the probe pulse, after it has passed the plasma wake, propagates mainly in one direction, and the imaging system has a certain numerical aperture (NA), i.e., acceptance angle. Here, we assume that the NA of our imaging system is small enough to justify a paraxial description of the imaging process. Transforming to spatial Fourier space allows to take into account the effect of the aperture by eliminating directions in k-space that do not propagate past it. Moreover, working in Fourier space we correct for the fact that the fields in the PIC code are not available on the object plane (which is within the interaction region) by virtual propagation back to the object plane. This allows to reconstruct simulated shadowgrams as in Fig. 1(e), which match very well the experimental shadowgrams [3].

The methodology developed here thus allows direct comparison with experimental shadowgrams and facilitates their interpretation. In particular, our ability to track probe propagation indicates that the strongest modulations in the shadowgrams originate from the front of the bubble, see Fig. 1, and this allowed the determination of bubble length in recent experiments [3]. Shadowgrams obtained at different delays allow to track the evolution of the size of the bubble as it propagates through the plasma. It is shown that, as suggested by recent models [5], the process of expansion of the bubble induced by self-focussing and self-compression of the pump laser pulse leads to self-injection of electrons into the bubble and their subsequent acceleration.

[1] E. Esarey, C. B. Schroeder, and W. P. Leemans, *Rev. Mod. Phys.* **81**, 1229, 2009.

[2] M. B. Schwab, et al., *Applied Physics Letters* **103**, 191118, 2013.

[3] A. Sävert, S. P. D. Mangles, M. Schnell, E. Siminos, J. M. Cole, M. Leier, M. Reuter, M. B. Schwab, M. Möller, K. Poder, O. Jäckel, G. G. Paulus, C. Spielmann, S. Skupin, Z. Najmudin, M. C. Kaluza, Direct observation of the injection dynamics of a laser wakefield accelerator using few-femtosecond shadowgraphy, Phys. Rev. Lett. **115**, 055002, 2015.

[4] P. K. Panigrahi and K. Muralidhar, *Schlieren and Shadowgraph Methods in Heat and Mass Transfer*, SpringerBriefs in Applied Sciences and Technology, Springer New York, 2012.

[5] S. Kalmykov, S. A. Yi, V. Khudik, and G. Shvets, *Phys. Rev. Lett.* **103**, 135004, 2009.

2.25 Mechanisms of backtrack recovery by RNA polymerases I and II

ANA LISICA, CHRISTOPH ENGEL, MARCUS JAHNEL, ERIC A. GALBURT, ÉDGAR ROLDÁN, PATRICK CRAMER, STEPHAN W. GRILL

Introduction. Transcription elongation is often interrupted by RNA polymerase (Pol) backtracking (Fig. 1), a reverse movement of the polymerase on the DNA template that displaces the RNA 3′-end from the active site, making the enzyme transcriptionally inactive [1–3]. Transcription resumes when the polymerase realigns the 3′-end of the RNA with its active site. This can be done via two distinct backtrack recovery (BR) mechanisms: by 1D diffusion of the enzyme along the DNA until it returns to an elongation competent state [4, 5] or by cleavage of the backtracked RNA which generates a new RNA 3′-end in the active site [6]. However, mechanisms that underlie the choice of backtrack recovery by either 1D diffusion or RNA cleavage are unknown. The aim of this work was to investigate BR mechanisms of eukaryotic RNA polymerases, Pol I and Pol II [7].

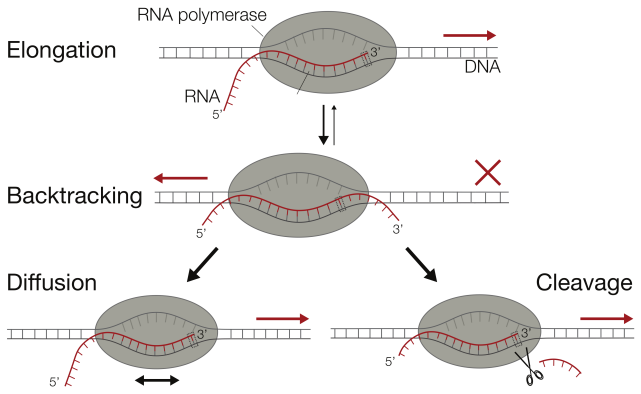

Figure 1: Scheme of transcription elongation, backtracking and backtrack recovery processes. In a backtracked state, the 3′-end of the RNA is displaced from the active site (dashed square) and the polymerase is transcriptionally inactive. Backtrack recovery can proceed through 1D diffusion of the polymerase along the DNA template, until the 3-end of the RNA realigns with the active site or through cleaving of the backtracked RNA and production of a new 3′-end that is aligned with the active site.

Backtrack recovery of Pol I and Pol II. To this end we used single-molecule optical tweezers and introduced an assay that analyzes BR kinetics after rapid force reduction (FR) and at low opposing force (Fig. 2). We found that BR depended on how far the polymerase had backtracked prior to FR. Pol I recovered from shallow, but not from deep backtracks, with the BR threshold set at the average depth of 22.4 ± 0.9 nt, whereas Pol II enzymes were unable to recover already at significantly lower depths (15.6 ± 0.6 nt, Fig. 2B). Furthermore, Pol I resumed elongation after an average time of 41.7 ± 17.5 s, whereas Pol II took 66.2 ± 21.2 s ($p \leq 0.05$, Wilcoxon rank sum test) to recover. These results show that both enzymes failed to recover from backtracks beyond a certain depth and that Pol I recovered faster and from deeper backtracks than Pol II.

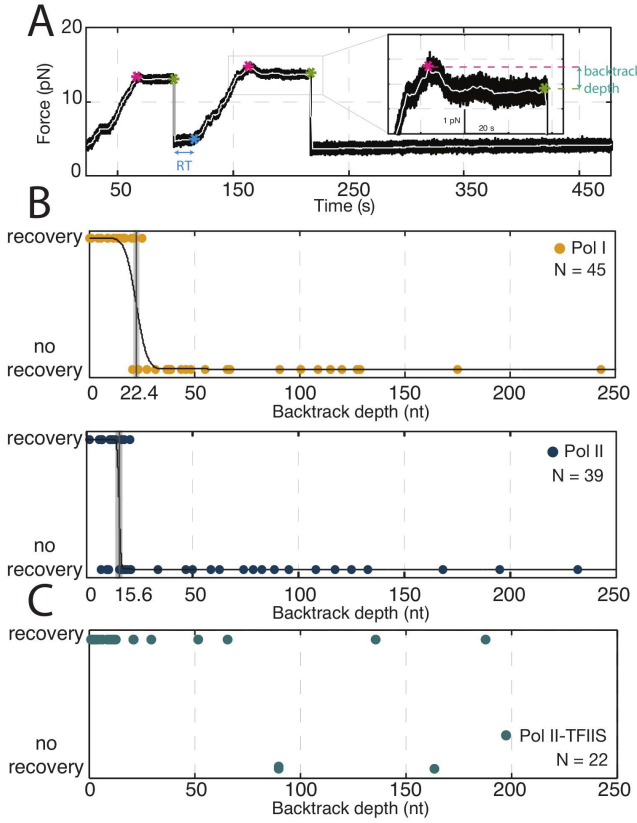

Figure 2: (A) Typical FR experiment: times of backtrack entry (magenta asterisk), FR (green asterisk) and BR (blue asterisk, setting a recovery time, RT) are indicated. Inset: zoomed view of the backtrack prior to FR. BR for Pol I and Pol II (B) and Pol II-TFIIS (C): each data point represents one FR event. The BR threshold (dark gray) with 68 % confidence interval (light gray) is determined via fitting to a complementary error function (black).

BR of Pol II can be enhanced by TFIIS [3,4,8]. To test this with our assay, we performed Pol II FR experiments in the presence of TFIIS. Indeed, with TFIIS, Pol II recovered from most backtracks, even the ones deeper than 100 nt and within an average BR time of 10.3 ± 2.7 s. These results confirm the role of TFIIS in BR of Pol II and show that Pol II with TFIIS is more efficient in backtrack recovery than Pol I.

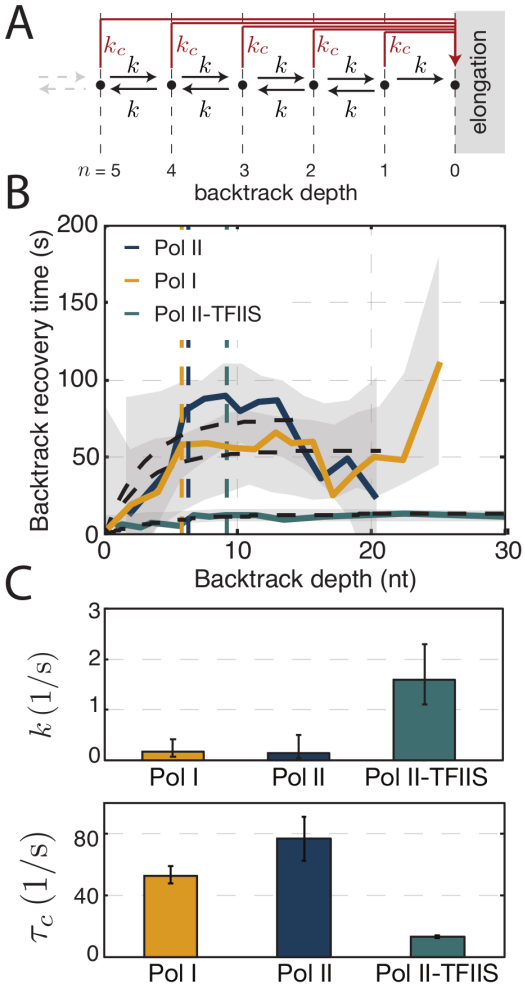

Figure 3: (A) BR time (solid lines) of Pol I, Pol II and Pol II with TFIIS plotted against backtrack depths, with standard deviations obtained via bootstrapping (gray, Methods). Black dashed lines are fits to the mean of the recovery time distribution. (A) Diffusion rates (k) and cleavage times (τ_c) obtained by fitting.

Backtrack recovery mechanisms. To better understand BR mechanisms, we modeled the random motion of the polymerase in a backtrack as a continuos time random walk with discrete states, where each state represents the backtracked distance in nucleotides, 0 being the elongation competent state [5,8,9]. The polymerase undergoes 1D diffusion between adjacent states, with a hopping rate k, until it either realigns the RNA 3'--end or until it cleaves the RNA, with a cleavage rate k_c (Fig. 3A). We calculated the distribution of the recovery time t as a function of the backtrack depth n at which the BR starts, and determined the mean recovery time. We found that the competition between diffusion and cleavage sets a characteristic backtrack depth, $n_c = 2\sqrt{k/k_c}$. Below this depth, BR is dominated by diffusion and the average BR recovery time increases with increasing starting depth n. Beyond it, BR is dominated by cleavage and the average BR recovery time saturates at $\tau_c = 1/k_c$.

To test our model and its predictions, we investigated how the BR time depends on backtrack depth (Fig. 3B). Consistent with our expectations, we observed that for Pol I, Pol II and Pol II with TFIIS, the BR time increases with increasing backtrack depth, however only until a certain distance beyond which it saturates. By fitting the model to the experimental data, we obtained the rates of 1D diffusion and RNA cleavage. We found that the diffusion hopping rates were comparable between Pol I and Pol II (Fig. 3C, top). However, the RNA cleavage rate of Pol I was higher than the one of Pol II, corresponding to shorter cleavage times. An even shorter cleavage time was obtained for Pol II in the presence of TFIIS (Fig. 3C, bottom). These values set the characteristic backtrack distance n_c to about 6 nt for both Pol I and Pol II, and to about 9 nt for Pol II in the presence of TFIIS. Beyond these distances, BR is dominated by RNA cleavage.

Conclusions. Here, we determine kinetic rates of RNA cleavage and diffusion during backtracking of Pol I and Pol II and show that the choice of backtrack recovery mechanism is determined by a kinetic competition between the two processes. Our results identify the distinct backtrack recovery strategies of Pol I and Pol II and shed light on the evolution of cellular functions of these key enzymes. Pol I likely evolved a strong intrinsic BR mechanism to ensure a fast production of ribosomal RNA in dividing and rapidly growing cells with a large demand for proteins. In contrast, Pol II evolved a weak BR mechanism, but at the advantage of being able to associate with the external factor TFIIS that provides a strong BR, which enables many co-transcriptional processes such as pre-mRNA splicing and polyadenylation.

[1] E. Nudler, A. Mustaev, A. Goldfarb, E. Lukhtanov, Cell **89**, (1997), 33.

[2] N. Komissarova, M. Kashlev, Proc. Natl. Acad. Sci. U.S.A. **94**, (1997), 1755.

[3] L. S. Churchmann, J.S. Weissman. **469**, (2011), 368

[4] E. A. Galburt et al. Nature **446**, (2007), 820.

[5] M. Depken, E. A. Galburt, S. W. Grill, Biophys. J. **96**, (2009), 2189.

[6] W. Ruan, E. Lehmann, M. Thomm, D. Kostrewa, P. Cramer, J. Biol. Chem. **286**, (2011), 18701.

[7] A. Lisica, C. Engel, M. Jahnel, E.A. Galburt, E. Roldan, P. Cramer, S. W. Grill, submitted.

[8] T. Ishibashi et al. Proc. Natl. Acad. Sci. U.S.A. **111**, (2014), 3419.

[9] M. Depken, J. M. R. Parrondo, S. W. Grill, Cell Rep. **5**, (2013), 521.

2.26 Improving Forward Genomics by directly accounting for phylogenetic relatedness and differences in evolutionary rates

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Background We previously introduced a computational "Forward Genomics" strategy that – given only an independently lost phenotype (trait) and whole genomes – predicts phenotype-genotype associations for these phenotypes [1]. Our approach utilizes predictions from evolutionary theory that genomic regions encoding trait-specific information evolve neutrally and diverge faster in trait loss species. We quantify per-species sequence divergence of conserved genomic regions by a comparison with the reconstructed DNA sequence of the common ancestor as

$$\%id = \frac{id}{(id + subs + ins + del)} * 100 \qquad (1)$$

where id, subs, ins, and del are the numbers of identical bases, substitutions, inserted bases, and deleted bases, respectively. In the following, this sequence divergence between an extant species and the ancestor of all species of interest is called *global %id* value. To associate specific genomic regions to the given phenotype, Forward Genomics searches for a region where all trait-loss species show a lower *global %id* value (increased sequence divergence). This method is called "Perfect-match" in the following. As a proof of concept, we applied Forward Genomics to "synthesis of vitamin C", a trait lost independently in primates, guinea pigs and many bats. Forward Genomics detected elevated sequence divergence in all vitamin C non-synthesizing lineages in the *Gulo* gene, which encodes the vitamin C synthesizing enzyme [1].

Limitations of the first Forward Genomics implementation Previously, we searched for loci where the two groups of species show a clear separation in their sequence divergence values. This approach has 3 limitations. First, it cannot compute a P-value for this association. Second, the fact that species are related via their phylogeny was only indirectly taken into account by requiring that the trait-loss species must represent at least two independent lineages. Third, we did not take into account that differences in evolutionary rates (proportional to the branch lengths in Figure 1) influence the sequence divergence (%id) values..

A new method using global divergence Given that hundreds of sequenced genomes will be available in the near future, approaches like Forward Genomics have the potential to detect associations between genomic and phenotypic change for many phenotypes. It is therefore worth to optimize the method in order to have maximal power to detect such associations.

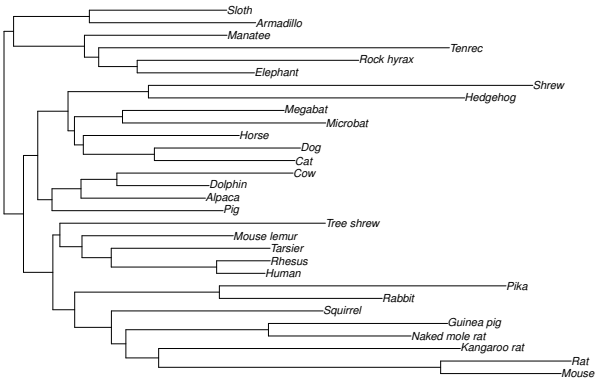

Figure 1: Phylogenetic tree of mammals. The branch lengths are proportional to the number of substitutions per site and show the evolutionary rate in every lineage.

We first improved the method that uses the *global %id* values by addressing the limitations mentioned above. We assume that the topology and the branch lengths of phylogenetic tree (Figure 1) are given. In fact, the tree can be estimated from the DNA sequence of the species and we only consider species with sequenced genomes. Then, the relatedness of these species can be converted into a covariance matrix. Given n species, we define the covariance $n \times n$ matrix R that captures the phylogenetic relatedness as:

$$\begin{aligned} R_{ii} &= L_i \\ R_{ij} &= L_{ij} \end{aligned}$$

where L_i is the total branch length (in substitutions per site) from the common ancestor of to the tip i, and L_{ij} is the total branch length shared by i and j (Figure 2).

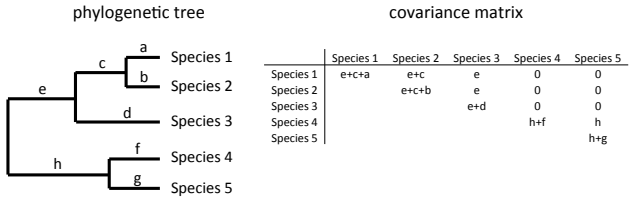

Figure 2: Illustration of how to compute a covariance matrix from a phylogenetic tree that captures the relatedness of the species. Lower case letters (a-h) indicate the branch lengths.

We define X and Y to be vectors of the *global %id* and the phenotype data, respectively:

$$X = (x_1, x_2, ..., x_n),\ Y = (y_1, y_2, ..., y_n).$$

Then, a Generalized Least Square (GLS) approach [2]

$$b = (X^T W^{-1} X)^{-1} X^T W^{-1} Y \qquad (2)$$

can be used to estimate the correlation between *global %id* and the phenotype by testing the significance of the slope.

A new method using local divergence In addition to the global method described above, we also developed a new method that measures local sequence divergence. The maximum likelihood method that we use to reconstruct the DNA sequence of the common ancestor can also be used to reconstruct the most likely sequence of every internal node in the phylogenetic tree. This means, we can define a *local %id* value for every branch (Figure 3). In contrast to the *global %id* values, these *local %id* values are all independent as every branch in the phylogenetic tree represents independent evolution, which solves the problem of relatedness in our data.

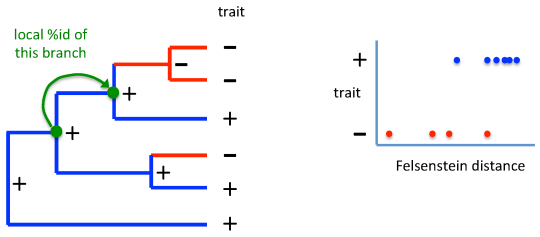

Figure 3: Left: Given the presence/absence of a trait (+/-), we can reconstruct the ancestral phenotype states by parsimony and classify each branch into a trait-loss branch (red) and a trait-preserving branch (blue). A *local %id* is computed between the sequences at the start and end of each branch, which is either a reconstructed DNA sequence or the sequence of an extant species (leave). Right: Given the Felsenstein distances of each branch, we expect that trait-involved genomic regions have lower values for trait-loss branches and higher values for trait-preserving branches.

To account for differences in evolutionary rates (i.e. differences in the branch lengths), we pre-compute the distribution $P(\%id, b|selection)$ of the %id values at the branch of length b that evolves under selection by simulating the evolution of a genome containing thousands of conserved elements. This distribution is then used to normalize for differences in evolutionary rates by computing for a given genomic element e the Felsenstein distance:

$$F(e, b) = \%id(e, b) - \text{mean}(P(\%id, b|selection)).$$

Hence genomic elements under selection will have $F(e, b) \sim 0$, while elements that evolve neutrally on that branch will have $F(e.b) < 0$. Then, we compute the significance of a positive Pearson correlation coefficient to test if there is a trend that trait-loss branches evolve neutrally (lower Felsenstein distances, Figure 3). Tests have shown that the Pearson correlation has substantially more power than the Spearman correlation or a Wilcoxon rank-sum test that ignore the quantitative information in our data.

Evaluation on simulated data Because we lack comprehensive real data that tells us which genomic loci are/are not involved in a phenotypic differences, we created test data by simulating genome evolution and trait loss. In these simulations, we randomly pick a number of conserved elements (trait-involved elements) and let them evolve neutrally in independent lineages. Afterwards, we compute *local* and *global %id* values and test how well our two new methods can find the elements that we let evolve neutrally.

We simulated over 50 different trait loss scenarios covering different numbers of independent losses in different lineages with different evolutionary rates as well as different trait loss ages. We found that both the new global and local method have a substantially increased performance compared to the "Perfect-match" method [1] (two examples are shown in Figure 4). Furthermore, the local method often outperforms the global method.

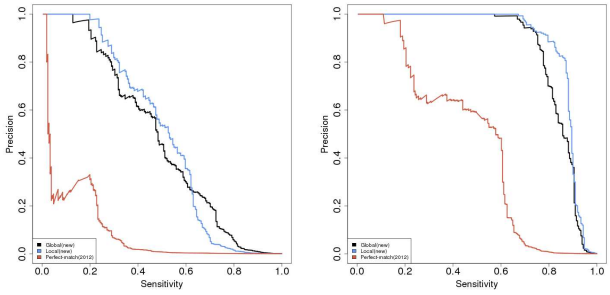

Figure 4: Plot showing the precision and sensitivity of the previous Forward Genomics method (Perfect-match) and our two new methods (Global and Local). The scenario is a trait loss in 3 independent lineages that happened 0.05 (A) and 0.1 (B) substitutions per site ago.

Future Plans We plan to apply both new methods to already available and new phenotypic differences. Promising candidate loci will be tested by us and by our collaborators. We also want to explore under which conditions one of the two methods has more power and we want to create a searchable web database that integrates information about the discovered genomic loci and associated phenotypes as a public resource.

[1] M. Hiller et al., Cell Rep **2** (2012) 817-823.

[2] A. Grafen, Philos Trans R Soc Lond B Sci **326** (1989) 119-157.

2.27 Development of a computational approach to accurately detect gene losses in genome sequences

VIRAG SHARMA, ANAS ELGHAFARI, BJOERN LANGER, LEO FOERSTER, MICHAEL HILLER

Motivation Gene losses are one important class of genomic differences with likely functional consequences for the organism. Individual case studies have shown that gene losses can be involved in both loss and gain of phenotypes during evolution. For example, the loss of alpha/beta-globin and myoglobin genes in Antarctic icefish led to one of the most remarkable phenotype losses in vertebrates, the absence of red blood cells [1]. This is an adaption to the artic environment as the loss of red blood cells reduces blood viscosity and enough oxygen dissolves in the plasma at these temperatures. Although counterintuitive, gene loss can also be beneficial; the so called "less is more" principle. For example, the loss of *ACTN3* that is associated with increased endurance athletic performance in mice and humans [2]. Here, we define a lost gene as a protein-coding gene with clear gene-inactivating mutations (frameshifting insertions and deletions, stop codon mutations, splice site disrupting mutations, larger deletions) that lead to a likely non-functional protein.

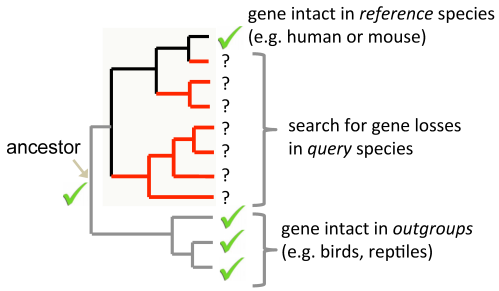

Figure 1: General framework: Genes that are functional in a chosen reference species and intact in phylogenetic outgroups must be ancestral, therefore we can search all for gene loss in all query species (indicated by ?). Red branches are branches in the phylogenetic tree where gene loss can be detected.

Development of a gene loss detection approach A key prerequisite to study how gene loss contributes to phenotypic change is a computational approach that systematically detects gene losses in any given species at high accuracy in an automatic fashion. While detecting gene losses at the level of individuals of the same species is essentially a solved problem, at the between-species level this is an unsolved challenge. The two main problems are: (i) over longer evolutionary timescales, genes can change their exon-intron structure and (ii) accurate sequence alignments are much more difficult due to an increased amount of sequence change and the fact that different species have genome assemblies of varying quality and completeness. We have developed a computational multi-step pipeline that addresses these issues and we describe here the concept and implementation steps.

Our general framework makes use of a selected reference species, where a set of genes is annotated, and query species, where we search for loss of these genes (explained in Figure 1). By definition, real loss necessitates that the gene was present in the ancestor, which we assure by only including genes who have a clear ortholog in phylogenetic outgroups.

Challenges in achieving high accuracy Our work identified a number of problems leading to false positives that we needed to solve in order to achieve an accuracy high enough that no manual curation of the results is necessary anymore.

First, assembly gaps (regions of the real genome that did not make it into the available genome assembly) mimic the deletion of exons or genes. As shown in Figure 2A, the first exon (blue box) of the human *CYP11A1* gene aligns to rat (black parts indicate aligning sequence). While this exon appears to be deleted in the cow 2007 assembly (double horizontal lines), where it overlaps an assembly gap, the newer 2011 assembly of the cow closes this assembly gap and shows that this exon does align to the cow. We solve this problem by ignoring deletion candidates that map to an assembly gap in the query species.

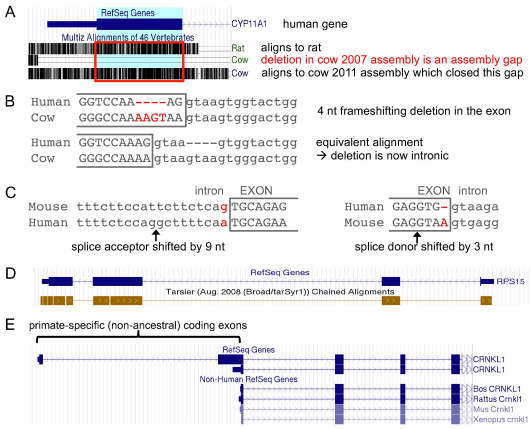

Figure 2: Types of False Positives: (A) Assembly gaps mimic exon deletions. (B) Alignment ambiguities and (C) splice site shifts mimic gene-inactivating mutations. (D) Genome alignments are contaminated with alignments to processed pseudogenes. (D) Lineage-specific exons in ancestral genes should be excluded.

Second, alignment ambiguities can be mistaken for real mutations. Figure 2B shows two alignments that have the same number of matching bases. The first alignment shows a 4 nt frameshifting deletion in the exon. However, the second alignment, where this 4 nt deletion is in the intron, shows that there is no mutation that inactivates a gene.

Third, over evolutionary time, splice sites (exon boundaries) can shift, which also leads to incorrect detection of gene-inactivating mutations. Figure 2C shows on the left an acceptor splice site disrupting mutation in human that becomes exonic as the real human acceptor has been shifted 9 nt upstream. On the right in Figure 2C, the frameshifting 1 nt insertion at the end of the exon in mouse becomes intronic as the mouse splice donor site has shifted 3 nt upstream. We solved both the alignment ambiguity and splice site shift problem by developing a Hidden Markov Model with a layout (Figure 3) tailored to our problem. The model consists of different states that correspond to the splice sites and codons of an exon. Each codon state emits the sequence in the given reading frame. States are connected by transitions that preserve the gene structure with a high probability (black, green and blue arrows) and low-probability transitions (red) that delete splice sites or introduce frameshifting insertions/deletions. We have trained the model parameters so that the most likely path (corresponding to a new sequence alignment) will avoid gene-inactivating mutations whenever possible. Otherwise, the model will give an alignment with a minimal number of gene-inactivating mutations.

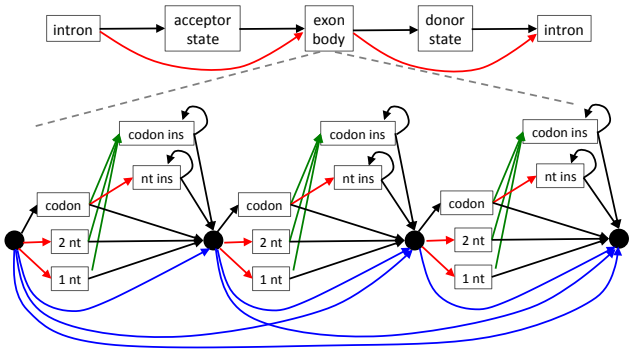

Figure 3: Hidden Markov Model layout. Boxes or black circles are the states, arrows represent the transitions. For each codon in the reference sequence, the model will have a set of states called "codon", "1 nt", "2 nt", "codon ins" and "nt ins". The figure shows only an excerpt with 3 codons.

Fourth, genome alignments (the basis for our approach) are contaminated with alignments of processed pseudogenes, which arise by reverse-transcribing a spliced mRNA and inserting this intron-less gene copy into the genome. Such processed pseudogene copies evolve neutrally and accumulate mutations. Figure 2D shows the *RPS15* gene (blue boxes are exons, blue lines are introns) that is not contained in the low-quality assembly of the tarsier, however a processed *RPS15* pseudogene aligns instead (brown boxes in an "alignment chain" represent aligning regions, the brown horizontal lines show the lack of all introns, a hallmark of a processed pseudogene). To avoid mistaking the alignment to such a pseudogene for the alignment to the real gene ortholog, we implemented a filtering procedure to remove such alignments. that only includes alignments that span multiple genes and have intronic sequences.

Fifth, while we only analyze ancestral genes (Figure 1), individual exons of a transcript of this gene can be non-ancestral. An example is shown in Figure 2E, where the first two exons of the longest transcript of *CRNKL1* are primate-specific and we incorrectly detect gene-inactivating mutations in these exons in non-primate species. In contrast, all exons of the shorter transcript are ancestral as they occur in cow, rat, mouse and frog ("Non-human RefSeq Genes") and no mutation is detected in the shorter transcript. To solve this problem, we now first determine which transcript is free of gene-inactivating mutations in our outgroup species and only analyze this transcript in the query species.

Value of this pipeline for future research We will apply our gene pipeline to create a resource of lost genes for many different species (mammals, fruit flies etc.). This provides a powerful resource for Forward Genomics to use this gene loss data to search for genes that are lost in all phenotype-loss lineages and will increase both the sensitivity and specificity compared to our existing approach that measures nucleotide divergence. Sensitivity will increase because a few gene-inactivating mutations in one lineage clearly indicate loss of the gene, however these mutations might not lead to an increased nucleotide divergence compared to other lineages. Such cases will be missed by the current Forward Genomics implementation. Specificity will increase because fast protein evolution (maybe due to positive selection) or lots of synonymous mutations result in increased nucleotide divergence, but do not indicate gene loss (in fact positive selection is rather a sign of gain of function). Such cases will erroneously detected by our current Forward Genomics implementation.

Furthermore, this resource enables use to determine general characteristics of lost genes by investigating if these genes differ in gene pleiotropy, evolutionary age, paralogy and lethal phenotypes from genes that are not lost in evolution.

[1] CH. Cheng et al., Philos Trans R Soc Lond B Sci **362** (2007) 2215-2232.

[2] DG. MacArthur et al., Nature Genetics **39** (2007) 1261-1265.

2.28 Spatio-temporal dynamics of Eg5 in mitotic spindles

CARLOS GARZON CORAL, ANITA JANNASCH, JAN BRUGUES

The mitotic spindle is a highly dynamic self-organized assembly, composed of microtubules, molecular motors, and other associated proteins, that segregates chromosomes during cell division. Hundreds of proteins have been found to contribute to spindle assembly [1] but how are they spatially and temporally organized in the spindle, and how their molecular activities control microtubule interactions and contribute to the overall spindle morphology is not known. A common approach to understanding how molecular activities control spindle behavior is to perturb those activities and follow the effects on spindle dynamics and shape.

As an illustrative example of these perturbations, spindles become monopolar after inhibiting the kinesin molecular motor Eg5, and have diffuse poles after inhibiting Dynein; but their simultaneous inhibition restores the shape of a regular spindle [2]. These observations may suggest that Eg5 and Dynein have opposing activities that cancel each other out. However, we recently shown using laser ablation perturbations [3] and measuring spatio-temporal correlation functions of microtubule density, orientation and stress [4], that the microtubule organization and mechanical properties of regular and Eg5-Dynein double inhibited spindles are dramatically different despite their similar overall shape. These preliminary results show a more complex interaction between these two motors, and indicate that Eg5 organizes microtubules and establishes a gradient of polarity in the spindle—which may be important for localizing proteins involved in chromosome segregation—, whereas Dynein forms poles in the spindle without affecting microtubule lengths or polarity. To better understand the relation between the spatio-temporal dynamics of motors and the overall microtubule organization in spindles, here we will concentrate on studying the dynamics of Eg5 in spindles.

Eg5 is a tetrameric motor which motor domains walk towards the plus ends of microtubules, see figure 1. Eg5 is responsible for the spindle architecture and its polarity by sliding anti-parallel microtubules apart [3]. Microtubule polarity changes almost linearly across the spindle, with antiparallel microtubules in the center, and parallel microtubules at the poles with plus ends pointing toward the center. Based on this microtubule organization, Eg5 is expected to concentrate in the center of spindles, where it can slide anti-parallel microtubules. Additionally, since the average polarity points towards the center of the spindle, Eg5 is expected to also walk and concentrate towards the center of spindles. Florescence imaging of Eg5-GFP shows, however, that Eg5 concentrates mainly at the poles [5], which is a priori inconsistent with its microscopic activity. Moreover, photo-activation experiments show that Eg5 appear to move towards the poles [5]. Conversely, in our measurements, single molecule Eg5 has very fast binding and unbinding dynamics (with a characteristic turnover time of ~ 225 ms) and appears everywhere in the spindle. To reconcile these two seemingly contradicting results between the large-scale concentration of Eg5 and its individual activities, we here aim to combine a theoretical model of Eg5 activity together with single molecule measurements using a custom build microscope to understand the spatio-temporal dynamics of Eg5 and its relation to spindle architecture.

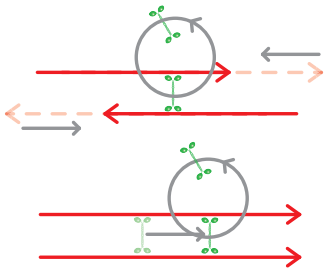

Figure 1: Schematics of Eg5 activity and dynamics. Top panel, when Eg5 binds to two anti-parallel microtubules, it slides microtubules apart (arrows indicate microtubule plus ends). Dotted microtubules indicate their position before sliding. Lower panel, when Eg5 binds to parallel microtubules, it walks towards their plus ends without sliding. Eg5 binds and unbinds to microtubules with a residence time depending on the force it exerts to microtubules.

We consider Eg5 as a two state model of bound and unbound species, characterized by their density ρ^b, and ρ^u respectively,

$$\frac{\partial \rho^b}{\partial t} = -\nabla(\mathbf{v}^b \rho^b) - k_d(\mathbf{x})\rho^b + k_a \rho^u \tag{1}$$

$$\frac{\partial \rho^u}{\partial t} = D\nabla^2 \rho^u + k_d(\mathbf{x})\rho^b - k_a \rho^u. \tag{2}$$

where we assume that diffusion of Eg5 in the bound state is negligible, and when bound, Eg5 walks with a velocity proportional to microtubule polarity $v^b \sim v_0 \mathbf{p}$, with $v_0 = 2.5\mu$m/min. We estimate the bulk diffusion constant as the diffusion constant of a rod with the size of Eg5, leading to $D \sim 5\mu\text{m}^2/s$. Finally, k_a and $k_d(\mathbf{x})$ are the rates of attachment and detachment from microtubules respectively. The detachment rate is assumed to follow a Kramer's-like kinetics,

$$k_d(x) = k_d^0 \exp\left[f(x)d/kT\right], \tag{3}$$

where d is a characteristic bond length in the nanometric scale, $f(x)$ is the force Eg5 applies to the microtubules, and k_0 the detachment at vanishing force

which we observe in our measurements to be $1/k_d \sim 225$ ms.

Eg5 only applies force when it binds to antiparallel microtubules (neglecting any drag from Eg5 moving on microtubules), and therefore $f(x)$ is given by the characteristic force a motor exerts (f_0) times the probability to find antiparallel microtubules in the spindle ($1 - |p(x)|$). We have previously shown that microtubule polarity in *Xenopus laevis* spindles increases linearly from pole to pole, $p(x) \sim \alpha(1 - 2x/L)$, where $L \sim 30\mu$m is the total spindle length [3]. The detachment rate is therefore maximum at the center of the spindle and minimum at the poles. The steady-state density of bound Eg5 in spindles can be approximated by

$$\rho^b(x) \sim \frac{k_a}{k_d}\rho^0 \exp\left[(1 - |\alpha(1 - 2x/L)|)d/kT\right], \quad (4)$$

where ρ^0 is the bulk concentration of unbound Eg5, which in extract is much larger than the bound fraction. This exponential dependence on the position along the spindle matches remarkably well the intensity profile of Eg5 in spindles as obtained from [5], see figure 2 A.

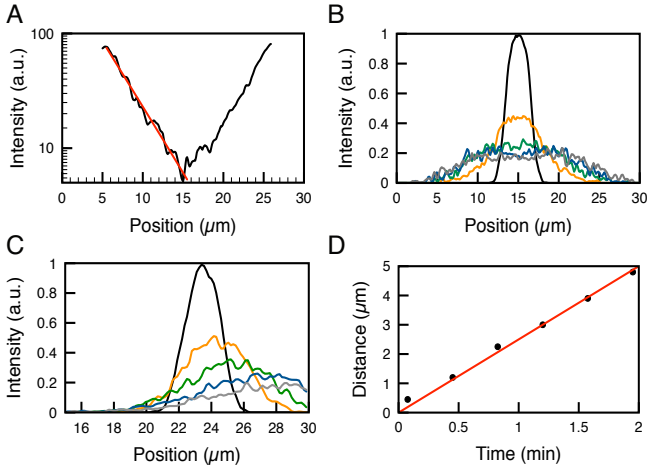

Figure 2: Theoretical predictions for Eg5 dynamics in spindles. A, log-linear plot of the density of Eg5 as a function of the position of the spindle (black, from [5]) and theoretical prediction (red). B, predicted temporal dependence of Eg5 photoactivation at the middle of the spindle. B, temporal dependence of Eg5 intensity after photoactivation of a stripe at 23 μm away from the left pole for 0.75, 0.45, 0.82, 1.57, and 1.95 minutes after photobleaching. C, dependence of the position of the intensity peak as a function of time (black dots), and corresponding linear fit (red line).

We next predict photo-activation experiments by simulating equations 1 and 2 with a stripe of bound Eg5-GFP at the center of the spindle and midway between the center and the pole as initial conditions, see figure 2. At the center, the residence time of Eg5 is symmetric with respect to the original photo-activation region and the stripe simply spreads away. Conversely, when photo-activating midway between pole and center, the residence time of Eg5 is larger towards the pole, which leads a biased diffusion motion towards it. Tracking of the peaks results in an apparent directed motion to the poles, figure 2 D. Our predictions are consistent with the photo-activation experiments from [5], however, our interpretation is fundamentally different; Eg5 has fast binding and unbinding dynamics that depends on the local polarity of microtubules. This fast dynamics results in a spatial organization of Eg5 that decreases exponentially from pole to center, were it slides antiparallel microtubules apart.

To validate experimentally our model, we are building a microscope capable of measuring the fast dynamics of Eg5 and providing enough spatial resolution to resolve individual molecules. To this end, we adapted the reflective light-sheet microscope (rLSM) from [6] to use in *X. laevis* egg extracts, see figure 3. Using speckle level Eg5-GFP in spindles we hope to validate our model and shed some light in the spatio-temporal dynamics of Eg5, and their role in the microtubule organization in spindles.

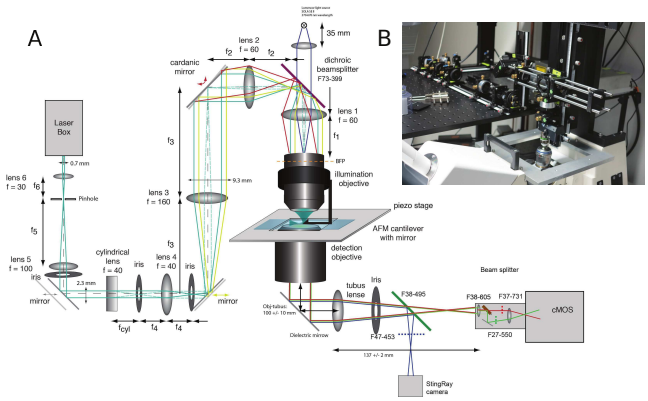

Figure 3: Reflective light-sheet microscope (rLSM). A, schematics of the optic path of the rLSM. B, Microscope set up.

[1] B. Neumann, et al., Nat. Rev. Mol. Cell Biol. 464, 721-727 (2010).

[2] T.J. Mitchison et al., Molecular Biology of the Cell, 16: 3064-3076 (2005).

[3] J. Brugues, et al., Cell 149:554-564 (2012).

[4] J. Brugues, D.J. Needleman, PNAS 111 (52), 18496-18500 (2014).

[5] M. Uteng, et al., Journal of Cell Biology, 10.1083/jcb.200801125 (2008).

[6] J.C. M. Gebhardt, et al., Nature Methods, 10 (5), 421-426 (2013).

2.29 Odd Bose condensation in non-equilibrium steady states

D. VORBERG, W. WUSTMANN, H. SCHOMERUS, R. KETZMERICK, A. ECKARDT

Introduction The dynamics of many-body quantum systems is a wide and widely unexplored terrain, which recently gained a lot of interest. Here, a paradigmatic scenario is given by driven-dissipative quantum systems [1]. In this context, we found that even the ideal Bose gas offers unexpected behavior, when it is driven into a steady state far from equilibrium. Namely, it can undergo a generalized form of Bose condensation, where an odd number of states acquires large occupations [2]. Let us describe the phenomenon starting from the equilibrium situation.

Equilibrium Bose gas and Bose condensation Consider a single-particle system with states $|i\rangle$ of sharp energy E_i, such that $E_0 < E_1 \leq E_2 \leq \cdots$. If the system operator v couples weakly to a heat bath of temperature $T = 1/(k_B\beta)$, the bath will induce transitions between states i and j. Their rates are given by a golden-rule type expression [3]

$$R_{ji} = \frac{2\pi}{\hbar}|\langle i|v|j\rangle|^2 \frac{J(E_j - E_i)}{e^{\beta(E_j-E_i)} - 1}, \tag{1}$$

where $J(E)$ is the spectral density of the bath that we assume to be Ohmic, $J(E) \propto E$. The rates obey

$$R_{ji}/R_{ij} = e^{-\beta(E_j-E_i)}, \tag{2}$$

implying that the steady state is of the form $\hat{\rho} = \sum p_i|i\rangle\langle i|$, with Boltzmann distribution $p_i = e^{-\beta E_i}/Z$.

In an ideal quantum gas of N non-interacting bosons, the rate for a transition where one particle is transferred from state i to j is given by $R_{ji}(n_j + 1)n_i$. It is not only proportional to the occupation n_i of the initial state i, but, as a result of the bosonic quantum statistics, it depends also on the occupation n_j of the final state j. As a simple theoretical tool, one can introduce a mean-field description in terms of the averaged occupation numbers $\bar{n}_i = \langle\hat{n}_i\rangle$, where $\hat{n}_i$ is the number operator for state i. For that purpose, two-particle correlations are assumed to be trivial, $\langle\hat{n}_i\hat{n}_j\rangle \approx \bar{n}_i\bar{n}_j$ for $i \neq j$, in order to arrive at the non-linear equations of motion

$$\dot{\bar{n}}_i = \bar{n}_i \sum_j \left\{R_{ij}\left[1 + \bar{n}_i\right]\bar{n}_j - R_{ji}\left[1 + \bar{n}_j\right]\bar{n}_i\right\}. \tag{3}$$

The steady state of this equation, with $\dot{\bar{n}}_i = 0$, reads

$$\bar{n}_i = \frac{1}{e^{\beta(E_i-\mu)} - 1}, \tag{4}$$

where the chemical potential μ has to be adjusted such that $\sum_i \bar{n}_i = N$. This familiar expression of statistical mechanics [4] reflects that the system is in thermal equilibrium with the bath.

The chemical potential grows with N, until it approaches its saturation value given by E_0, such that $E_0 - \mu \ll E_1 - E_0$. We can then approximate

$$\bar{n}_{i>0} \simeq \frac{1}{e^{\beta(E_i-E_0)} - 1}, \quad \bar{n}_0 \simeq \frac{1}{\beta(E_0 - \mu)} = N - \sum_{i>0} \bar{n}_i. \tag{5}$$

Roughly, all particles that cannot be accomodated in the depletion $N^* = \sum_{i>0}[e^{\beta(E_i-E_0)} - 1]^{-1}$ will occupy the ground state. This is the phenomenon of Bose condensation, occurring when N exceeds N^*. In a finite system it is a crossover; in the thermodynamic limit it either disappears (namely if N^* grows superlinearly with system size) or it becomes a sharp phase transition. An example for finite-size Bose condensation in a tight-binding chain is depicted in Fig. 1(a). For N above $N^* \sim 10^2$ all occupations saturate, except that of the ground state.

Driven-dissipative Bose gas and Bose selection A simple way of driving the system away from equilibrium is to couple it to two heat baths, 1 and 2, of different inverse temperatures $\beta_1 \neq \beta_2$, so that the rates are now given by

$$R_{ij} = R^{(1)}_{ij} + R^{(2)}_{ij}. \tag{6}$$

As a consequence, condition (2) is not valid anymore and equation (3) does not possess a stationary solution of the form (4) anymore, for which its right-hand side vanishes term by term. This indicates the breaking of detailed balance. Such scenarios are depicted in Fig. 1(b) and (c).

In panel (b) both baths are of (different) positive temperature, whereas in panel (c) one bath is population inverted and described by a negative temperature, so that it favors larger occupations in states of higher energy. We can now make two observations. First, for two baths of different positive temperature we can observe that Bose condensation into the ground state still occurs in a similar fashion as in thermal equilibrium. Second, in the presence of the population inverted bath, again most occupations saturate in the limit of large N. But now, as a striking effect, condensation occurs into a whole group of *multiple* (three) selected states. We call this effect *Bose selection* [2]. It can occur when the notion of the single-particle ground state becomes meaningless. Such a situation occurs also when a periodically driven Bose gas, whose quasienergies are defined modulo the driving frequency only so that no ground-state exists, is coupled to a heat bath. This can be observed in Fig. 1(d). Moreover, equations of the form (3) not obeying condition (2) are used in various contexts, such as network dynamics, classical transport, chemical reactions, or evolutionary game theory [5].

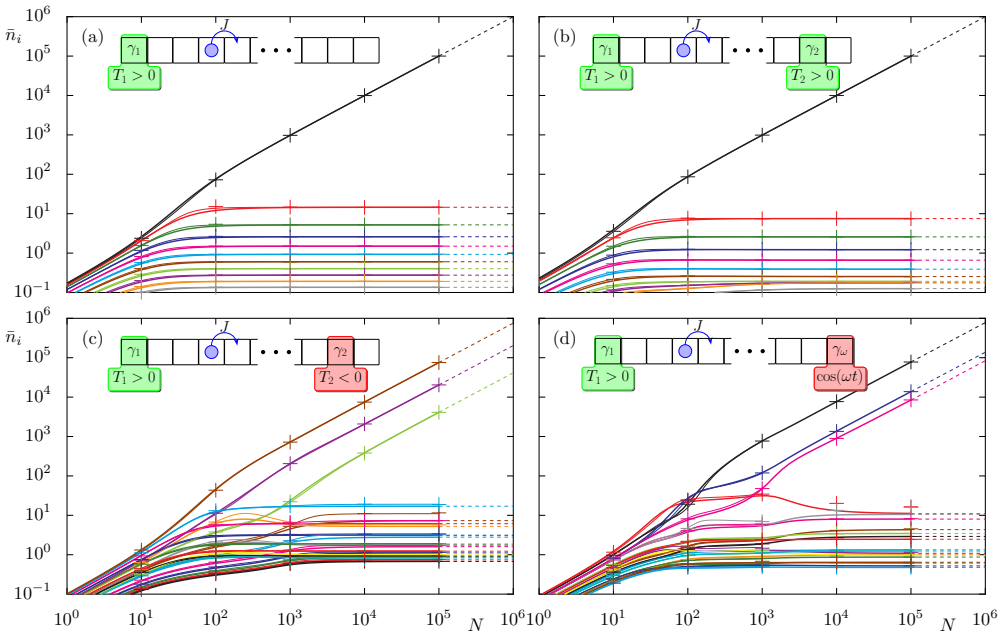

Figure 1: Occupations $\bar{n}_i$ versus particle number for a tight-binding chain of $M = 20$ sites and tunneling parameter J, from mean-field theory (thick solid lines) and exact Monte-Carlo simulations (crosses). (a) Equilibrium, chain coupled to one bath with $\beta = 1/J$. (b) Non-equilibrium situation, with the chain coupled to two heat baths with $\beta_1 = 1/J$, $\beta_2 = 2/J$. (c) Like in (b), but with $\beta_2 = -1/J$. (d) Chain coupled to a bath with $\beta = 1/J$ and subjected to periodic potential modulation at the last site with amplitude $\gamma_\omega = 2.3J$ and frequency $\hbar\omega = 1.5J$.

For a theoretical description of Bose selection, we can use that it occurs for large N. Approximating $\bar{n}_i + 1 \simeq \bar{n}_i$ in Eq. (3), for the steady state we obtain

$$0 = \bar{n}_i \sum_j A_{ij}\bar{n}_j, \qquad A_{ij} = R_{ij} - R_{ji}. \tag{7}$$

Generically, on this level of approximation only a (yet to be determined) subset $\mathcal{S}$ of selected states can have nonzero occupations. For these states Eq. (7) implies

$$0 = \sum_{j\in\mathcal{S}} A_{ij}\bar{n}_j, \quad \text{with} \quad i \in \mathcal{S}. \tag{8}$$

These linear equations possess a meaningful solution only for an appropriate set $\mathcal{S}$. Namely, without fine tuning the skew-symmetric matrix $A_{ij} = -A_{ji}$ possesses a finite kernel only if $\mathcal{S}$ contains an *odd* number M_S of states and, moreover, not every solution gives rise to physically meaningful positive occupations. This restricts the set $\mathcal{S}$. The occupations of the non-selected states are predominantly determined by transitions from or into the highly occupied selected states. Neglecting transitions among non-selected states in a Bogoliubov-type fashion, from Eq. (3) we obtain

$$\bar{n}_i = \frac{1}{g_i - 1}, \quad \text{with} \quad g_i = \frac{\sum_{j\in\mathcal{S}} R_{ji}\bar{n}_j}{\sum_{j\in\mathcal{S}} R_{ij}\bar{n}_j}, \quad i \notin \mathcal{S}. \tag{9}$$

Since the g_i do not depend on N, these equations explain the saturation of non-selected-state occupations. They also determine the total occupation of the selected states,

$$N_S = \sum_{i\in\mathcal{S}} \bar{n}_i = N - \sum_{j\notin\mathcal{S}} \bar{n}_j. \tag{10}$$

Equations (9) and (10) are analogous to the equilibrium Eqs. (5) for the Bose-condensed state. Bose selection is expected to occur when N exceeds the depletion $N^* = \sum_{i\notin\mathcal{S}}[g_i - 1]^{-1}$. However, the set $\mathcal{S}$ has still to be determined from the requirement $\bar{n}_i \geq 0 \forall i$. This is typically a non-trivial task, which reflects the many-body character of the driven-dissipative ideal Bose gas. We can show that condensation into a single state k, like in Fig. 1(a,b), occurs if $R_{ki} > R_{ik} \forall i$ [2]. However, otherwise an odd number of states $M_S \geq 3$ will be selected.

[1] Markus Müller, Sebastian Diehl, Guido Pupillo, Peter Zoller, Adv. At. Mol. Opt. Phys. 61, 1 (2012).

[2] Daniel Vorberg, Waltraut Wustmann, Roland Ketzmerick, André Eckardt, Phys. Rev. Lett. **111**, 240405 (2013).

[3] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002)

[4] R.K. Pathria *Statistical Mechanics, Second Edition* (Butterworth-Heinemann, Oxford, 1996)

[5] G. Bianconi and A.-L. Barabasi, Phys. Rev. Lett. **86**, 5632 (2001); M.R. Evans and T. Hanney, J. Phys. A: Math. Gen. **38**, R195 (2005); A. Schadschneider, D. Chowdhury, and K. Nishinari, *Stochastic Transport in Complex Systems—From Molecules to Vehicles* (Elsevier, New York, 2011); J. Knebel, M.F. Weber, T. Krüger, E. Frey, Nat. Comm. **6**, 6977 (2015).

2.30 Hierarchical fractal weyl laws for chaotic resonance states in open mixed systems

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Introduction A century ago, Hermann Weyl published his celebrated theorem on the asymptotic distribution of eigenmodes of the Helmholtz equation in a bounded domain [1] which has found fundamental applications in the context of acoustics, optical cavities and quantum billiards. For a quantum billiard with a d dimensional phase space the number $\mathcal{N}(k)$ of eigenmodes with a wave number below k is asymptotically given by $\mathcal{N}(k) \sim k^{d/2}$. Only recently, this fundamental question has been addressed for open scattering systems, where for the case of fully chaotic systems a fractal Weyl law was found [2, 3]. Due to the opening of the system one classically obtains a fractal chaotic saddle [4], which is the invariant set of points in phase space that do not escape, neither in the future nor in the past. Its fractal dimension δ plays an important role quantum mechanically: The number $\mathcal{N}$ of long-lived resonance states is given by a fractal Weyl law,

$$\mathcal{N}(h) \sim h^{-\delta/2}, \tag{1}$$

which here is stated for open chaotic maps, where the k dependence is replaced by the dependence on the effective size h of Planck's cell.

Generic Hamiltonian systems exhibit a mixed phase space where regular and chaotic motion coexist, see Fig. 1(a). Regular resonance states of the open system obey a standard Weyl law, while for chaotic resonance states one would naively expect that their number follows the fractal Weyl law, Eq. (1). This ignores, however, that the dynamics in the chaotic region of generic two-dimensional maps is dominated by partial transport barriers [5], see Fig. 1(a). A partial barrier is a curve which decomposes phase space into two almost invariant regions. The small area enclosed by the partial barrier and its preimage (dotted line in Fig. 1(a), magnification) consists of two parts of size Φ on opposite sides of the partial barrier, which are mapped to the other side in one iteration of the map. This flux Φ is the characteristic property of a partial barrier. It is well known that such partial barriers strongly impact the system's classical and quantum mechanical properties. Their influence on fractal Weyl laws for open systems with a mixed has been studied recently in Ref. [6], which we review here.

Fractal chaotic saddle We start with the classical properties of the chaotic saddle in a generic mixed system and illustrate them for the prototypical example of the standard map as shown in Fig. 1(a). We open the system by defining absorbing stripes on the left and right, see Fig. 1(b). This leads to a chaotic saddle Γ, for which a finite-time approximation is shown in Fig. 1(b).

The chaotic saddle Γ of the open system is strongly structured by the presence of partial barriers. Partial barriers provide a hierarchical tree-like decomposition of the chaotic component of phase space into regions A_j. Using the box-counting method, one can associate a fractal dimension δ_j to the intersection $\Gamma \cap A_j$ of the chaotic saddle Γ with each of the regions A_j. It turns out that the chaotic saddle in generic two-dimensional open maps gives rise to an individual fractal dimension for each region of the hierarchical decomposition of phase space [7]. The number $N_j^{\mathrm{bc}}(\varepsilon)$ of occupied boxes of side length ε scales like $N_j^{\mathrm{bc}}(\varepsilon) \sim \varepsilon^{-\delta_j}$, see Fig. 1(c), with $\delta_0 = 1.68$ and $\delta_1 = 1.86$. To emphasize the difference between such dimensions close to two, the ordinate is rescaled by ε^2, yielding the rescaled counting function $\widetilde{N}_j^{\mathrm{bc}}(\varepsilon) = N_j^{\mathrm{bc}}(\varepsilon) \cdot \varepsilon^2$. It is important to stress that these are *effective* fractal dimensions, which are constant over several orders, while in the limit of arbitrarily small scales, they approach two.

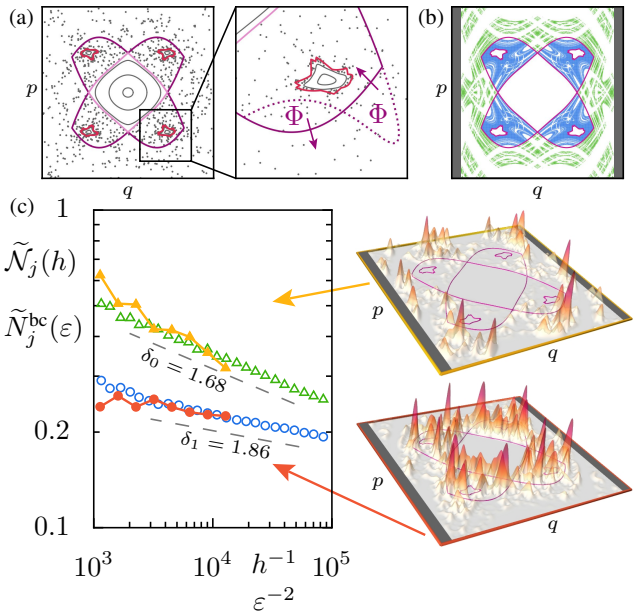


Figure 1: (a) Phase space of the standard map with regular (solid gray lines) and chaotic (gray points) orbits, three partial barriers (solid colored lines) and the preimage of the outermost partial barrier (dotted magenta line). (b) Chaotic saddle of the opened map (gray-shaded absorbing stripes) colored according to the regions (A_0: green, A_1: blue). (c) Rescaled hierarchical fractal Weyl laws $\widetilde{\mathcal{N}}_j$ vs. h^{-1} (filled symbols) counting hierarchical resonance states in the outer (A_0, triangles) and inner (A_1, circles) chaotic regions (with corresponding typical Husimi representations for $h = 1/1000$). Their power-law scaling is compared to the rescaled box-counting scaling $\widetilde{N}_j^{\mathrm{bc}}$ vs. ε^{-2} (open symbols) with fractal dimension δ_j in region A_j of the chaotic saddle.

Hierarchical resonance states Resonance states ψ of the open quantum system are given by $U_{\text{open}}\psi = \exp[-i(\varphi - i\gamma/2)]\psi$, where U_{open} denotes the corresponding time-evolution operator. Regular resonance states are predominantly located in the regular region. Chaotic resonance states are predominantly located in either of the hierarchical regions A_j, see Fig. 1(c). Hence, we call them *hierarchical resonance states* (of region A_j). Such a localization of chaotic eigenstates on different sides of a partial barrier is well known for closed quantum systems [8]. It requires that the classical flux Φ across a partial barrier is small compared to the size h of a Planck cell, i. e. $\Phi \ll h$. In the opposite case, eigenstates would be equidistributed ignoring the partial barrier. Quite surprisingly, in open quantum systems we find that this condition from closed systems is irrelevant for hierarchical resonance states. In the standard map, we have $\Phi \approx 1/80$ and for $h = 1/1000$, such that the condition $\Phi \ll h$ is violated, typical resonance states still predominantly localize in one of the regions A_j, as shown in Fig. 1(c). This is still the case for $h = 1/12800$, see Fig. 2. This highlights the strong impact of the opening.

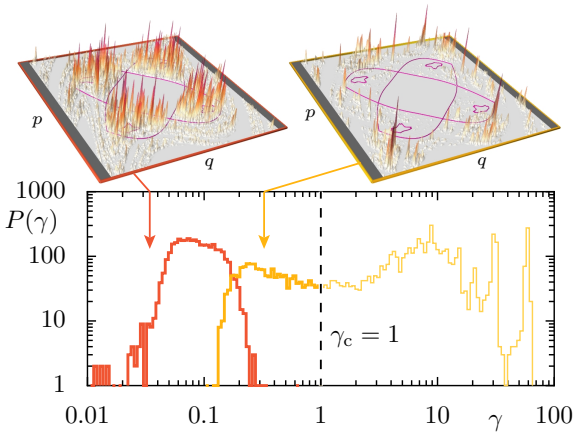


Figure 2: Distributions $P(\gamma)$ of decay rates γ for hierarchical resonance states of the standard map located in regions A_0 (right, yellow) and A_1 (left, red) for $1/h = 12800$ and corresponding Husimi representations of typical states. Short-lived states ($\gamma > \gamma_c$) are not counted in the fractal Weyl law.

A detailed study of this localization of chaotic resonance states in the presence of partial barriers due to the opening is currently carried out [9]: we find that this localization is already present classically for the corresponding conditionally invariant measures. Based on this insight we can predict the localization of quantum states in the semiclassical limit showing that hierarchical resonance states exist because the classical escape rates of neighboring regions A_j are sufficiently different.

Hierarchical fractal Weyl laws The localization of hierarchical resonance states in either of the regions A_j allows their classification. Numerically, we use their relative local Husimi weight in A_j and discard states with more than 50% Husimi weight in the regular region and the deep hierarchical region (A_j, $j \geq 2$). This classification is supported by the distribution of the decay rates γ of the corresponding resonance states, see Fig. 2. States which are located deeper in the hierarchy have smaller decay rates.

For each region A_j of the hierarchical phase space we now relate the number $\mathcal{N}_j$ of hierarchical resonance states of that region to the fractal dimension δ_j of the chaotic saddle in that region. To this end we use the fractal Weyl law of fully chaotic systems [2, 3], Eq. (1), individually for each region A_j. This gives our main result that in open systems with a mixed phase space one obtains a hierarchy of fractal Weyl laws, one for each phase-space region A_j,

$$\mathcal{N}_j(h) \sim h^{-\delta_j/2}. \tag{2}$$

We stress that this result is based on the surprising existence of hierarchical resonance states. Note that as a consequence of Eq. (2) the total number of long-lived hierarchical resonance states is a superposition of power laws with different exponents and not a single power law. This holds over ranges of h where on the corresponding classical scale the effective fractal dimension δ_j is constant.

The numerical investigation of the standard map supports the existence of hierarchical fractal Weyl laws. We restrict ourselves to the consideration of small h such that $\Phi/h \gtrsim 10$ where quantum mechanics can very well mimic classical transport in phase space [8]. Short-lived states are discarded by defining an arbitrary cut-off rate $\gamma_c = 1$, as usual for the fractal Weyl law. We obtain distinct behavior for each rescaled counting function $\tilde{\mathcal{N}}_j(h) = \mathcal{N}_j(h) \cdot h \cdot f_j$, see Fig. 1(c), corresponding to the previous classical rescaling. We fitted prefactors f_j to the quantum results to better demonstrate their scaling with power laws in agreement with the classical counterparts ($f_0 = 2.6$, $f_1 = 0.85$). Apart from the smallest values of $1/h$, one observes the power-law scaling of Eq. (2) and good agreement with the box-counting results for the fractal dimensions δ_j of the chaotic saddle in region A_j.

[1] H. Weyl, *Math. Ann.* **71**, 441 (1912).

[2] W. T. Lu, S. Sridhar, and M. Zworski, *Phys. Rev. Lett.* **91**, 154101 (2003).

[3] H. Schomerus and J. Tworzydło, *Phys. Rev. Lett.* **93**, 154102 (2004).

[4] E. G. Altmann, J. S. E. Portela, and T. Tél, *Rev. Mod. Phys.* **85**, 869 (2013).

[5] J. Meiss, *Rev. Mod. Phys.* **64**, 795 (1992).

[6] M. J. Körber, M. Michler, A. Bäcker, and R. Ketzmerick, *Phys. Rev. Lett.* **111**, 114102 (2013).

[7] A. E. Motter, A. P. S. de Moura, C. Grebogi, and H. Kantz, *Phys. Rev. E* **71**, 036215 (2005).

[8] M. Michler, A. Bäcker, R. Ketzmerick, H.-J. Stöckmann, and S. Tomsovic, *Phys. Rev. Lett.* **109**, 234101 (2012).

[9] M. J. Körber, A. Bäcker, and R. Ketzmerick, in preparation.

2.31 Extraordinary behavior in networks of introverts and extroverts

KEVIN E. BASSLER

Social networks are common in nature and show a fascinating variety of complex, collective behaviors. Examples of social networks include not only ones involving people, but also quorum sensing bacteria, colonies of ants, starling murmurations, and whale pods. There are, however, many challenges to understanding them. Among these challenges is the fact that the dynamics of these networks is typically driven by exogenous mechanisms, preventing them from reaching an equilibrium state. Non-equilibrium statistical mechanics (NESM), therefore, must be employed to describe them. Unfortunately, many of the fundamental principles of NESM and of non-equilibrium systems in general are poorly understood. Thus, understanding and predicting the evolution of social networks is extremely difficult. In this effort, the study of simple models that show some collective effects can be quite instructive. This is also a prerequisite for tackling more complex and realistic models.

In this spirit, consider a simple model of a dynamic social network in which each person (node) has a preference for the number of social contacts (links) they maintain. People tend to add links when they have fewer than they would like to have, and cut links when they have too many. The preferred number of links of each node, their preferred degree, can vary from node to node, for instance when some nodes are introverts who prefer few friends and others are extroverts who prefer many, The preferred degrees of the nodes can also vary from time to time. This occurs for instance when a person is medically quarantined. Incorporating some randomness in the actions of individuals, such preferred degree networks undergo stochastic evolution. What are the statistical properties of such a network (for example, its degree distribution)? Are they mundane or surprising? Are some properties more robust, independent of details of evolution rules, similar to the universality seen in equilibrium phase transitions?

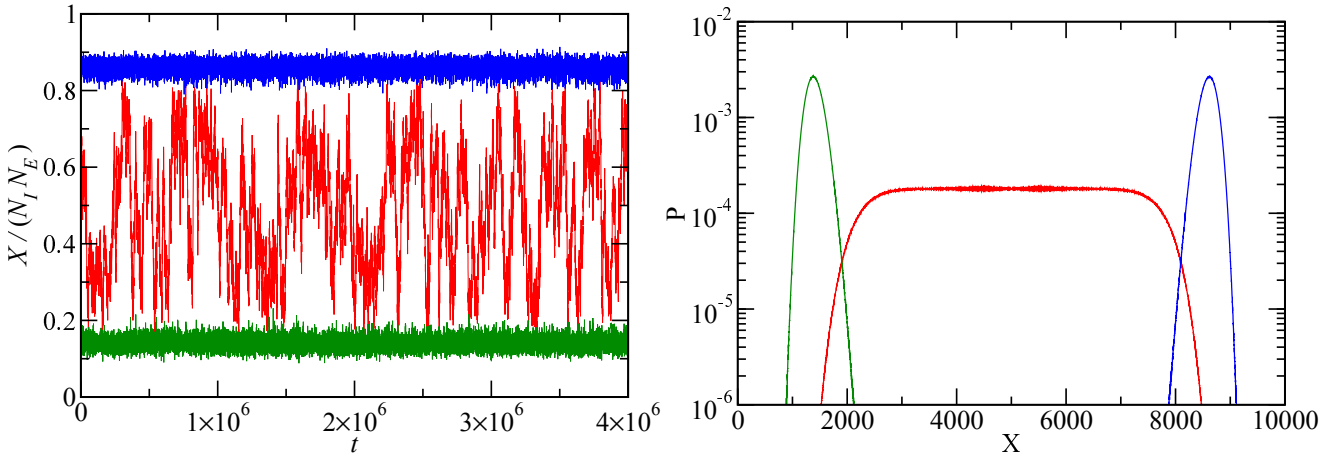


Figure 1: A 'mixed order' phase transition displaying an extreme Thousless effect in a preferred degree network consisting of extreme introverts and extroverts. Steady state time traces of the number of cross-links between introverts and extroverts X (left) and its steady state probability distributions P(X) (right) for three cases with (N_I ,N_E) near/at criticality, shown in green (101, 99), red (100, 100), and blue (99, 101). From [2].

We have studied a number of variants of preferred degree networks and have found that they display a wide variety of remarkable behavior [1]. Perhaps the most remarkable of all of the behavior we have discovered, though, is that when the network consists of introverts and extroverts an extraordinary type of phase transition can occur [2]. In common descriptions of phase transitions, first order transitions are characterized by discontinuous jumps in the order parameter and normal fluctuations, while second order transitions are associated with no jumps and anomalous fluctuations. Outside this paradigm are unusual systems that exhibit 'mixed order transitions' that possess a mixture of these characteristics. When the jump is maximal and the fluctuations range over the entire range of allowed values, the behavior has been coined an *extreme Thouless effect*. Preferred degree networks composed of introverts and extroverts display an *extreme Thouless effect*.

A mixed order phase transition with an extreme Thouless effect is clearly seen in a particularly simple version of preferred degree networks. Assume that the introverts and extroverts are extreme in the sense that they prefer to have contacts with, respectively, no one or everyone. The system is updated by randomly choosing a

node and then either cutting or adding a link depending on whether it is an introvert or an extrovert. Evidence of an extreme Thouless effect in the model can be seen in Fig. 1, showing the time traces and distribution of X, the total number of links between introverts and extroverts (cross links) for a system with 200 nodes. On either side of the symmetry point (N_I, the number of introverts, being the same as the number of extroverts, N_E), X is substantially different from being half of its maximum value. The right subfigure shows that there is a huge, first-order-like jump in the mean value of X when just one node switches between being an introvert and an extrovert. Further, as the left subfigure shows, the fluctuations in X away from the symmetry point are "normal," while at the critical transition point fluctuations are anomalously large, consistent with continuous transition behavior.

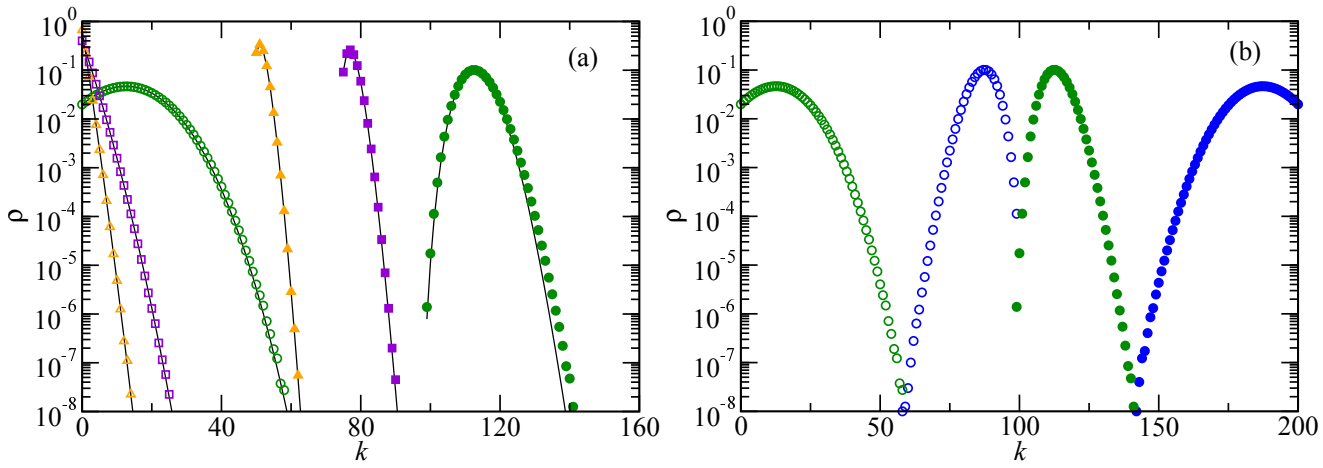


Figure 2: Degree distributions, $\rho(k)$, in the steady state of a preferred degree network consisting of N_I introverts and N_E extroverts for several cases with $N_I + N_E = 200$. Simulation results for the low or high k components, associated with introverts or extroverts, are denoted by open and solid symbols, respectively. (a) The symbols for (N_I ,N_E) are orange triangles (150,50), purple squares (125,75), and green circles (101,99). The solid black lines are predictions from a self-consistent mean-field theory. (b) When two introverts "change sides," a dramatic jump in $\rho(k)$ results, with the case of (99,101) shown as blue circles. From [2].

Remarkably, this extreme variant of introvert and extrovert preferred degree networks also results in a useful simplification for its analytic description. Unlike what happens when the temperament of the individuals is not extreme, detailed balance is restored in the asymptotic dynamics of the extreme variant. Thus, the steady state of this system behaves effectively as one in thermal equilibrium, allowing use of many of the theoretical tools and principles known about equilibrium systems. From the dynamics, we have derived an exact distribution of microstates in the stationary state. In addition to simulations, we have formulated a self-consistant mean-field theory that provides evidence that this system displays an extreme Thouless effect. Specifically, the fraction X/ ($N_I N_E$) jumps from 0 to 1 (in the thermodynamic limit) when N_I crosses N_E, while all values appear with equal probability at $N_I = N_E$. Furthermore, as shown in Fig. 2, the mean-field theory can accurately predict the degree distributions of even near (but not exactly!) critical states. Note also, as the figure shows, the dramatic change in the degree distribution as the transition is crossed.

Finding a mixed order phase transition with an extreme Thouless effect in such a simple model of social networks was surprising and illustrates the remarkable variety of behavior that can occur in such non-equilibrium systems. Similar transitions are also found in other, very different systems, including in some models of wetting, DNA denaturation, glass and jamming transitions, and active biopolymer gels. As these transitions have properties of continuous transitions, it may be that their critical properties are 'universal,' and that, like systems with more usual continuous transitions, there may be universality classes of systems that display an extreme Thouless effect. In on-going work, we are seeking to determine the precise critical properties of preferred degree networks with extreme introverts and extroverts and other variants. It will be very interesting and will provide a deep insight into the fundamental nature of non-equilibrium systems to learn if indeed there is a broad class of systems displaying mixed order phase transitions, including both social networks and a variety of physical systems, which have essentially the same critical properties.

[1] K. E. Bassler, D. Dhar, and R. K. P. Zia, Networks with preferred degree: A mini-review and some new results, J. Stat. Mech. (2015) P07013.

[2] K. E. Bassler, W. Liu, B. Schmittmann, and R. K. P. Zia, Extreme Thouless effect in a minimal model of dynamic social networks, Phys. Rev. E **91** (2015) 042012.

2.32 Isomorphism of pulsing and bursting between laser models

JASON GALLAS

Introduction Since first introduced by Leibniz in 1676, differential equations are indispensable across all disciplines of physics and the natural sciences. Despite extensive use and knowledge accumulated during 339 years, the persistent lack of general analytical methods to solve nonlinear differential equations prevented the discovery of the full spectrum of phenomena supported by them, and universalities lurking across different branches of classical dynamics and in phenomena governed by rate equations. Mathematical models of natural phenomena involve many control parameters. How to transcend the century-old limits of linear stability analysis or the determination of Hopf bifurcations, i.e. transcend the onset of the most trivial oscillations possible? What else exists beyond the birth boundaries of prosaic single-peaked periodic oscillations? How do periodic oscillations self-organize themselves while becoming more and more complicated, eventually turning into fully developed chaos? Computer clusters provide answers: They allow one to explore large sets of nonlinear equations, massively and systematically, over extended parameter intervals and with high-resolution, constructing stability (phase) diagrams which invariably reveal a host of unanticipated organizations and surprising global regularities.

Isomorphism between unrelated dynamical systems Recent simulations of stability phases for distinct types of dynamical systems shed new light on the nature of the global organization of their oscillatory modes, regular and chaotic. This means that rather different dynamics may, after all, lead to similar unfolding and scaling of complex behaviors. Furthermore, simulations reveal an elevated degree of similarity between certain hypersurfaces embedded in the control parameter space of dynamical systems. In the continuation, we present an example of isomorphism between two distinct and popular lasers.

The equations used to predict the laser behaviors are derived from careful considerations of experimental observations and typically contain a host of parameters needed to represent the degrees of freedom characteristic of the laser media, the pump mechanisms driving the laser, and other relevant factors. The dimensionality of such models can be high or low, depending of the quantum structure of the levels underlying the lasing transition. After deriving a model one faces the strenuous task of exploring a huge parameter space in order to delimit physically relevant regions for stable operation. As mentioned, prediction of suitable parameter ranges presupposes solving model equations for all possible sorts of oscillatory modes, periodic or chaotic, a task not feasible analytically. However, it may be efficiently done with ad-hoc computer routines that combine standard numerical methods and ideas stemming from dynamical systems with efficient MPI (Message Passage Interface) programming in order to obtain high-resolution information about oscillatory modes of systems of interest, in the present case of two types of CO_2 lasers, as illustrated in the next section.

State-of-the-art modeling Two distinct models of CO_2 lasers have been used frequently in the literature, each one for selected sets of parameters or varying over restricted intervals. Is there something new to learn from the dynamics predicted by such models, when comparing their stability (phase) diagrams?

First model: Experimentally, the most accurate model of a CO_2 laser with feedback is governed by a six-dimensional set of differential equations [1]:

$$\begin{aligned}
\dot{x_1} &= k_0 x_1\big(x_2 - 1 - k_1 \sin^2(x_6)\big),\\
\dot{x_2} &= -\Gamma_1 x_2 - 2k_0 x_1 x_2 + \gamma x_3 + x_4 + P_0,\\
\dot{x_3} &= -\Gamma_1 x_3 + x_5 + \gamma x_2 + P_0,\\
\dot{x_4} &= -\Gamma_2 x_4 + \gamma x_5 + z x_2 + z P_0,\\
\dot{x_5} &= -\Gamma_2 x_5 + z x_3 + \gamma x_4 + z P_0,\\
\dot{x_6} &= \beta\big(B_0 - x_6 - R x_1/(1+\alpha x_1)\big).
\end{aligned}$$

Here, x_1 represents the laser output intensity, x_2 the population inversion between the two resonant levels, while x_6 stands for the feedback voltage signal which controls the cavity losses. The three coupled equations involving these variables are sufficient to generate chaos. However, due to the interplay of the different energy levels of the CO_2 molecule one must introduce three additional variables, acting as linear filters, thereby increasing the phase-space dimension from three to six.

Second model: In contrast, a single-mode non-autonomous CO_2 laser with modulated losses involves just two coupled degrees of freedom and a time-dependent parameter which we write as usual [2]:

$$\dot{u} = \frac{1}{\tau}\,(z-k)u, \qquad \dot{z} = (z_0 - z)\gamma - uz.$$

Here, u is proportional to the radiation density, z and z_0 are the gain and unsaturated gain in the medium, respectively, τ denotes the transit time of the light in the laser cavity, γ is the gain decay rate, and $k \equiv k(t)$ represents the total cavity losses. The losses are modulated periodically according to

$$k(t) = k_0(1 + a\cos 2\pi f t),$$

where k_0 is the constant part of the losses and a and f, the amplitude and frequency of the modulation, are the bifurcation parameters of interest here.

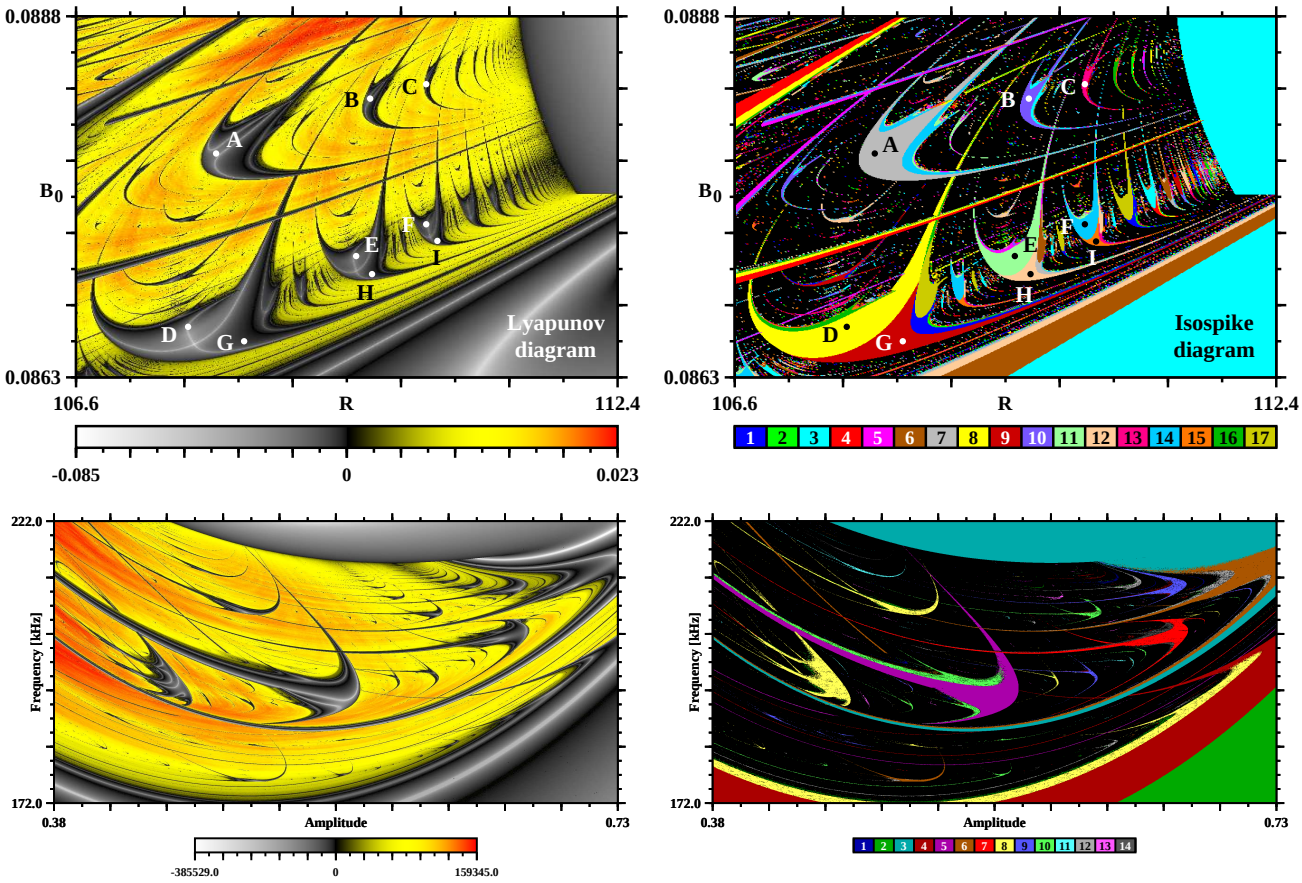


Figure 1: Top row: A section of the control parameter space the CO_2 as predicted by the 6-dim model, shown in two complementary ways: Standard Lyapunov stability diagram (left column), and *isospike* diagram (right column), i.e. counting the number of spikes per period in the laser intensity. Bottom row: similar diagrams, but predicted by the smaller 3-dim model of a CO_2 with modulated losses. Despite the completely distinct modeling, the control space of both laser shows a striking resemblance, including the cascades of systematic accumulations.

Comparing stability charts of lasing modes The distribution of periodic and chaotic stability phases are compared in Fig. 1 for the 6-dim model (top row) and the 3-dim model (bottom row). On the left column (showing Lyapunov diagrams) chaos is represented with colors (positive exponents). In contrast, chaos is represented in black on the right column, where colors represent the number of spikes per period of the periodic modes. All stability diagrams display self-similar islands of regularity profusely. The most conspicuous organizations are the systematic accumulations of periodic modes along certain "specific directions", converging towards smooth boundary curves. To detect these specific directions one needs to tune two control parameters simultaneously. Along such accumulations, the distinction between phases is the number of spikes contained in their wave patterns. Thus, accumulations represent a "route of mode complexification". The spiking and bursting behaves similarly. Both lasers share additional similarities, despite their totally distinct natures and models.

Conclusion We have shown that the control space of standard lasers models displays systematic similarities, in particular scaling of mode complexification occurs along specific direction of the control space. These remarkable and unexpected similarities seem to be clues that both lasers contain some sort of similar recurrent organization in their control spaces. A crucial open question is about the genericity of such regularities. We have seen that rather distinct differential equations lead to a similar-looking class of stability phases. The key point now is to check how generic such class might be and with many distinct classes do we have to deal when classifying oscillations in nonlinear dynamics.

[1] J.G. Freire, R. Meucci, F.T. Arecchi, and J.A.C. Gallas. Invited review paper, 25th Anniversary Focus Issue: Chaos **25**, 097607 (2015).

[2] C. Bonattto, J.C. Garreau, and J.A.C. Gallas Phys. Rev. Lett. **95**, 143905 (2005).

2.33 Quantum criticality in the Hubbard model on graphene's honeycomb lattice

FAKHER ASSAAD, IGOR HERBUT

In numerical simulations, spontaneously broken symmetry is often detected by computing two-point correlation functions of the appropriate local order parameter. This approach, however, computes the square of the local order parameter, and so when it is small, very large system sizes at high precisions are required to obtain reliable results. Alternatively, one can pin the order by introducing a local symmetry breaking field, and then measure the induced local order parameter infinitely far from the pinning center. The method is applied to the Hubbard model on honeycomb lattice, within the realm of the projective auxiliary field quantum Monte Carlo algorithm. With our enhanced resolution we find a direct and continuous quantum phase transition between the semi-metallic and the insulating antiferromagnetic states with increase of the interaction. The single particle gap in units of the Hubbard U tracks the staggered magnetization. An excellent data collapse is obtained by finite size scaling, with the values of the critical exponents in accord with the Gross-Neveu universality class of the transition. [1]

Introduction Honeycomb lattice is a bipartite, non-frustrated lattice, which at half filling and small Hubbard repulsion U hosts the semi-metallic state of electrons, as in graphene. When the repulsion is increased one expects eventually a phase transition into an insulating state with antiferromagnetic order [2], which due to gapless Dirac fermionic excitations being present on the semimetallic side, should belong to a particular, Gross-Neveu universality class [2, 3]. Starting from the strong coupling limit and noting that the insulator to metal transition occurs at values of the Hubbard interaction lesser than the bandwidth, allows for the proliferation of higher order ring exchange terms in an effective spin model aimed at describing the magnetic insulating state in the vicinity of the transition. This point of view opens the possibility that the melting of the magnetic order is unrelated to the the metal-insulator transition. Previous quantum Monte Carlo calculations [4] suggested that there is an intermediate spin liquid phase with a single-particle gap but no magnetic ordering, separating the semi-metal and magnetic insulator. The results of Ref. [4] have been challenged by other studies: Ref. [5], for example, shows that extrapolating from significantly larger system sizes would suggest almost complete disappearance of the spin-liquid from the phase diagram. The latter conclusion is reinforced here, where we exhibit excellent data collapse and identical finite-size scaling of both single-particle gap and staggered magnetization, [1] with the distinct values of critical exponents, in accord with the Gross-Neveu universality class [2, 3].

By introducing a local magnetic field at say the origin, we explicitly break the SU(2) spin symmetry. In the presence of long range order and in the thermodynamic limit, any field will pin the order along the direction of the external field. Thereby, order can be detected by computing directly the magnetization infinitely far from the pinning field. The upside of such an approach is that one measures directly the order parameter rather than its square. The downsides are three-fold. One explicitly breaks SU(2) spin symmetry such that spin sectors mix and it becomes computationally more expensive to reach the ground state. Since the computational cost scales linearly with the projection parameter, however, this problem is tractable. The second difficulty lies in the ordering of limits. To obtain results which are independent on the magnitude of the pinning field, it is important to first take the thermodynamic limit and then the limit of infinite distance from the pinning field. In a practical implementation, this ordering of limits has as a consequence some leftover dependence of the magnetization on the magnitude of the pinning field. The final drawback is that it is not always possible to introduce a pinning field without generating a negative sign problem. Nevertheless, the method is applicable to SU(N) symmetric Hubbard-Heisenberg models.

Model and the method The half-filled Hubbard model on the Honeycomb lattice is

$$H_{tU} = t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + U \sum_{\mathbf{i}} \left(n_{\mathbf{i},\uparrow} - \frac{1}{2} \right) \left(n_{\mathbf{i},\downarrow} - \frac{1}{2} \right). \tag{1}$$

The hopping is restricted to nearest neighbors such that the bipartite nature of the lattice allows us to avoid the negative sign problem.

Generically, to detect anti-ferromagnetic ordering we compute spin-spin correlations:

$$m = \lim_{L\to\infty} \sqrt{\frac{1}{N} \sum_{\mathbf{i}=1}^{N} e^{i\mathbf{Q}\cdot\mathbf{i}} \langle \mathbf{S_0} \cdot \mathbf{S_i} \rangle_{H_{tU}}}. \tag{2}$$

Here $N = 2L^2$ corresponds to the number of orbitals, and L is the linear length of the lattice. A finite value of m signalizes long range order and is equivalent to spontaneous symmetry breaking. In particular, including a magnetic field term with appropriate Fourier component,

$$H_h = h \sum_{\mathbf{i}} e^{i\mathbf{Q}\cdot\mathbf{i}} S^z_i, \tag{3}$$

gives

$$m = \lim_{h\to 0} \lim_{L\to\infty} \frac{1}{L^2} \sum_{\mathbf{i}} e^{i\mathbf{Q}\cdot\mathbf{i}} \langle S^z_{\mathbf{i}} \rangle_{H_{tU}+H_h}. \qquad (4)$$

The local pinning field is given by the term $H_{loc} = h_0 S^z_{\mathbf{0}}$ in the Hamiltonian. Using the representation $\delta_{\mathbf{i},\mathbf{0}} = (1/L^2)\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{i}}$ of the Kronecker symbol shows that each Fourier component comes with an amplitude h_0/L^2 so that taking the thermodynamic limit is equivalent to taking the amplitude of the relevant Fourier component to zero. With the local field construction, the appropriate ordering of limits for an $L \times L$ lattice reads:

$$m = \lim_{\mathbf{i}\to\infty} \lim_{L\to\infty} e^{i\mathbf{Q}\cdot\mathbf{i}} \langle S^z_{\mathbf{i}} \rangle_{H_{tU}+H_{loc}}. \qquad (5)$$

That is, one first has to take the thermodynamic limit – again to guarantee the collapse of the tower of states in the presence of long range order – and only then can one take the distance from the pinning center to infinity. As an efficient estimator for the evaluation of the ordered moment we use:

$$m = \lim_{L\to\infty} \frac{1}{L^2} \sum_{\mathbf{i}} e^{i\mathbf{Q}\cdot\mathbf{i}} \langle S^z_{\mathbf{i}} \rangle_{H_{tU}+H_{loc}}. \qquad (6)$$

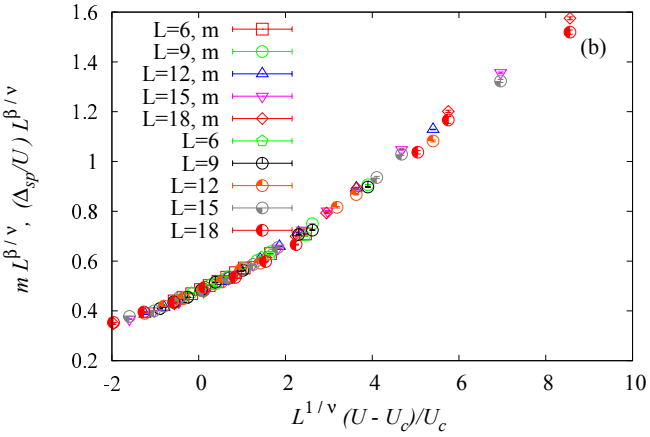


Figure 1: Data collapse for both the single particle gap and the staggered magnetization, with the exponents from the ϵ-expansion and the critical point at $U_c/t = 3.78$.

Ground state calculations were carried out with the projective auxiliary field Quantum Monte Carlo (QMC) algorithm which is based on the equation:

$$\langle O \rangle_H = \lim_{\theta\to\infty} \frac{\langle \Psi_T | e^{-\theta H/2} O e^{-\theta H/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-\theta H} | \Psi_T \rangle}. \qquad (7)$$

Here θ is a projection parameter, and the trial wave function is required to be non-orthogonal to the ground state. For $H = H_{tU} + H_{loc}$ the inclusion of the magnetic field does not generate a negative sign problem. We have chosen the trial wave function to be the ground state of the non-interacting Hamiltonian $H_T = H_t + H_{loc}$ in the $S^z = 0$ sector. The implementation of the algorithm follows closely Refs. [4]. The major difference is the use of a symmetric Trotter breakup which ensures hermiticity of the imaginary time propagator for any value of the time discretization $\Delta\tau$. It also leads to smaller systematic errors.

Results To look for the signs of the Gross-Neveu criticality in the Hubbard model we have carried out a finite size scaling analysis based on the usual scaling form

$$X = L^{-\beta/\nu} F(L^{1/\nu}(U - U_c)). \qquad (8)$$

where X is the staggered magnetization (m) or the single particle gap (Δ_{sp}). The ϵ-expansion value of the correlation length exponent reads [3], $\nu = 1/2 + 21\epsilon/55 + \mathcal{O}(\epsilon^2)$. With this value of ν with $\epsilon = 1$, we obtain an excellent single data collapse for both the magnetization and the single particle gap (see Fig. 1). This is a strong indication that there is a direct continuous transition between the magnetically ordered and disordered phase in the Hubbard model, at which Dirac fermions play a crucial role.

Conclusion and outlook The application to the Hubbard model on the honeycomb lattice sheds new light on the phase diagram of this well known problem. The enhanced precision in comparison to Refs. [4] and [5] reveals that the staggered moment has the same functional form as the single particle gap. Remarkably, an excellent data collapse onto a single universal curve is found in the finite size scaling of both quantities, with the values of the critical exponents characteristic of the Gross-Neveu criticality between the semimetallic and the magnetic insulating phases.

Further extensions of this work, which include a study of the effects of the long-range Coulomb interaction on the critical point [6] and the state-of-the-art analysis of the corrections to scaling [7], have lent an additional support to the presented results and to the overall physical picture of the phase transition. Closely related fermionic quantum critical points in generalized Hubbard models on honeycomb and pi-flux lattices have also been studied, [8,9] with the results being broadly in agreement with the Gross-Neveu universality classes.

[1] F. F. Assaad, I. F. Herbut, Phys. Rev. X, **3**, 031010 (2013).

[2] I. F. Herbut, Phys. Rev. Lett. **97**, 146401 (2006)

[3] I. F. Herbut, *et al.*, Phys. Rev. B **80**, 075432 (2009).

[4] Z. Y. Meng, *et al.*, Nature **464**, 847 (2010).

[5] S. Sorella, *et al.*, Sc. Rep. **2**, 292 (2012).

[6] M. Hohenadler, *et al.*, Phys. Rev. B **90**, 085146 (2014).

[7] F. Parisen Toldin, *et al.*, Phys. Rev. B **91**, 165108 (2015).

[8] L. Wang, *et al.*, N. Journal of Phys. **16**, 103008 (2014).

[9] E. F. Huffman, S. Chandrasekharan, Phys. Rev. B **89**, 111101(R) (2014).

Chapter 3

Details and Data

3.1 PhD Program

The training of PhD students is one of the central tasks of the mpi**pks**. It is realized through a large PhD program, our leading role in the IMPRS *Dynamical Processes in Atoms, Molecules and Solids* (see next section) and our participation in the IMPRS *Cell, Developmental and Systems Biology* 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. Applications for PhD positions funded through the Visitors Program are accepted at all times and invited via the internet pages of the institute, workshop announcements and print publications.

In 2013, a total of 77 PhD students were working at the mpi**pks**, including 41 students from abroad (these numbers count all students, also those who finished or started their studies during that year). The respective numbers for 2014 were 98 PhD students working at the mpi**pks**, including 42 students from abroad. We counted 11 successful final PhD exams for the year 2013 and 9 for the year 2014.

In addition to the scientific training by their supervisor, PhD students at the mpi**pks** benefit from a variety of opportunities to develop their expertise, skills, and career: The students are admitted to the lecture courses offered by the TU Dresden and the mpi**pks** (p. 171). Presentation skills can be practised in regular group seminars or through active participation in the events of the Workshop and Seminar Program. The institute organizes soft skill training and career coaching events ranging from a seminar for scientific writing to invited talks by alumni, who provide first-hand information about possible career opportunities (p. 172). Students from foreign countries receive financial and logistic support for joining German language courses.

The majority of the PhD students at the mpi**pks** receive their degree from the TU Dresden (p. 173). After graduation, most continue their research and move to postdoc positions at research institutions all over the world, a smaller fraction takes up non-academic positions in applied research, computer science, finance or consulting.

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. Close to the end of the present funding period, expiring in December 2016, the IMPRS was evaluated for a second time in September 2015, going along with a prolongation application of the program beyond 12 years.

The IMPRS is currently a collaboration of the following 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)
- University of Chemistry and Technology — UCT (Prague/Czech Republic)

The participating research groups cover an intentionally broad area, including the fields of theoretical and quantum chemistry, atomic, molecular, optical and condensed matter physics, materials science, and scientific computing. The general focus is on modelling in the natural sciences, featuring algorithms as well as applications in simulations of microscopic and mesoscopic systems. In the future, we intend to shift the focus towards many-particle systems in structured environments.

PhD students

There are currently 52 students enrolled in the program. Approximately half of them are from Germany, the other students come from all over the world. The distribution by geographical origin is as follows, Europe: 36 (Germany: 22, Czech Republic: 6, Poland: 2, Austria, Greece, Italy, Netherlands, Sweden, UK: 1), Asia: 8 (India: 5, Iran: 2, Indonesia: 1), America: 7 (Mexico 2, Brazil 2, Colombia, Cuba, Peru: 1), Africa: 1 (Ethiopia). The distribution among the affiliated partner institutions is TUD: 17, mpi**pks**: 25, IOCB: 2, UCT: 4, MPI-CPfS: 2, ILTSR: 2.

Scientific events

Since the foundation of the IMPRS, we have been organizing an annual retreat for the students. These are normally held in autumn at different locations on the countryside around Dresden, e.g. in Gohrisch in 2013 and in Kreischa in 2014 (see picture). In these meetings, with a total duration of three days, the PhD students present their work in talks to stimulate discussions among all students including those working in different fields. Furthermore, the retreats are an important component which facilitates the initiation of recently enrolled PhD students of the IMPRS and strengthens their interaction with IMPRS students who are at an advanced stage of their PhD. Sometimes, also senior scientists affiliated with our research school are invited to join the retreat on its first day. They introduce themselves and their research topics to the IMPRS students, contributing particularly to the acquaintance of the recently enrolled students with the scientific landscape of Dresden, and of the IMPRS in particular.

In order to closely integrate our Polish and Czech partner institutions, we organize joint block seminars or summer/winter schools in Wrocław and Prague, which are also open to local participants not necessarily affiliated with the IMPRS. The latest event was a summer school in Prague, held in July 2015. The lecture program focused on photoinitiated molecular processes.

In May 2013, our institute hosted a new kind of scientific IMPRS event. Together with three other International Max Planck Research Schools, with which our scientific focus partly overlaps, we organized a joint workshop. The primary aim was to bring together the PhD students of the four research schools, but also to strengthen the interaction between the Max Planck institutes and the affiliated partner institutions involved. Scope and details of this workshop are described in section 3.3.4. This pilot project was received very positively by the participants, and thus a similar event was organized in June 2015, this time by the IMPRS at the MPI for Quantum Optics.

IMPRS meeting in Kreischa in October 2014.

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 also open to non-members of the IMPRS; participation of the IMPRS students in the lectures is monitored by a credit-point system.

In fall 2014, we launched a presentation series in which IMPRS faculty members share their expertise on professional skill topics with the doctoral students (p. 172). In order to provide the students with first-hand information about possible career opportunities, especially outside of academia, IMPRS alumni who left the academic sector are also invited as speakers for such seminars, to share their experiences and to answer questions. The presentations are normally scheduled for the day after one of the monthly IMPRS seminars, so that students from the associated institutions outside of Dresden may stay overnight and attend. Due to the positive response, we intend to make the professional skill talk series a regular part of the IMPRS curriculum.

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.

3.3 Workshop and Visitors Program

The Visitors Program of the mpi**pks** hosts guest scientists for a period of up to two years. Excellent working conditions are offered to qualified, mostly young, scientists. In close collaboration with the other service departments of the mpi**pks** , the Visitors Program is dedicated to support the scientists in every possible way to allow them to focus on their research. This also includes logistic help, e.g., for finding suitable accommodation, solving visa problems, etc.

A Mentoring Program, a Platform for Social Activities and financial support for joining German language courses are installed to make it easy for guests to integrate fast and smoothly into the local community.

International Workshop "Charge Transfer meets Circuit Quantum Electrodynamics", June 29 - July 3, 2015

During 2013, the number of guest scientists including predocs with contracts for at least three months hosted by the mpi**pks** was 262, and 261 during 2014.

Guest scientists either join the in-house research groups or work independently. Alternatively, they may form small temporary groups of their own, working intensively on a particular problem. Many guest scientists participate actively in the Workshop and Seminar Program (see p. 135).

In addition to the regular positions of the Visitors Program, the institute annually offers a Distinguished PKS Postdoctoral Position for experienced postdoctoral scientists. PKS Fellows conduct independent studies and complement research areas pursued at the institute and are appointed for three years. Between 2013 and 2015, we had four PKS Fellows working at the mpi**pks**: *Dr. Achilleas Lazarides* on *Collective phenomena*, *Dr. Benjamin Friedrich* on *Regulation of the cytoskeleton*, *Dr. Robert Johne* on *Light-matter interaction at the single photon level*, and *Dr. Alexander Croy* on *Nonlinear phononics using atomically thin membranes* (see reports on p. 127).

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 last awardee *Prof. A. P. Young* (University of California Santa Cruz) spent four months at the mpi**pks** (see report below on this page).

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 timey topic from the field of the physics of complex systems. From 2013-2015, we enjoyed large scale activities of three Advanced Study Groups: From December 2012 on, we hosted the group *Topological Band Structures and Their Instabilities* under its convenor *Prof. I. Herbut*, in 2013 and 2014 the group *Coevolution: A proving ground for non-equilibrium statstical mechanics* coordinated by *Prof. K. Bassler*, and in 2014, the group *Optical rare events: A challenge in Laser Dynamics* headed by *Prof. J. Gallas* (see reports on p. 43).

In addition to the long-term guest scientist positions, the Visitors Program 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 263 during the year 2013, and 256 during the year 2014.

A considerable number of guest scientists leave the institute for permanent positions in the academic sector, beside many others who continue with postdoctoral positions at other institutions in Germany or abroad. Several guest scientists take up 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-Fellow

Spin glasses and other frustrated systems
(Prof. Peter Young)

My research covers two main areas. Firstly, I have a long-standing interest in phase transitions in (classical) disordered systems, especially those with frustration which are known as spin glasses. My work uses numerical simulations to ascertain under what circumstances phase transitions occur (e.g. dimension of space, number of spin components, presence or not of a magnetic field), what are the universal properties at those transitions (e.g. the values of critical exponents), and what is the nature of the spin glass phase at temperatures below the transition temperature. Secondly, I am interested in problems involving quantum phase transitions motivated by the active topic of quantum computing. In particular I have been looking at whether the method of the Quantum Adiabatic Algorithm (QAA), which is a form of Quantum Annealing (QA), could solve optimization problems more efficiently on a quantum computer than could a classical computer. Early numerical work used very small sizes, those for which all 2^N states could be enumerated, but it was clearly necessary to go to larger sizes to determine the asymptotic behavior of how the computer time varies with N in the limit of $N \to \infty$. For someone like myself with a statistical mechanics background it was clear that one needed to do a random sampling of the states using Quantum Monte Carlo (QMC) simulations.

My residence at the mpi**pks** as Gutzwiller Fellow for 2014 was split into three visits: two months in September–November 2014, five weeks in May–June 2015, and a final visit of three weeks will take place in December 2015. I am most grateful that the Fellowship allows for this flexibility. During the first of these three visits, my graduate student Matthew Wittmann accompanied me, with support from the Gutzwiller Fellowship for which I am also most grateful.

During my stays at the mpi**pks** I have worked primarily on three topics:

1. With my student Wittmann, we addressed the question of what is the "right" way to describe the spin glass state below T_c using statistical mechanics, given that a spin glass is never truly in equilibrium since it gets trapped in "valleys" surrounded by high barriers. Experimental measurements on a system at finite-temperature involve a *time average*. Dynamics is harder to calculate than statics, so, in theoretical work, the time average is usually replaced by a static calculation using statistical mechanics in which one *sums over all configurations* with the Boltzmann probability distribution. Most systems are ergodic, so theory agrees with experiment even though different averages are

performed. One situation where more care is needed is that of a phase transition where symmetry is spontaneously broken. A simple case is the Ising ferromagnet, which has just two ordered states below the transition temperature T_c, the "up" spin state with a net positive magnetization, and the "down" state. On cooling, the system will choose one of these symmetry-related states and acquire a non-zero magnetization. The Boltzmann sum is then not the "right" thing to calculate because it unphysically includes both the up and down states and give zero net magnetization. However, for this ferromagnetic case it is straightforward to disentangle the two states because they are related by symmetry. However, in spin glasses, the situation is much more complicated. *Dynamically*, below the spin glass transition temperature T_c a macroscopic system is not in thermal equilibrium because relaxation times are much too long. Rather, in a typical experiment the system is quenched from a high temperature to a temperature below T_c and the subsequent dynamic evolution of the system is observed. *For statics*, the state (or states) of thermal equilibrium are very complicated and are not related to any symmetry. As for the ferromagnet we would like to find a static calculation which will predict the experimental behavior, at least to some extent. We showed *quantitatively* that the theoretical idea called the "metastate" [1, 2], combined with the technique of "replica symmetry breaking" (RSB) [3] provides such a description for spin glasses, at least in high dimensions, where the critical behavior is described by mean field theory.

We did this by performing large scale, non-equilibrium Monte Carlo simulations on a one-dimensional model with long-range interactions which is argued to represent a short-range model in higher dimension with the value of this effective dimension determined by the rate at which the interactions in the one-dimensional model fall of with distance. We chose values corresponding to eight dimensions, which is greater than the "upper critical dimension" $d_u = 6$, and so is in the mean field regime.

Our results represent a simplification of the theory of spin glasses, at least in the mean field regime since the observed dynamical behavior (which is inevitably out of equilibrium) can be described by a static theory (the metastate). Whether this equivalence holds outside the mean field regime remains to be seen.

These simulations were very demanding and could not have been carried out without the generous amount of computing time from mpi**pks** made available to my student Wittmann, both during and after his stay. We are very grateful to the institute for providing this computer support. This work has been written up [4] and is currently under consideration at Physical Review Letters.

2. After extensive effort, the static properties of the spin glass transition in three dimensions are now quite well understood. In particular, Hasenbusch et al. [5] extracted not only the leading singular behavior at the transition but also the dominant correction to scaling. This gives confidence that the asymptotic critical region has been reached (which it had not in much of the earlier work, see, e.g., discussion in Ref. [6]), and hence that the critical exponents are accurate. Subsequently, massive simulations by Baity-Jesi et al. [7], using a special-purpose computer, obtained even more accurate results, which are consistent with the earlier work of Ref. [5].

   However, the dynamical critical behavior, in particular the value of the dynamical exponent z, is less well understood. In a visit to the mpi**pks** prior to the start of my Gutzwiller fellowship, Arnab Das suggested using a non-equilibrium method, in combination with scaling first used in the Kibble-Zurek (KZ) mechanism in cosmology, to determine the value of z. During my first Gutzwiller stay, I began interacting with Anders Sandvik and collaborators at Boston University, who already had a code for doing KZ scaling for related models. A specific focus of our study is to accurately determine the value of z for models with two very different bond distributions to test whether universality, according to which critical exponents don't depend on microscopic details, holds for spin glasses. There have been a series of papers by Ian Campbell and collaborators proposing that universality does *not* hold, quite a revolutionary claim since universality is one of the cornerstones of the modern theory of critical phenomena. The calculations were done with great precision and yield the most accurate values obtained so far for the dynamical critical exponent. Furthermore, the values are the same for both bond distributions within fairly small error bars, thus strongly supporting universality.

   This work has been written up [8] and is currently under consideration at Physical Review E.

3. One problem that has interested me for a long time is precisely what are the conditions for spin

glass behavior. The usual intuition is that the system should have disorder and frustration, but these can be present in different ways, not just as in the canonical spin glass model of Edwards and Anderson. I was therefore very interest to learn of a project of my mpi**pks** host, Roderich Moessner, and collaborators, involving spins which are placed in random positions on a lattice, interacting via non-random, very long-range, potential. Moessner et al. considered a classical Heisenberg model, but my experience with short-range spin glasses is that vector spin models such as Heisenberg are much harder than the Ising spin glass, so I proposed to Moessner that we look at the Ising version, starting in two dimensions where the potential is logarithmic in the distance. The goal is to see if this is a spin glass, and if so, whether screening effects make it effectively a short-range spin glass in the same universality class as the Edwards-Anderson model. The project is a collaboration between Moessner, his student Jorge Rehn, and myself. The simulations are ongoing. The model is computationally challenging even though we use the state-of-the-art technique of parallel tempering, since, in the first version of the code, the acceptance rate for Monte Carlo moves goes down very fast with decreasing temperature and increasing size. We are currently looking into a new version which we expect will equilibrate faster.

I expect that this project will be finished off and written up during my last Gutzwiller stay in December this year (2015).

I have also enjoyed stimulating discussions with Frank Pollmann, Jens Bardarson, and Shivaji Sondhi, on the topic of many body localization (MBL) and connections to spin glasses. These have been extremely informative but have not yet led to a publication.

[1] "Metastate approach to thermodynamic chaos", C. Newman and D. L. Stein, Phys. Rev. E **55** 5194 (1997).

[2] "Rounding Effects of Quenched Randomness on First-Order Phase Transitions", M. Aizenman and J. Wehr, Comm. Math. Phys. **130**, 489 (1990).

[3] "The order parameter for spin glasses: a function on the interval 0–1", G. Parisi, J. Phys. A. **13**, 1101 (1980).

[4] "The connection between statics and dynamics of spin glasses", M. Wittmann and A. P. Young, arXiv:1504.07709, (submitted to Phys. Rev. Lett.)

[5] "The critical behavior of three-dimensional Ising glass models", M. Hasenbusch, A. Pelissetto, and E. Vicari, Phys. Rev. B **78** 214205 (2008).

[6] "Detailed study of universality in three-dimensional Ising spin glasses", H. G. Katzgraber, M. Körner, and A. P. Young, Phys. Rev. B, P**73**, 224432 (2006).

[7] "Critical parameters of the three-dimensional Ising spin glass", M. Baity-Jesi et al., Phys. Rev. B, **88**, 224416 (2013).

[8] "Universal dynamic scaling in three-dimensional Ising spin glasses", C.-W. Liu, A. Polkovnikov, A. W. Sandvik and A. P. Young, arXiv:1411.6745, (submitted to Phys. Rev. E).

3.3.1.2 PKS-Fellows

Scaling and regeneration of self-organized patterns
(Dr. Benjamin Friedrich)

Spatial patterns emerge in systems out of thermodynamic equilibrium: sand ripples are sculptured by wind, chemical spirals form in a Belousov-Zhabotinsky reaction. These patterns are characterized by fixed length scales set by physical parameters. Pattern formation is abundant also in biology, from the development of a single fertilized egg into a multicellular organism, or the regeneration of lost body parts in certain species like flatworms, polyps, salamanders. Biological pattern formation can display unconventional features, not commonly found in non-living systems, such as scaling of patterns with system size: in developing fruit flies, chemical patterns of signaling molecules, termed morphogens, scale proportionally with the size of the tissue [2]. Flatworms scale their body plan over more than one order of magnitude in length, when they grow and degrow in response to feeding conditions [3], see Fig. 1. Additionally, a tiny amputation fragment of these worms will re-pattern itself into a complete miniature version of the original worm within days. The astonishing scaling and regeneration capabilities of animals such as flatworms prompt patterning mechanisms that can cope with highly variable initial conditions as well as variable sizes of the organism.

Together with a PhD student, Steffen Werner, we use concepts from nonlinear dynamics to address physical mechanisms of pattern scaling. We enjoy a close collaboration with the experimental group of Jochen Rink at the Max Planck Institute for Cell Biology and Genetics, which resulted in two joint publications [6, 7].

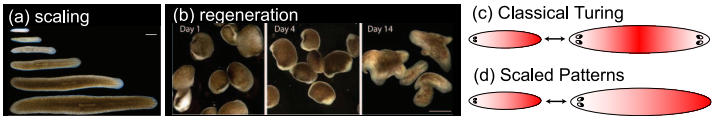


Figure 1: (a) Scaling: flatworms scale their body plan proportionally during growth and degrowth. (b) Self-organization: small amputation fragments repattern into miniature versions of the original worm. Images courtesy of Rink lab (MPI-CBG). Scalebar: 1 mm. (c) Turing patterns are self-organized, but do not scale, showing more periodic repeats in larger systems as a result of fixed intrinsic length scales. (d) Inspired by biology, we ask how self-organized patterns may scale with system size.

The genesis of form in biology can be studied theoretically as problem of pattern formation, a viewpoint pioneered by Alan Turing. In a seminal paper published in 1952, he proposed a minimal mechanism that spontaneously establishes stable chemical patterns by a self-organization mechanism [4]. Today, we know that spatial concentration profiles of signaling molecules termed morphogens indeed specify the future body plan in developing and regenerating organisms [1], for example, high or low morphogen concentrations could induce tail or head formation, respectively. However, it took 50 years of advances in molecular biology and genetics to find evidence that Turing-like self-organization operates in a number of developmental systems, ranging from finger patterning to stripe formation in zebra fish [5]. There are notable exceptions, like the formation of body segments in vertebrates, which results from a sequential process that starts with a pre-patterned egg. Nonetheless, Turing mechanisms provide an appealing minimal model for robust pattern formation from highly variable initial conditions, as applies to regeneration.

Turing patterns do not naturally scale with system size, see Fig. 1(c). Instead, they are commonly characterized by fixed intrinsic length scales that result from the interplay of diffusion and degradation of morphogens. Inspired by biological examples of pattern scaling, we asked for a minimal mechanism that yields patterns, which are both self-organized and self-scaling. We present a new class of patterning systems, which comprises a self-tuning mechanism that regulates the intrinsic length scales of a Turing system [7]. As a specific implementation, we consider a Turing system with two chemical species (concentrations A and B) that diffuse in a one-dimensional domain of size L (with respective diffusion coefficient D_A, D_B, reflecting boundary conditions), while being subject to degradation

$$\begin{aligned} \partial_t A &= \alpha_A\, P(A,B) - k_A E\, A + D_A\, \partial_x^2\, A, \\ \partial_t B &= \alpha_B\, P(A,B) - k_B E\, B + D_B\, \partial_x^2\, B\,. \end{aligned} \tag{1}$$

Importantly, production of both morphogens with production rates α_A and α_B occurs in a dynamic source region, which constantly re-adjusts its size and position according to $P(A,B) = \theta(A-B)$, *i.e.* a local source forms, whereever the activator concentration A exceeds the inhibitor concentration B. In Eq. (1), E is the concentration of a third molecular species, the expander.

For a constant level of expander E, Eq. (1) represents a classical Turing system. We have shown that in a classical Turing system, several stable steady-state patterns co-exist. In Turing systems of increasing size, low wavenumber patterns are characterized by increasingly smaller basins of attraction, rendering them unstable with respect to perturbations of finite amplitude. Thus, classical Turing patterns do not scale.

We now consider the case of a dynamic expander that is produced everywhere in the system, diffuses, and is subject to degradation with a rate that depends on the level of Turing morphogens,

$$\partial_t E = \alpha_E - \kappa_E\, B\, E + D_E\, \partial_x^2\, E\,. \tag{2}$$

The mutual coupling between the Turing instability of Eq. (1) and the expander dynamics of Eq. (2) results in a nonlinear feedback loop, which generates patterns that scale with system size, see Fig. 2. To quantify pattern scaling, we define the relative source size $\ell/L = \langle P \rangle$ and the expander-dependent pattern length scales $\lambda_A = (D_A/\langle \kappa_A E \rangle)^{1/2}$, $\lambda_B = (D_B/\langle \kappa_B E \rangle)^{1/2}$, where brackets denote a spatial average over the system. We numerically find that the source size of steady-state patterns scales with system size over several orders of magnitude. Concomitantly, we obtain a scaling of the effective Turing length scales $\lambda_A^* \propto L$ and $\lambda_B^* \propto L$, where the asterisk denotes steady-state.

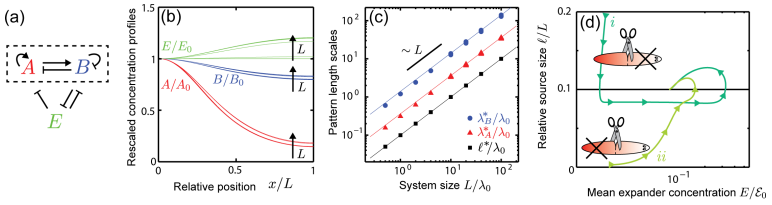


Figure 2: Scalable pattern formation in a Turing system with expander feedback: (a) Turing system and expander mutually control their degradation rates, resulting in a stable feedback loop. (b) Scaling corresponds to morphogen profiles that collapse as a function of relative position x/L (normalized by respective concentrations A_0, B_0, E_0 at $x = 0$). (c) The feedback self-consistently adjusts the length scales λ_A, λ_B of the morphogen profiles and thus the source size ℓ with system size (symbols: numerical solution, lines: analytic result) (d) Example trajectories, mimicking amputation experiments (labeled *i,ii*). Here, $\varepsilon_0 = (\alpha_A/\kappa_A)^{1/2}$ and $\lambda_0 = [D_A/(\varepsilon_0\kappa_A)]^{1/2}$ denote characteristic concentration and length scales of the system.

We can probe pattern regeneration by mimicking amputation experiments, see Fig. 2(d). Two example trajectories, corresponding to head and tail fragments, respectively, converge to an appropriately re-scaled head-tail gradient, after a transient over-shoot of the source size.

We can formally show that any steady-state of Eqs. (1), (2) perfectly scales with system size in the limit of fast expander diffusion. One crucial step in the reasoning is that the relative source size ℓ/L is independent of system size at steady state. This can be seen from Eqs.(1), (2) at steady-state by noting $0 = \alpha_B\langle P\rangle - k_B\langle BE\rangle$ and $0 = \alpha_E - k_E\langle BE\rangle$, from which we conclude $\ell/L = k_B\alpha_E/(k_E\alpha_B)$. Additionally, in the limit of adiabatically slow expander dynamics, we find that the simple head-tail gradient shown in Fig. 2 represents a stable fixed point.

Our model identifies minimal requirements for robust, self-scaling pattern formation and captures essential features of body plan regeneration in animals such as flatworms as observed in experiments. We predict specific signatures such as non-monotonic dynamics of source size after amputation and size-dependent degradation rates. Current experiments by the Rink lab at MPI-CBG are testing these signatures in flatworms.

[1] L. Wolpert and C. Tickle: Principles of Development (Oxford University Press, New York, 2011).
[2] O. Wartlick, P. Mumcu, A. Kicheva, T. Bittig, C. Seum, F. Jülicher, and M. González-Gaitán, Science **331**, 1154, 2011
[3] P. A. Newmark and A. Sánchez Alvarado: Nat. Rev. Genet. **3**, 210, 2002
[4] A. M. Turing: Philos. Trans. R. Soc. London B **237**, 37, 1952
[5] L. Marcon and J. Sharpe, Curr. Op. in Gen. & Dev. **22**, 578 (2012).
[6] S. Werner, I. Riedel-Kruse, J. Rink, B.M.Friedrich: PLoS ONE **9**(11), e113083, 2014
[7] S. Werner, T. Stückemann, M. Beiran, J. Rink, F. Jülicher, B.M. Friedrich: Phys. Rev. Lett. **114**(13), 138101, 2015 (selected as "Editor's suggestion").

Non-equilibrium dynamics of isolated systems

(Dr. Achilleas Lazarides)

The bulk of our work over the past two years has been on non-equilibrium dynamics, in particular on

- The dynamics of closed many-body quantum systems with a time-periodic Hamiltonian, for which we have set up a general framework analogous to statistical mechanical ensembles for systems with static Hamiltonians. This was in collaboration with A. Das (mpi**pks** and IICS, Kolkata, India) and R. Moessner (mpi**pks**) and has resulted so far in three publications [1–3]
- The effect of disorder on classical interacting systems (that is, classical systems the equations of motion of which are not linear). This was done in collaboration with O. Tieleman (mpi**pks**) and Ch. Skokos (University of Stellenbosch, South Africa) and has resulted in Ref. [4]

Periodically-driven quantum many-body systems

Background: Equilibrium and non-equilibrium physics. Much of condensed matter physics over the last century has been concerned with equilibrium states, where statistical mechanics applies and the behavior of a system with a large number of microscopic degrees of freedom is well-characterised by a small number of emergent degrees of freedom.[1]

Recently, the approach to equilibrium in closed quantum many-body systems with a time-independent Hamiltonian has been the subject of intense activity using the twin concepts of *equilibration*, the approach of a large, closed system's time-dependent state to some steady state, and *thermalization*, when this steady state depends only upon a small number of quantities. This subject, which may be thought of as the study of the emergence of statistical mechanics from purely unitary quantum dynamics, has now developed into a mature field of research.

Periodically-driven systems. In this context, our focus has been to extend this understanding to systems with Hamiltonians depending periodically on time but otherwise isolated, which is the simplest extension of time-independent Hamiltonians to the time-dependent domain. Our approach has been to first map the time-dependent problem to a time-independent problem by constructing an effective Hamiltonian for the system, then use results developed for the static case. This allows us to show that a driven system generically approaches a long-time steady-state that is synchronized with the driving; that is, a state in which physical observables have expectation values that are periodic with the period of the driving [2]. The details of that steady-state then depend on whether the system is ergodic or not, with the ergodic case leading to a fully-mixed ("infinite-temperature") final state for any initial state.

An obvious question is what happens if ergodicity is broken. One way of doing so is by tuning to an integrable point; this however is not robust, in that small perturbations restore ergodicity. A more robust way is by introducing disorder, so that the system is localized. In this case, small perturbations do not restore ergodicity. We have also studied both of these situations.

In what follows we explain in more detail what happens in the three regimes (ergodic, integrable and disordered).

Non-integrable systems. For generic, non-integrable systems, we have found [1] that the completely featureless, fully-mixed or "infinite temperature" steady state can be understood in terms of the set of ideas referred to as the "Eigenstate Thermalization Hypothesis" (ETH). For static (undriven) systems, the form of this ETH convenient for us is that the expectation value of an observable calculated in each eigenstate (eigenstate expectation value, EEV) is a smooth function of the energy of that eigenstate.

In [1] we show that the effective Hamiltonian for non-ergodic driven systems generically satisfies a special form of the ETH, namely, one in which EEVs are identical for all eigenstates of the effective Hamiltonian (for physical observables). This implies that these observables acquire a value that is independent of the initial state of the system and equal to the average over all states;[2] this is a fully-mixed state.

The mechanism by which this happens is that each eigenstate of the effective Hamiltonian is a linear superposition of eigenstates from throughout the spectrum of the undriven Hamiltonian (that is, the part of the Hamiltonian that does not depend on time), since the time-dependent perturbation couples not just nearby states in energy but also equally states distant by the driving frequency. Thus, periodic driving may be thought of as delocalizing the eigenstates of the effective Hamiltonian over the basis of the eigenstates of the unperturbed Hamiltonian.

Let us now discuss in turn the two ways of preventing this mixing.

Integrable systems. Systems that are mappable to free fermions via a Jordan-Wigner transformation, such as hard-core bosons (HCBs) in one dimension, form a particularly simple class of integrable systems. In the undriven case, one can easily identify an extensively large set of conserved quantities for this class of integrable systems. This implies that neither the Gibbs nor the microcanonical ensembles apply, as those assume that the only conserved quantity is the energy. The appropriate ensemble may be derived using Jaynes' idea of maximizing entropy subject to the expectation values of the conserved quantities being fixed to the correct values, yielding the so-called "Generalised Gibbs Ensemble" (GGE).

[1] A simple example would be a gas, which is made up of a large number of interacting particles but the macroscopic behavior of which may be described using only its global temperature, pressure and density.

[2] That is, the trace of the operator divided by the dimension of Hilbert space.

Our work [2] generalises and extends this idea to the domain of genuine out of equilibrium states. Our approach is to identify a set of operators that

- Reduce to the static conserved quantities in the undriven limit,
- Have expectation values that are time-independent, i.e., are dynamically conserved in time,
- Are periodic in time.

Maximising the entropy in the space of time-periodic function and subject to these operators being conserved, we obtain the "Periodic Gibbs Ensemble" (PGE), which we then show analytically to correctly reproduce the expectation values of all possible operators in the thermodynamic limit. This constitutes a generalization of the usual techniques of statistical mechanics to the periodically-driven case.

This class of integrable systems allows for a complete analytical understanding but has the disadvantage of being fine-tuned: a slight perturbation to the Hamiltonian away from the integrable point immediately renders all our analysis invalid. A class of "robustly integrable" systems is formed by disordered interacting systems displaying "many-body localization" (MBL).

Many-body localized systems. MBL refers to disorder-induced localization in the presence of interactions. For our purposes, it is of interest because it is one of the few examples of "emergently integrable" generic systems available. That is, in an MBL system, ergodicity is broken and thermalization does not set in despite the fact that the Hamiltonian is not, on the face of it, integrable.

In [3] we study two different systems displaying MBL.

The first is a system of interacting hard-core bosons or equivalently a spin-1/2 XXZ-type system with disorder. For strong enough disorder the entire spectrum (all eigenstates) is localized. Whether or not this system delocalizes under driving depends on the frequency of the driving term: For low frequency the system fully mixes, while for high frequency it does not. This may be understood by appealing to the existence of local conserved quantities [3].

We have also studied driving the so-called Quantum Random Energy Model (QREM), which is a paradigmatic model displaying a mobility edge (that is, part of the spectrum is localised and part delocalised). In this case, driving causes delocalisation (mixing) for any frequency by virtue of coupling all eigenstates to others spread throughout the spectrum (thus inevitably to delocalised eigenstates).

In conclusion, disorder may lead to a robust mechanism of preventing interacting systems from reaching a fully-mixed, featureless state. This result may be of practical significance in connection with recent theoretical proposals to engineer desirable Hamiltonians by periodically driving cold atoms, as these are usually presented in the context of non-interacting systems.

Classical nonlinear disordered systems: Lyapunov exponents and ergodicity

An independent but related direction has been to study classical nonlinear disordered systems. In these systems the question of localisation by disorder is not yet completely settled.

Our contribution was to point out that chaos indicators, such as the maximal Lyapunov exponent, are not good indicators of ergodicity. In particular, we have developed a novel symplectic integrator and used it to show [4] that for the example of the Gross-Pitaevskii model with disorder positive Lyapunov exponents do not necessarily imply ergodicity in contrast to previous claims in the literature. In this case, the phase space of the system separates into subspaces that are disjoint on experimentally relevant timescales. It is therefore for all intents and purposes non-ergodic, despite the presence of positive Lyapunov exponents.

[1] A. Lazarides, A. Das and R. Moessner, Phys. Rev. E **90** (2014) 012110
[2] A. Lazarides, A. Das and R. Moessner, Phys. Rev. Lett. **112** (2014) 150401
[3] A. Lazarides, A. Das and R. Moessner, Phys. Rev. Lett. **115** (2015) 030402
[4] O. Tieleman, Ch. Skokos and A. Lazarides, EPL **105** (2014) 20001

Light-matter interaction at the low photon number level

(Dr. Robert Johne)

My main research interest is the interaction of light and matter in various settings. Not only does this interaction set the basis for quantum light sources, lasers and optical detectors, but it is also, since photons do not interact in vacuum, of fundamental importance to mediate photon-photon interactions by

exploiting strong nonlinearities in the material system. I am particularly interested in the quantum regime, where the light field typically contains only a few photons. The ultimate goal is to generate nonlinearities at the sinlge photon level mediated by atoms or artificial atoms such as semiconductor quantum dots in the optical regime and superconducting qubits in the microwave regime. The light-matter interaction is governed by the coupling strength between the material excitation and its electromagnetic environment. In optical resonators light can be confined in small volumes resulting in a dramatic increase of the local optical density of states. Thus, placing the material system in cavities provides the basis for strongly interacting light and matter systems opening the emergent field of cavity quantum electrodynamics (cQED) and efficient light-matter interfaces. In my research I have been investigating the interaction of light and matter in different resonator coupled material systems. The specific research topics range from solid state to atomic systems and are detailed in the following.

Semiconductor quantum dots in photonic crystal cavities

If quantum emiters are placed in optical resonators, all the dynamics are governed by a coupling constant given by the dipole moment of the quantum emitter and the electric field associated with the cavity mode. This interaction constant is thus given by intrinsic device properties, which are difficult to modify. In collaboration with an experimental group from the Eindhoven University of Technology we have theoretically developed and experimentally implemented two schemes, which allow for the ultrafast control of the interaction constant in a solid state cQED system, namely quantum dots in photonic crystal cavities. The first scheme is to manipulate the emission frequency of quantum dot excitons via electric fields [1]. This allows for the indirect control of the light-matter coupling by tuning the spectral overlap between the quantum emitter and the cavity mode. A second scheme is based on a coupled cavity approach and enables the direct control of the light-matter interaction and the cavity loss rates [2]. In this approach the dynamics of a quantum dot placed in a target cavity can be engineered by an adjacent control cavity. If the two resonant cavities are strongly coupled, two new eigenmodes appear hybridizing the initial properties of the uncoupled cavity modes. This leads to the delocalization of the electric field as well as the mixture of the loss rates of the two cavities. Hence, the cavity coupling directly affects the light-matter interaction, since the maximum electric field amplitude associated with the target cavity mode determines the coupling strength. Furthermore, by ultrafast control of the resonance condition between the adjacent cavity modes, it is possible to tune the light-matter coupling by a factor of two on timescales much faster than the spontaneous emission time of the quantum dot. The experimental implementation has led to the demonstration of the ultrafast and nonlocal control of spontaneous emission of quantum dot excitons in a coupled cavity environment [2]. Also, an extension to three coupled cavities has been theoretically studied, which enables the on-off switching of the light matter coupling between a quantum emitter and a cavity mode [3]. Therefore, it provides the full control of the light-matter coupling and can be used for switching Rabi-oscillations, for shaping photon pulses, and also as a basis for a new class of gain-modulated lasers. Implementations are not limited to quantum dot systems but also possible in superconducting circuits. Our work on the ultrafast control of spontaneous emission by electrical and optical means has been additionally covered by two invited news articles [4, 5] and an invited article for a public audience [6].

Semiconductor excitons

Exciton-polaritons are quasi particles which arise from the strong coupling of (semiconductor) excitons and photons. They are mixed light-matter particles combining the properties of excitons and photons with a characteristic non-parabolic dispersion and a light effective mass. Exciton-polaritons have excellent transport characteristics as well as the capacity to interact with each other and the environment. As a result of the enormous technological progress in recent years, semiconductor microcavities are currently the most advanced system to investigate and to explore the unique properties of exciton-polaritons. In collaboration with an experimental group from the University of Leipzig, we have studied the dynamics of exciton-polaritons in a complex multimode whispering gallery mode resonator. We have observed condensation of polaritons and a cascade-like relaxation within the multimode polariton dispersion [7]. The developed theory unambiguously shows that this relaxation is dominated by parametric polariton-polariton scattering induced by the excitonic component and the numerical simulations are in very good agreement with the experimental observations.

There is an ongoing effort at mpi**pks**, in collaboration with the group of Dr. Thomas Pohl, to theoretically

study the exciton-exciton interaction in semiconductor systems. This field is getting even more attention as Rydberg excitons have been recently observed in two dimensional semiconductor monolayers. Owing to the large extend of the wavefunctions of these excited exciton states, strong and long-range exciton-exciton interactions are expected and currently investigated. These novel features may eventually push forward the polariton physics in the quantum regime, where nonlinearities at the single photon level start to play a role.

Ion crystals in cavities

Crystals of cold ions are among the most advanced systems for the implementation of quantum information science. Due to the formation of crystals, effective ion-ion interactions can be engineered via state dependent optical forces and collective vibrational modes of the crystal. These in its range and strength engineerable interactions are a fruitful playground for experiments in the framework of quantum simulations. Again in collaboration with Dr. Thomas Pohl, we have studied the possibilities to explore the ion-ion interactions for the generation of optical nonlinearities by combining the spin-physics with cavity quantum electrodynamics. We have shown that by implementing a long-range Ising interaction in the spin system placed in a cavity, a single photon nonlinearity is obtained, which is independent of the cavity loss rate, while the enhanced collective light-matter interaction is maintained [8]. Furthermore, the combination of spin-spin interactions and coherent rotation of the spin states allows for the generation of arbitrary photon Fock states with high fidelity. This system represents a versatile platform for advanced applications in quantum nonlinear optics and quantum information processing.

Summary and conclusions

I have been intensively working on different aspects of the light-matter interaction such as spatio-temporal control of the coupling strength as well as optical nonlinearities induced by interactions in the material system. In particular, effects arising from exciton-exciton interactions in polariton systems or spin-spin interactions in ion crystals with a direct backaction on the incident light field pave the way for generating effective photon-photon interactions, which is a long standing goal of fundamental and technological significance.

Collaborations

I have been collaborating with several interal and external scientists. First, I collaborate with an experimental group led by Prof. Andrea Fiore (Eindhoven University of Technology,The Netherlands) working on quantum dots in photonic crystal cavities. A second collaboration has been established with Dr. R. Schmidt-Grund (University of Leipzig, Germany) working on polariton systems in hexagonal whispering gallery mode resonators based on ZnO. Within this polariton project, I have been also cooperating with Prof. P. Eastham (Trinity College Dublin, Ireland) and with Dr. C. Dietrich (St. Andrews University, United Kingdom). I also have an ongoing internal collaboration with the group of Dr. Thomas Pohl at the mpi**pks**.

[1] F. Pagliano, Y. Cho, T. Xia, F. van. Otten, R. Johne, A. Fiore, Nature Communications **5** (2014) 5786

[2] C.-Y. Jin, R. Johne, M.Y. Swinkels, T.B. Hoang, L. Midolo, P.J. van Veldhoven, A. Fiore, Nature Nanotechnology **9** (2014) 886

[3] R. Johne, R. Schutjens, S. Fattah poor, C.-Y. Jin, A. Fiore, Phys. Rev. A **91** (2015) 063807

[4] C.-Y. Jin, R. Johne, M.Y. Swinkels, T.B. Hoang, L. Midolo, P.J. van Veldhoven, A. Fiore, Optics and Photonics News - Optics in 2014 (2014)

[5] C.-Y. Jin, R. Johne, M. Swinkels, R. Schutjens, T.B. Hoang, L. Midolo, R. van Veldhoven, A. Fiore, SPIE Newsroom (2015) DOI: 10.1117/2.1201502.005792

[6] A. Fiore, F. Pagliano, M.Y. Swinkels, C.-Y. Jin, R. Johne, Nederlands Tijdschrift voor Natuurkunde (2015) in press

[7] C. P. Dietrich, R. Johne, T. Michalsky, C. Sturm, P. Eastham, H. Franke, M. Lange, M. Grundmann, R. Schmidt-Grund, Phys. Rev. B **91** (2015) 041202(R)

[8] R. Johne, T. Pohl, in preparation

Nanomechanics of 2d materials
(Dr. Alexander Croy)

Since August 2014 I am working at the mpi**pks** on various aspects related to nanomechanical systems. In particular, I am interested in modeling mechanical properties of 2d materials (like graphene or phosphorene) in order to evaluate their potential in the context of phononics. The emerging field of phononics

deals with tailoring acoustic and thermal properties of (artificial) materials. Although phononic crystals and acoustic metamaterials are known for a long time, nonlinear elements are still lacking. Using 2d materials might provide a viable route to obtain them [1].

In addition, my research activities include the application of concepts of open systems to transport in nano-scale devices.

Strain-displacement relations for 2d materials

In recent years continuum elasticity was shown to be a valuable tool for the description of mechanical properties of 2d materials. However, in some cases additional knowledge about the relation between (macroscopic) strain and (microscopic) displacements of the atoms in the unit cell is required. For example, by stretching a material, one changes the distance between atoms and thus the overlap of neighboring orbitals, which in turn results in a modification of the electronic structure.

Together with Dr. Daniel Midtvedt (mpi**pks**) and Prof. Caio Lewenkopf (Universidade Federal Fluminense, Brazil) I have investigated the derivation of strain-displacement relations from valence force models (VFM) [2]. Since 2d materials have non-Bravais lattices (more than 1 atom in the unit cell), we found that a simple transformation of the bond-vectors by the strain tensor is not sufficient. An additional correction vector is required and can be related to the parameters of the VFM. We found a straight-forward procedure to obtain this vector. We have also shown that the correction leads to a renormalization of the strain dependence of the electronic band-gap for graphene nanoribbons and phosphorene.

Strain tuning of vacancy-induced magnetism in graphene nanoribbons

Defects, such as vacancies or chemisorpted hydrogen, provide a simple way of creating localized electronic states in graphene. Moreover, those states are predicted to have a finite magnetic moment. Since strain can modify the electronic properties of 2d materials, it might offer the possibility to in-situ tune the magnetic properties and realize spintronic applications.

Together with Dr. Daniel Midtvedt (mpi**pks**) I investigated the influence of strain on localization and magnetic properties of vacancy-induced states in semiconducting armchair nanoribbons [3]. We found that both properties sensitively depend on uniaxially applied strain. Using a mean-field Hubbard model and an effective double-quantum dot description we found that exchange splitting of a single vacancy and the singlet-triplet splitting for two vacancies can be widely tuned.

In the future we are planning to combine vacancy-induced magnetism with mechanical resonators to investigate the potential for creating magneto-mechanical devices.

Nanoelectromechanical motor

Together with Dr. Alexander Eisfeld (mpi**pks**), I had studied the dynamics of an electromechanical nanomotor, which is driven by the tunneling of electrons. Treating the rotor classically we found different modes of operation (stand-still, oscillatory and rotatory motion) depending on the ratio between driving strength (bias voltage) and damping. Our motor can thus be seen as an extension of the seminal electron shuttle, which only has stand-still and oscillatory motion. Recently, we started to use a full quantum description of this system, which is relevant for molecular motors. We also want to understand to which extent the different types of motion survive in the quantum regime and if there is a clear feature to identify them.

Non-adiabatic electron pumps.

In collaboration with Prof. Ulf Saalmann (mpi**pks**) I worked on non-adiabatic charge pumping through a single-level quantum dot with periodically modulated parameters [4]. By using a quantum master equation approach we obtained the full counting statistics of the system and found a trinomial probability distribution of the charge transfer, which adequately describes the reversal of the pumping current by sweeping the driving frequency – a feature found in the non-adiabatic pumping regime. We also derived equations of motion for the current and the noise, which can be solved numerically for arbitrary time-dependencies. This approach can also be extendend to treat nanoelectromechanical systems, like nanomotors, in order to obtain an additional characterization of transport and motion in those systems.

[1] D. Midtvedt, A. Isacsson and A. Croy, Nature Comm. 5, 4838 (2014).
[2] D. Midtvedt, C. H. Lewenkopf and A. Croy, submitted (arXiv:1509.02365).
[3] D. Midtvedt and A. Croy, submitted (arXiv:1504.06956).
[4] A. Croy and U. Saalmann, submitted (arXiv:1508.03977).

3.3.2 Conferences, Workshops and Symposia

1. *Wetting and Capillarity in Complex Systems*
   Workshop: February 18 - 22, 2013 — 76 participants
   Scientific coordinators: S. Dietrich, G. Oshanin, M. N. Popescu, M. Tasinkevych
2. *Flat Bands: Design, Topology, and Correlations*
   Focus Workshop: March 06 - 09, 2013 — 80 participants
   Scientific coordinators: M. Franz, R. Moessner, S. Parameswaran
3. *Spin-Orbit Interaction for Light and Matter Waves*
   Workshop: April 15 - 19, 2013 — 62 participants
   Scientific coordinators: A. Aiello, K. Bliokh, J. Götte, W. Löffler
4. *Quantum Dynamics and Photon-Matter-Interactions*
   IMPRS Workshop: May 14 - 17, 2013 — 73 participants
   Scientific coordinators: A. Di Piazza, M. Genkin
5. *Photoemission and Electronic Structure of 4f and 5f Systems*
   Focus Workshop: May 28 - 30, 2013 — 27 participants
   Scientific coordinators: T. Durakiewicz, J. van den Brink
6. *Connecting Theory and Experiments in Active Matter*
   Focus Workshop: June 05 - 07, 2013 — 41 participants
   Scientific coordinators: H. Chaté, K. Kruse, S. Ramaswamy
7. *Methods of Chaos Detection and Predictability: Theory and Applications*
   Focus Workshop: June 17 - 21, 2013 — 64 participants
   Scientific coordinators: G. Gottwald, J. Laskar, H. Skokos
8. *Ultracold Rydberg Physics 2013*
   Seminar and Workshop: July 01 - 12, 2013 — 118 participants
   Scientific coordinators: T. Pohl, J.-M. Rost
9. *Origins of Life - At the crossroads between Biochemistry and Astrophysics*
   International Symposium: July 10 - 12, 2013 — 69 participants
   Scientific coordinators: A. Lupas, J.-M. Rost
10. *Spin Orbit Entanglement: Exotic States of Quantum Matter in Electronic Systems*
    Seminar and Workshop: July 15 - August 02, 2013 — 93 participants
    Scientific coordinators: R. Thomale, B. Trauzettel, S. Trebst
11. *Quantum Many Body Systems out of Equilibrium*
    Seminar and Workshop: August 12 - 30, 2013 — 136 participants
    Scientific coordinators: J.-S. Caux, T. Esslinger, M. Haque, C. Kollath
12. *Advances in Quantum Chaotic Scattering: From (Non-)Linear Waves to Few-Body Systems*
    Workshop: September 09 - 13, 2013 — 101 participants
    Scientific coordinators: R. Ketzmerick, U. Peschel, K. Richter, P. Schlagheck
13. *Topology and Nonequilibrium in Low-Dimensional Electronic Systems*
    Workshop: September 16 - 20, 2013 — 103 participants
    Scientific coordinators: A. Mirlin, F. v. Oppen
14. *Korrelationstage 2013*
    Workshop: September 23 - 27, 2013 — 100 participants
    Scientific coordinators: H. Fehske, C. Pfleiderer, F. Pollmann

15. *Synergetic Approaches to Complexity*
    Focus Workshop: September 30 - October 01, 2013 — 47 participants
    Scientific coordinators: H. Haken, J. Peinke, G. Radons

16. *Astrophysical Turbulence: From Galaxies to Planets*
    Workshop: October 07 - 11, 2013 — 32 participants
    Scientific coordinators: E. Bodenschatz, U. Christensen, S. Dreizler

17. *Small Systems far from Equilibrium: Order, Correlations, and Fluctuations*
    Workshop: October 14 - 18, 2013 — 44 participants
    Scientific coordinators: M. Henkel, D. Mukamel, M. Pleimling, G.M. Schütz

18. *From Dynamics to Statistical Physics and Back*
    Focus Workshop: October 21 - 23, 2013 — 52 participants
    Scientific coordinators: H. Kantz, A. Politi

19. *Atomic Physics 2013*
    Workshop: November 25 - 29, 2013 — 81 participants
    Scientific coordinators: J.-M. Rost

20. *Weak Chaos and Weak Turbulence*
    Workshop: February 03 - 07, 2014 — 42 participants
    Scientific coordinators: E. Kartashova, A. Pikovsky, D. Shepelyansky

21. Recent Progress and Perspectives in Scaling, Multifractality, Interactions, and Topological Effects Near Anderson Transitions
    Focus Workshop: March 11 - 14, 2014 — 58 participants
    Scientific coordinators: F. Evers, I. Gruzberg, V. Kagalovsky

22. Brownian Motion in Confined Geometries
    Workshop: March 17 - 21, 2014 — 64 participants
    Scientific coordinators: S.M. Bezrukov, L. Schimansky-Geier, G. Schmid

23. Topological Matter Out of Equilibrium
    Focus Workshop: March 27 - 29, 2014 — 64 participants
    Scientific coordinators: R. Moessner, S. Parameswaran

24. Circle Meeting on Biological Physics
    Focus Workshop: April 23 - 25, 2014 — 62 participants
    Scientific coordinators: G. Salbreux, F. Jülicher

25. DNA-Based Nanotechnology: Digital Chemistry
    Workshop: May 05 - 09, 2014 — 83 participants
    Scientific coordinators: M. Mertig, C. Richert, H. Yan

26. ETW Program: Nonlinear Physics at the Nanoscale: A Cross-Fertilization on Stochastic Methods
    Workshop: May 12 - 16, 2014 — 51 participants
    Scientific coordinators: J. Brand, S. Flach, P. Schwerdtfeger

27. Causality, Information Transfer and Dynamical Networks
    Seminar and Workshop: May 12 - July 04, 2014 — 83 participants
    Scientific coordinators: J. Davidsen, P. Grassberger, B. Schelter

28. Topology and Entanglement in Correlated Quantum Systems
    Seminar and Workshop: July 14 - August 08, 2014 — 104 participants
    Scientific coordinators: E. Berg, N. Cooper, F. Pollmann, X.-G. Wen

29. Arbeitstreffen Rydbergphysik 2014
    Focus Workshop: July 15 - 16, 2014 — 25 participants
    Scientific coordinators: J.-M. Rost, T. Pfau

30. Quantum Spin Dynamics: From Exotic Excitations to Novel Transport and Non-Equilibrium Phenomena
    Seminar and Workshop: September 01 - 12, 2014 — 74 participants
    Scientific coordinators: W. Brenig, A.L. Chernyshev, M. Zhitomirsky

31. Echoes in Complex Systems
    Workshop: September 22 - 26, 2014 — 52 participants
    Scientific coordinators: A. Goussev, R. Jalabert, D. Wisniacki

32. New States of Matter and their Excitations
    Workshop: September 29 - October 02, 2014 — 66 participants
    Scientific coordinators: J.H. Bardarson, F. Pollmann

33. Pressure and Strain Effects in Correlated Electron Materials
    Workshop: October 06 - 10, 2014 — 53 participants
    Scientific coordinators: J.P. Attfield, J. Hamlin, P. Hirschfeld, R. Valenti

34. Cellular Mechanisms of Sensory Processing
    Workshop: October 14 - 17, 2014 — 47 participants
    Scientific coordinators: M. Göpfert, T. Moser, F. Wolf

35. Atomic Physics 2014
    Workshop: November 24 - 28, 2014 — 91 participants
    Scientific coordinators: J.-M. Rost, T. Pfeifer

36. Many-body Dynamics out of Equilibrium
    Workshop: March 10 - 14, 2015 — 68 participants
    Scientific coordinators: J.H. Bardarson, S. Parameswaran, F. Pollmann

37. Activity meets Biology
    Focus Workshop: March 23 - 24, 2015 — 28 participants
    Scientific coordinators: S. Grill, G. Salbreux, V. Zaburdaev

38. Criticality in Biology: A Critical Assessment
    Seminar and Workshop: April 07 - 17, 2015 — 60 participants
    Scientific coordinators: H. Chaté, M.A. Muñoz

39. Novel Light Sources from Laser-Plasma Interaction
    Workshop: April 20 - 24, 2015 — 66 participants
    Scientific coordinators: M. Bussmann, M. Grech, E. Siminos

40. Random Walks and Nonlinear Dynamics in the Life of Cells
    Workshop: May 18 - 22, 2015 — 60 participants
    Scientific coordinators: S. Denisov, L. Manning, V. Zaburdaev

41. Dynamics of Multi-Level Systems
    Seminar and Workshop: June 01 - 09, 2015 — 76 participants
    Scientific coordinators: F. Atay, K. Lindgren, E. Olbrich

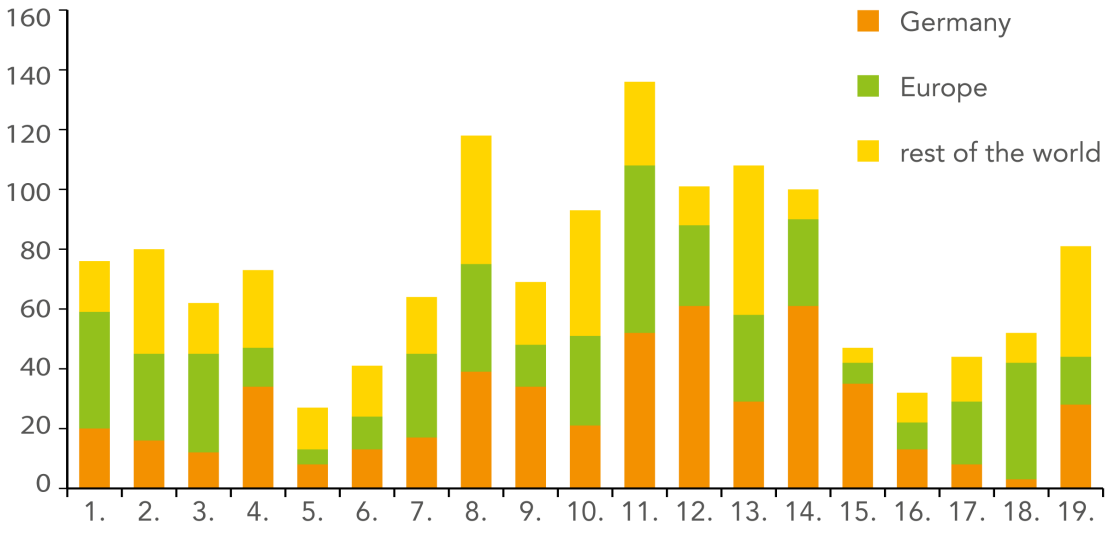
42. Quantum Hardness
    Focus Workshop: June 03 - 04, 2015 — 11 participants
    Scientific coordinators: R. Moessner, S. Sondhi

43. Quantum Correlated Matter and Chaos - A Workshop in Honor of the Life and Work of Richard Prange
    Workshop: June 22 - 26, 2015 — 95 participants
    Scientific coordinators: S.M. Anlage, S. Fishman, G. Radons

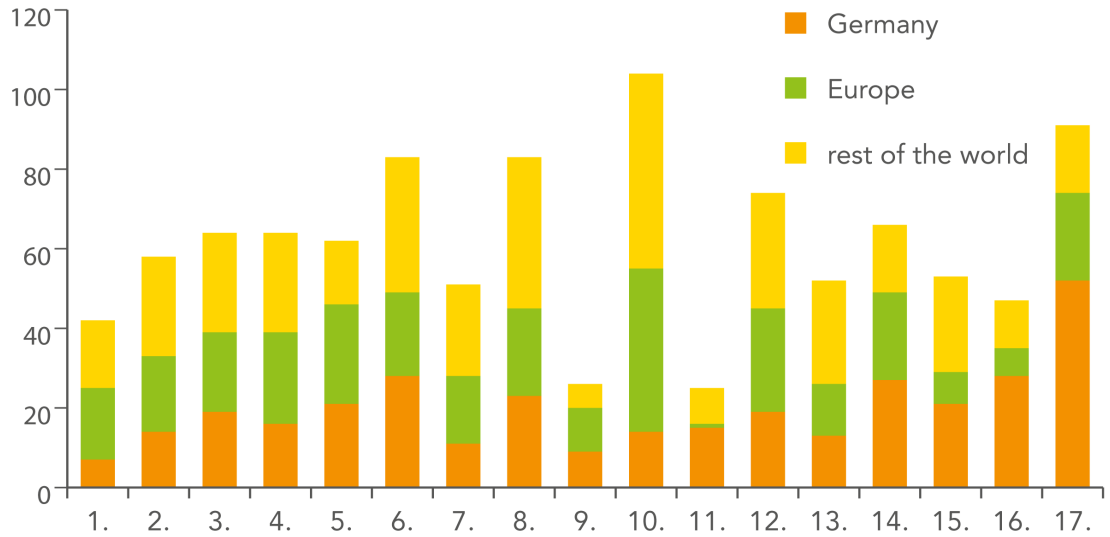
44. Charge Transfer meets Circuit Quantum Electrodynamics
    Workshop: June 29 - July 03, 2015 — 60 participants
    Scientific coordinators: M. Blencowe, B. Huard, B. Kubala

3.3.3 Workshop Participation and Dissemination of Results

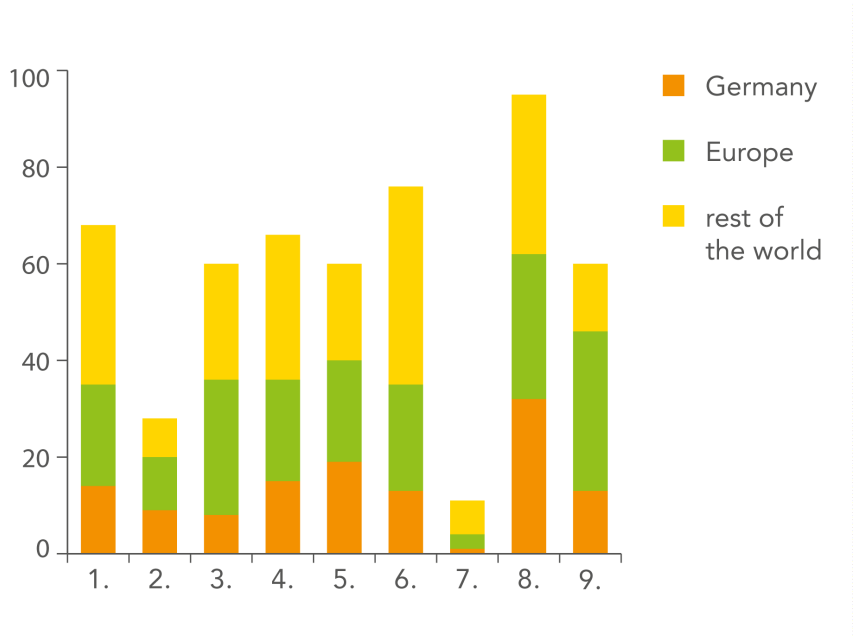
Statistics of Workshop participation



Number of Workshop/Seminar participants in the year 2013.



Number of Workshop/Seminar participants in the year 2014.



Number of Workshop/Seminar participants in the year 2015.

Dissemination of Workshop Results

As the Workshops Program of the **mpipks** focus on new and emerging topics, it is often attractive for scientific coordinators of Workshops and Seminars to compile and publish the results of their event in proceedings, lecture notes or monographs. The **mpipks** supports such efforts in various ways. The following list summarizes publications which resulted from scientific events at the institute:

- Workshop *Connecting Theory and Experiments in Active Matter*
  E. Bertin, H. Chate, F. Ginelli, S. Mishra, A. Peshkov, S. Ramaswamy: Mesoscopic theory for fluctuating active nematics. New Journal of Physics 15, 085032 (2013)
- Workshop *Methods of Chaos Detection and Predictability: Theory and Applications*
  G. A. Gottwald, C. Skokos: Chaos Detection Methods and Predictability. Chaos Focus Issue 24, 024201 (2014)
- Seminar and Workshop *Spin Orbit Entanglement: Exotic States of Quantum Matter in Electronic Systems*
  E. K. Lee, R. Schaffer, S. Bhattacharjee, Y. B. Kim: Heisenberg-Kitaev model on the hyperhoneycomb lattice. Physical Review B 89, 045117 (2014)
  I. Kimchi, J. G. Analytis, A. Vishwanath: Three-dimensional quantum spin liquids in models of harmonic-honeycomb iridates and phase diagram in an infinite-D approximation. Physical Review B 90, 205126 (2014)
- Seminar and Workshop *Topology and Entanglement in Correlated Quantum Systems*
  M. P. Zaletel, R. S. K. Mong, F. Pollmann: Flux insertion, entanglement, and quantized responses, Journal of Statistical Mechanics 2014, P10007 (2014)
- Seminar and Workshop *Recent Progress and Perspectives in Scaling, Multifractality, Interactions, and Topological Effects Near Anderson Transitions*
  A. L. Chudnovskiy, V. Kagalovsky: Thermal and electrical quantum Hall effects in ferromagnet/topological insulator/ferromagnet junction. Physical Review B 91, 195105 (2015)

3.3.4 Workshop Reports

Wetting and Capillarity in Complex Systems 2013, Workshop
Scientific coordinators: S. Dietrich, G. Oshanin, M.N. Popescu, M. Tasinkevych

Aim and Focus. The workshop was organized in response to the growing interest in the interfacial properties of complex fluids (such as colloidal suspensions, organic ionic liquids, electrolytes, and liquid crystals) in contact with patterned or responsive substrates. This interest is nurtured by the potential to exert controlled manipulation of fluids at mesoscopic length scales. The underlying feature is that the hierarchical structure of patterned (responsive) substrates introduces a wealth of length and time scales which interplay with the intrinsic length and time scales of complex liquids. The complexity of such systems requires highly innovative approaches, which bundle experimental, theoretical, and computational skills. The goal of this international workshop was to achieve crossfertilization between the various fields in Physics, Physical Chemistry, and Materials Science which deal with wetting and capillarity in experiment, theory, and simulations. This was facilitated by bringing together leading experts (36) and junior scientists (8) who delivered talks on various theoretical, experimental, or numerical topics, as well as a number of invited participants (10) and applicants presenting posters (17; three additional ones canceled their participation on short notice due to health or travel issues).
Most important participants. It is difficult to single out specific contributions because more than half of the participants are leading, senior experts in the field. All the talks have been of high scientific quality and the presentations included numerous open questions, which significantly facilitated discussions and interactions between the participants. The topics dealt with experimentally or theoretically (via analytical and numerical approaches) and presented in the talks included: static and dynamic Cassie-Wenzel transitions, liquid flow over uniformly textured substrates with inhomogeneous chemical composition, imaging and characterization of microscopic droplets condensing on patterned substrates, wetting of patterned substrates by ionic liquids, liquid crystals, or colloidal suspensions, electrowetting with ionic liquids, surface tensions of electrolytes, pair and multibody interactions between colloidal particles trapped at fluid-fluid interfaces, capillary induced clustering and self-assembly for colloids trapped at fluid-fluid interfaces, hydrodynamics of active gels, catalytically active droplets, wetting of hairy-elastic surfaces, Leidenfrost-levitated and propelled drops and solids, and wetting and spreading of liquid metals in the presence or absence of surface alloying. Among these presentations, one may eventually make a special note of the workshop Colloquium: "Wetting and drying of fibers", a very insightful and thought provoking overview of the complex behavior resulting from the interplay between capillarity and elasticity given by Howard Stone, a renowned and leading expert of capillarity and wetting phenomena.
Newcomers. The talks and posters by the early career scientists (PhD students, postdocs, Assistant Professors) attending the workshop were of excellent quality and significantly added to the scientific content of the workshop. As an example one can mention the talks on the self-propulsion of chemically active drops by Y. Sumino (experiment) and N. Yoshinaga (experiment and theory), an emerging area that generated a lot of interest for the participants. It was very pleasing to see this sizeable group of young scientists taking part in the workshop, engaging in lively collegial discussions during the talks, the coffee breaks, the poster sessions, as well as during the free time, and establishing contacts for future collaborations or strengthening existing ones.
Scientific results in the broader sense. The response of the scientific community, and in particular from leading experts in the field, on the invitations to participate in this workshop was very enthusiastic, which led to vivid on-site discussions. These were facilitated by the balanced schedule of formal scientific presentation time and time for informal scientific discussions. The need for comprehensive collaborations between complex, powerful experimental techniques and intensive theoretical and numerical work in the studies of complex liquids in contact with complex substrates was strongly re-enforced by the workshop participants. This, together with the identification of new, emerging topics of significant academic and industrial interest (for example, self-assembly and dynamics enabled by interactions with (in) complex fluids) is expected to lead to a long lasting impact of this meeting.

Flat Bands: Design, Topology, and Correlations, Focus Workshop
Scientific coordinators: M. Franz, R. Moessner, S. Parameswaran

The mpi**pks** workshop "Flat Bands: Design, Correlations, Topology" was held from March 6-9, 2013. The primary focus of the workshop was the study of emergent strongly correlated phases of matter in systems that exhibit an extensive degeneracy in the absence of inter-particle interactions. This quenching of kinetic energy leads to non-dispersing energy levels colloquially termed 'flat bands', in which the efficacy of interactions is enhanced. This leads to interesting phases with both conventional broken symmetries, such as ferromagnets, as well as topologically ordered phases such as lattice versions of fractional quantum Hall states and fractional topological insulators. A flurry of recent numerical observations of

fractionalized phases in lattice models with 'topological' flat bands, has renewed interest in the study of flat bands of electronic insulators. There have also been various proposals to realize and study flat bands in experimental systems, ranging from oxide heterostructures to optical lattices of ultracold fermions with an artificial gauge field. In a different vein, the realization of various frustrated hopping models of ultracold bosons in optical lattices has motivated interest in the rather less well-studied problem of bosons in flat bands. In all these cases, the fundamental role played by correlations simultaneously leads to novel behavior while complicating the understanding of these phases from numerical and analytical approaches. The goal of the workshop was to bring together researchers working on diverse aspects of flat band physics.
Some key questions that speakers were asked to focus on included: Is there a reliable route to designing flat bands in experimentally relevant systems, be they electronic or cold atomic systems? What correlated phases and new physical phenomena can occur (generically or as a result of careful fine-tuning)? Is there a systematic understanding and/or classification of (topological) phases in flat bands, and how does one characterise them?
The workshop itself was organized along three broad directions, roughly paralleling current work in the field:

- Fractional Topological Phases in Lattice models
- Flat band physics: Energetics, Anderson localization, and Magnetism
- Experimental work on Realizing Flat/Topological bands in Solid-State systems and Ultracold Atomic Gases

Tutorial Session. Since one of the major new directions in the field is the study of topological phases in lattice models, and we had a significant student participation, Prof. Nicolas Regnault very generously gave a brief tutorial on this field, well attended by both junior and senior participants. The aim of this was to replace repetitive introductory material of several talks in a well-focused field by one in-depth overall tutorial, thereby allowing for a more focused presentation of material by the following speakers.
The organizers attempted to have a wide representation of participants from different fields. These included many of the key workers in the theory of fractional topological phases (Prof. C. Mudry, Prof. C. Chamon, Prof. R. Roy, Prof. G. Murthy); in the realization of such phases in cold atom systems (Prof. N. Cooper, Prof. D. Stamper-Kurn, Dr. L. Leblanc) and solid-state systems (Prof. H. Manoharan); as well as a wide range of speakers discussing fundamental theoretical aspects of flat bands (Prof. G. Volovik, Prof. M. Oshikawa, Prof. J. Chalker), as well as numerical studies of these systems (Prof. M. Milovanovic, Prof. N. Regnault, Prof. K. Sun, Dr. E. Bergholtz.)
Younger participants. As this is a relatively young field, much of our participation was from PhD/Masters students and Postdocs. Indeed, several nice talks were given by postdoctoral fellows and junior faculty: Prof. R. Roy, Dr. E. Bergholtz, Prof. K. Sun, Dr. L. Hormozi, Dr. M. Daghofer, Dr. L. Leblanc, and Dr. C. Laumann. We also had an excellent selection of posters (both by junior and senior participants); indeed, from the poster submissions a handful were selected for oral presenations.
Summary. The workshop substantially achieved its stated goal of bringing together a diverse range of participants actively engaged in research on a wider variety of topics within the umbrella of flat band physics. There were several fruitful interactions across the different subtopics represented at the workshop; hopefully these will stimulate further work and collaborative research in new directions. Participants particularly appreciated the abundant time for discussions that were an integral part of the program, and commented on the insightful discussions that ensued.

Spin-Orbit Interaction for Light and Matter Waves, Workshop
Scientific coordinators: A. Aiello, K. Bliokh, J. Götte, W. Löffler

In quantum theory spin-orbit interaction describes any coupling of the spin of a particle with its motion. For central fields this coupling is proportional to the product of spin and orbital angular momentum. Whereas many effects based on this coupling are hard to detect directly for particles, light beams with angular momentum offer a highly controllable and accessible system. Intriguingly, the angular momentum of light also has a spin and orbital part, and we can therefore expect a spin-orbit interaction for light. In addition, the recent creation of electron vortex beam offers another avenue of investigation, extending the topic of the workshop to relativistic particles with mass. The aim of this workshop was to bring together the experts on spin-orbit coupling in light and matter waves together with world leading

researchers in optics and condensed matter physics to explore novel concepts in this field.
The session were organized around six main themes: spin-orbit conversion in optical materials, electron vortex beams, optical helicity, quantum weak measurements, spin-orbit coupling in condensed matter, and atomic systems. The colloquium by Erez Hasman (Technion and Stanford) on spin-optics offered many exciting analogies to condensed matter systems, such as optical realisations of spin-Hall effect and Rashba or Dresselhaus interactions. It culminated in the demonstration of coherent and spin-dependent thermal emission from nanoscale structures.
Through a series of outstanding talks by Etienne Brasselet (Bordeaux), Byoungho Lee (Seoul), Natalia Litchinitser (Buffalo) and Aristide Dogariu (CREOL) other aspects of material based spin-orbit coupling were explored on the first day. Mohamed Babiker (York) and Lorenzo Marrucci (Naples) drew on analogies between optical and electron vortices, while Jo Verbeeck (Antwerp), Jun Yuan (York) and Ebrahim Karimi presented the experimental and theoretical advances in manipulating the angular momenta of electrons in microscopes. The subtleties of optical helicity and duality transforms are crucial for a complete understanding of momenta in all fields and were introduced in talks from Steve Barnett (Glasgow), Kostya Bliokh (RIKEN), Gabriel Molina-Terriza (Macquarie) and Gerard Nienhuis (Leiden). David Andrews (University of East Anglia) gave a very lucid talk that the angular momentum of the light is not readily translated into its atomic counterpart. Spin-orbit coupling in optical beam shifts and its connection to the Abraham-Minkowski dilemma, spatial coherence, and quantum weak measurements were brought to the audience respectively by invited talks from Vladimir Fedoseyev (Tartu), Marco Ornigotti (MPI for the Science of Light) and Mark Dennis (Bristol). The talk by Iwo Bialynicki-Birula (Warsaw) touched on many aspects of the workshop simultaneously, including the underlying geometry of spinorbit coupling as well as some important differences between electrons and photons. Maarten de Kievit (Heidelberg) and Klaus Morawetz introduced a new theme by talking about spin-orbit coupling in atomic and condensed matter systems, which was continued by Sonja Franke-Arnold (Glasgow) and Manuel Valiente (Heriot-Watt). The workshop closed with a theme on focal properties of optical angular momentum with talks by Pepijn Pinkse (Twente) on spin-orbit coupling of focussed field in resonators, as well as surface and transverse angular momentum by Andrea Aiello and Peter Banzer (both MPI for the Science of Light). The final talk was given by Miles Padgett (Glasgow) on the transfer of angular momentum to light by spinning disks.
Five promising young postdocs gave invited talks, and five shorter talks were presented by excellent PhD students. The session of 3-4 minute talks to introduce the posters on the first day was a formidable icebreaker and helped in integrating the younger participants into the more senior audience. As a result, the two poster sessions with 20 posters were very lively and lasted well into the night.
Spin orbit interaction for light and matter waves is an emerging field and this workshop came at a crucial moment in its development, perfect for taking stock and reviewing the progress by relating it to established strands of research in optics and condensed matter physics.
In short the workshop was a complete success. The scientific and social programme was extremely well received by the participants, with many attendees taking home new insight and ideas. We would like to thank the **mpipks** for allowing us to host this workshop and in particular Mandy Lochar for the impeccable organisation. JBG also acknowledges support from the Royal Society for individual attendees.

Quantum Dynamics and Photon-Matter-Interactions, IMPRS Workshop
Scientific coordinators: A. Di Piazza, M. Genkin

The workshop resulted as a joint initiative of four International Max Planck Research Schools (IMPRSs): the IMPRS for Ultrafast Imaging and Structural Dynamics, hosted by the Max Planck Research Department for Structural Dynamics at the University of Hamburg, the IMPRS for Quantum Dynamics in Physics, Chemistry and Biology, hosted by the MPI for Nuclear Physics in Heidelberg, the IMPRS for Advanced Photon Science, located at the MPI for Quantum Optics in Garching, and the IMPRS for Dynamical Processes in Atoms, Molecules and Solids, hosted by the MPI for the Physics of Complex Systems in Dresden.
The research focuses of the four IMPRSs have an overlap in the fields of quantum dynamics and photon-matter-interactions. At the same time, the involved research groups within the schools approach the fields from different perspectives and with different emphases. The rather general focus thus included various topics, from the generation and the analysis of attosecond laser pulses from the perspective of photonics, over XFELs and their applications in chemistry, biology and medicine, to dynamical quantum processes in microscopic systems induced by these novel light sources. The primary aim of the event

was to bring together the PhD students from the involved schools and to facilitate an exchange among them. For this reason, it was strongly envisaged that the majority of the presentations should have been given by the PhD students of the IMPRSs.
The scientific program was organized as follows. Each day started with a plenary talk by a senior member of one of the IMPRSs. Jan Michael Rost (Dresden) presented an overview of the applicability of classical and semi-classical theoretical methods to describe the response of matter to light pulses in different energy ranges. The presentation of Matthias Kling (Garching) focused on possibilities to control electron dynamics on the attosecond timescale in nanostructures exposed to short pulses. Henry Chapman (Hamburg) demonstrated recent advances in the imaging of macromolecules with XFEL-pulses. Selim Jochim (Heidelberg) gave an overview of recent techniques to trap ultracold atoms. The institute colloquium of the mpi**pks** was embedded into the workshop program and given by Thomas Elsässer (Berlin), showing how x-ray diffraction can be used to resolve the charge dynamics in ionic crystals on the femtosecond timescale.
The plenary talks were followed by sessions, which typically started with a presentation introducing a certain sub-field by a group leader of one of the IMPRS research groups: Thorsten Uphues (Hamburg), Martin Eckstein (Hamburg), Petra Imhof (Heidelberg/Berlin), Pavel Jungwirth (Prague), Armin Scrinzi (Munich), Alexander Eisfeld (Dresden), Mathias Nest (Munich) and Andrey Surzhukov (Heidelberg/Jena). After the group leader contribution, a few PhD students from different groups presented their projects, methods and results. The scientific program comprised 39 oral presentations, out of which 26 were given by PhD students. In addition to the talks, poster sessions took place on two of the evenings, which stimulated the PhD students to discuss in an informal atmosphere, exchange their experiences and establish new ties. In total, 73 participants attended the workshop, with 52 of them being PhD students.
The coordinators have received a very positive feedback from many of the participating PhD students, but also from the involved senior scientists. The workshop provided a great atmosphere and resulted in numerous lively discussions. Further, it gave several young scientists the opportunity to present themselves and the results of their projects, which they mastered splendidly. Also, the workshop gave the PhD students of the IMPRSs an insight into current research within the four research schools and facilitated new bonds among them.
Last but not least, the entire organization was flawlessly handled by the visitors program of mpi**pks**, for which the coordinators would like to express their gratitude. In conclusion, the workshop was a full success.

Photoemission and Electronic Structure of 4f and 5f Systems, Focus Workshop
Scientific coordinators: T. Durakiewicz, J.v.d. Brink

The current progress in Angle-Resolved Photoemission (ARPES) techniques brings this most direct tool for band structure visualization to many a scientific laboratories. The focus of ARPES on strongly correlated systems over the last two decades was extremely fruitful in e.g. the field of high temperature superconductivity, where ARPES proves to be pivotal in shaping our understanding of the superconducting state.
In the meantime, the field of heavy fermion physics and unconventional superconductivity emerged, where (mostly) the f-electron systems based on lanthanides and actinides show a plethora of fascinating and novel groundstates, often coexisting. These states include magnetism, heavy fermion state, unconventional superconductivity or the exotic Hidden Order state. ARPES is a natural tool to investigate those states, but the field is in relatively early stages of development.
The need to get together the dominant players in the field of f-electron ARPES and simulate the development of the field was the primary reason for organizing our Workshop. This is driven by the need to create a critical mass of researchers in the early stages of the field, and enable the flow of information between different teams.
The workshop structure was designed to allow presentation of current discoveries in focused sessions, and afternoon round-table discussions. During the first day we enjoyed a focused session of 8 talks on URu_2Si_2 and a following discussion moderated by Andres Santander-Syro. The aim of this first day was to identify and focus on the areas of agreement between different teams. Disagreements and differences in interpretation are a necessary and normal part of the scientific process. But: finding common ground, even if sometimes difficult, is needed for progress in understanding the Nature. Four different ARPES teams and two theory teams presented their findings on Hidden Order, and the areas of convergence: (i) the general band structure, (ii) itinerancy of 5f electrons and (iii) Fermi Surface instability were all

agreed upon. One outstanding problem, namely the onset of hybridization remains unresolved, but the majority opinion emerged, linking hybridization with the coherence temperature scale. In that sense the first day was a tremendous success.
On the second day the cutting - edge research in 4f electrons was presented. Just to give a few examples, we had a presentation on Ce systems from Jim Allen, Ce heavy fermions from Andreas Koitzsch and most excellent, high resolution show of data from Denis Vyalikh, whose Yb ARPES example showing the first example of the valence band structure renormalized by crystal field levels was also used as a workshop logo. The afternoon discussion led by Peter Riseborough was focused on the theory aspects of f-electrons.
The last half-day was centered around the higher energy ARPES and x-ray scattering, which is rapidly emerging as a complex, but most helpful tool in aiding our understanding of f-electron physics.
The participants and organizers alike would like to thank MPI for providing the funds and especially thank Mrs. Lantsch, whose organization skills are impeccable. We have enjoyed the dinner and the art exhibition at the Albertinum very much. Most likely in two years we will organize the second issue of the workshop on a different continent, but also very likely, we will try to come back to Dresden in four or in six years. There is indeed no better place to organize such small to medium-size events than MPI.

Connecting Theory and Experiments in Active Matter, Focus Workshop
H. Chaté, K. Kruse, S. Ramaswamy

Main Focus of the Workshop. In active matter studies, collective motion occupies an important place. To a large extent, and notably thanks to the ASG and related events, theory is now "ahead" of experiments and thus in crucial need of confrontation to them. This situation largely arises from the difficulties of setting up controlled, quantitative, experiments / observations on animal groups and in vivo biological situations.
In this context, the remarkable in vitro experiments performed recently using purified proteins are an exception. These assays are of great values for the theorists, but they nevertheless retain some relevance to in vivo situations.
The workshop has been a wonderful opportunity to bring together the main players in this context: the theorists at the origin of most of the recent advances in the field, and most of the researchers already performing in vitro experiments using bio-components.
Format of Workshop. The initial plan to have a relatively small workshop where everybody would sit around the same table was maintained, in spite of logistic problems due to the unannounced participation of a fairly large group of people from the biophysics division of mpi**pks**. This setting, and the long discussion periods scheduled with each talk, did facilitate exchanges of frequency and spontaneity seldom seen in larger events.
Remarkable Talks and Participants, Newcomers. It is fair to say that the most noted and applauded talks were given by the experimentalists: K. Oiwa, Z. Dogic, A. Bausch, M. Murrell, and L. Blanchoin delivered remarkable talks during which they impressed the audience by the quality and novelty of their results obtained on relatively well-controlled systems of biofilaments, motor proteins, and various polymers/crosslinkers. The general consensus after that was that indeed we can look forward to tremendous progress in our understanding of active matter in the next few years thanks to this sort of experiments.
Also notable has been the update about our understanding of the actin cortex in cells, in particular thanks to the talks of F. MacKintosh, G. Koenderink, C. Sykes, C. Schmidt, A. Bernheim, and S. Grill, and the interactions with the theorists in the room.
Among the above people, L. Blanchoin, Z. Dogic, and M. Murrell, were all "newcomers" and were clearly very well regarded by others. They also said that they were very happy to have been invited. Everybody was impressed by the quality of the work of these young researchers.
Interactions with Theorists. With, in particular, J. Toner, F. MacKintosh, J. Prost and J.F. Joanny in the room, there were lively debates and many questions in the room. We could not avoid that the discussion sometimes went into important but rather technical issues!
Generals Outcome, Perspectives. There was general a posteriori consensus that the workshop was timely and fruitful: again, we now expect strong development in the area of controlled active matter experiments using bio-components, with particularly strong interactions between theory and experiments. Our opinion is that the near future will see more events organized on this topic.
Regarding the "focus" format of the workshop, participants found it refreshing, nicely different from the usual bigger conferences where they often meet each other. It is our opinion that such smaller-scale

events should be encouraged as they provide rare opportunities for high-frequency interactions in an informal-enough setting so that one can go to the heart of the problems.

Methods of Chaos Detection and Predictability: Theory and Applications, Workshop
Scientific coordinators: G. Gottwald, J. Laskar, H. Skokos

The main aim of the interdisciplinary workshop "Methods of Chaos Detection and Predictability: Theory and Applications" was to comprehensively review the theory and numerical implementation of the existing methods of chaos detection and predictability, as well as report recent applications of these techniques to different scientific fields like astronomy, mathematical physics, accelerator physics, geophysics, fluid dynamics, applied mathematics, and numerical analysis, with data coming from computer simulations, laboratory experiments and natural systems.
Being able to distinguish chaoticity from regularity in deterministic dynamical systems and to be able to determine the subspace of the phase space in which instabilities are expected to occur is of utmost importance in as disparate areas as astronomy, particle physics and climate dynamics. Is the solar system stable? Are accelerators beams consisting of elementary particles stable? How can we improve the behavior of these accelerators by avoiding chaotic zones, how shall we construct ensembles in numerical weather prediction or climate dynamics in order to capture most of the dynamics on a given time scale and to increase predictability? These are some of the questions that were lively discussed among the participants.
The workshop involved 65 participants coming from 15 different countries; a healthy mix of senior world experts and young early career researchers and postgraduate students met to discuss the latest developments.
Tangible outcomes of the workshop are a focus issue in the AIP journal *Chaos* with peer reviewed original research articles related to the workshop and a Springer *Lectures Notes in Physics* book compiling the current state of the art of chaos detection methods written by a select group of world experts drawn from the workshop. Furthermore the organizers have proposed a multi-author paper coauthored by those groups which have proposed chaos detection indicators, in which these methods are compared, with the aim of clarifying situations and problems for which the methods may be best suited, and making the codes which were used for the paper publicly available. We hope that this joint work emerging from the workshop will have high impact; providing guidance to the wider community and making it easier for the user to find the appropriate method.

Spin Orbit Entanglement: Exotic States of Quantum Matter in Electronic Systems, Seminar and Workshop
Scientific coordinators: R. Thomale, B. Trauzettel, S. Trebst

The major aim of the international workshop and seminar on Spin Orbit Entanglement: Exotic States of Quantum Matter in Electronic Systems was to bring together some of the leading theoretical and experimental physicists that share a common interest in the complex interplay of strong spin orbit coupling, Coulomb interaction and other correlation effects in novel electronic systems. We achieved this aim by inviting experts from a variety of different fields of condensed matter physics with their respective focus areas spanning a broad range from material physics, such as iridium oxides or topological insulators, to spin liquid phases and chiral magnets as well as superconductors and fractional topological states.
The three weeks including the workshop and seminar were organized as follows: In the first and last week, we scheduled a light program with roughly six talks per week and a lot of discussion time. In the intermediate week, we organized an international workshop with roughly eight invited talks per day and excellent speakers/participants from all over the world. In addition we organized an evening session of contributed talks, offering three promising junior researchers – Tobias Meng (Basel University), Andreas Schnyder (MPI for Solid State Physics, Stuttgart), and Sebastian Huber (ETH Zurich) – an opportunity to present their latest scientific results. We were particularly happy to host the most promising young researchers in the field, including the beforemetioned speakers but also e.g. Titus Neupert (Princeton).
Two very stimulating colloquia were given by Shoucheng Zhang (Stanford University) in the first week on the "Three cheers for the quantum Hall trio" and by Achim Rosch (University of Cologne) in the second week on "Skyrmions and monopoles in chiral magnets".
During the conference, a significant number of inspiring talks were given on the physics of iridium oxides – both by theoretical and experimental researchers. A particular focus was on material systems believed to

be well described by a Heisenberg-Kitaev model of spin-orbit entangled degrees of freedom. The deeper motivation to focus on these materials was the possible realization of rather exotic physics including, for instance, a quantum spin liquid phase. To mention a few highlights along these lines, Giniyat Khaliullin (MPI for Solid State Physics, Stuttgart) spoke about magnetic order and excitations in layered iridium oxides. Radu Coldea (University of Oxford) gave an experimental talk on the spin dynamics of different iridium oxides based on inelastic neutron scattering. In addition, Roderich Moessner (MPI for the Physics of Complex Systems, Dresden) told us about the dynamical structure factor of the Kitaev model and Roser Valenti (University of Frankfurt) about an ab initio analysis of hexagonal iridates and rhodates.
The physics of topological superconductors and insulators also played a major role during our seminar and workshop. Stimulating presentations on topological metals in proximity to superconductors were given by Eun-Ah Kim (Cornell University) and Patrik Recher (University of Braunschweig). Onedimensional topological superconductors based on semiconducting nanowires were discussed in the presence of Coulomb interactions by Roman Lutchyn (Microsoft Research Station Q, Santa Barbara), in the presence of disorder by Pavel Ostrovsky (MPI for Solid State Physics, Stuttgart), and in the presence of hyperfine interaction by Daniel Loss (University of Basel).
The interplay of topological physics and Coulomb interactions was in the focus of a number of talks by Stephan Rachel (TU Dresden), Karyn Le Hur (Ecole Polytechnique, Lozere), Fakher Assaad (University of Würzburg), and Lars Fritz (University of Cologne). Laurens Molenkamp (University of Würzburg) gave an excellent presentation on his pioneering experiments on HgTe as a topological insulator. This high level was likewise met regarding the discussion of Heusler compounds presented by Claudia Felser (MPI for Chemical Physics of Solids, Dresden).
More general theoretical aspects of symmetry-protected topological phases were presented by Shinsey Ryu (University of Illinois at Urbana Champaign) and of statistical topological insulators by Anton Akhmerov (Harvard University). Gregory Fiete (University of Texas at Austin) told us about topological phases in transition metal oxides where interesting physics, for instance, that of Chern insulators and topological crystalline insulators, plays a substantial role.
Two leading experimentalists on the physics of skyrmions in chiral magnets – Christian Pfleiderer (TU Munich) and Peter Milde (TU Dresden) – presented their latest results on impressive experimental signatures of skyrmions such as a topological Hall signal and the appearance of quantized magnetic monopoles that can be detected by magnetic force microscopy.
Finally, fractional topological insulators and the fractional quantum Hall effect were the main topics of a series of excellent talks given by Nicolas Regnault (ENS Paris), Duncan Haldane (Princeton University), and Andrei Bernevig (Princeton University). In this research area, new conceptual and numerical developments allow to explore exotic models (such as Read Rezayi states and the Gaffnian state describing a critical quantum Hall scenario) by the determination of so-called entanglement spectra which can yield new insights in the unconventional physics of these systems.
In summary, we believe that the workshop and seminar on Spin Orbit Entanglement: Exotic States of Quantum Matter in Electronic Systems was definitely a great success – mostly due to the excellence and liveliness of its participants. The latter is also testimony of a field that is rapidly evolving and with a number of new collaborations generated during this event we expect to hear a lot more about new and fascinating physics in this area of research in the near future.

Quantum Many Body Systems out of Equilibrium, Seminar and Workshop
Scientific coordinators: J.-S. Caux, T. Esslinger, M. Haque, C. Kollath

Background. The three-week programme was conceived as an extended meeting on the topic of non-equilibrium situations in quantum many-body systems, treated as an emerging coherent field of study. It was intended that the programme would bring together several communities interested in quantum dynamics in systems out of equilibrium. These communities include experimentalists working with laser-cooled trapped atomic systems, pump-probe spectroscopy of correlated solid-state materials, non-equilibrium transport, and theoreticians addressing fundamental conceptual issues that arise out of equilibrium.
The programme was very successful in fulfilling this goal.
The event was well-timed for this purpose. In very recent years, the topic of out-of-equilibrium evolution has started to be recognized as an important subfield of condensed matter physics, quantum optics and quantum information theory. The explosive growth of interest in the topic makes it difficult to cover the important issues in a one-week meeting. The extended three-week format allowed the meeting to obtain a snapshot of a significant fraction of current activity in the field. It was widely recognized as the

most important meeting of 2013 on the topic of non-equilibrium dynamics, as indicated by the prominent speakers and participants.
Format. The central week was a higher-intensity "Workshop week" with about a hundred participants. The first and third weeks were lighter "Seminar weeks" with lighter programmes, more time for discussion and collaboration, and 35-40 participants each.
In the central "Workshop week", there were 36 regular talks (each of 25-minute duration), one colloquium, and an after-dinner talk. The first week had fifteen regular 40-minute research talks and a special overview talk. The final week had 13 regular 40-minute research talks and two special sessions. In addition, each week had two poster sessions.
The poster sessions were held two afternoons each during the Seminar weeks, and as afterdinner sessions during the Workshop week. The poster sessions were well-attended, and the accompanying vibrant discussions continued well beyond the scheduled time. There were more than 60 posters presented in total. The sessions were not organized by subtopic; instead different subtopics were mixed into each session. This seemed to work well as participants at each session got exposure to a variety of emerging themes.
Scientific Highlights. As intended, a number of themes were addressed in the workshop. We mention a few here:
A significant fraction of presentations addressed cold-atom experiments on non-equilibrium phenomena, including transport, Bloch oscillations, soliton dynamics, matter-wave scattering, and spin dynamics. There were also a few talks on pump-probe spectroscopy experiments. Among the theory talks, many addressed particular types of existing or feasible experimental systems, such as cold atom experiments, cavity and polariton experiments, and non-equilibrium transport. A number of theory talks addressed conceptual issues such as the nature of thermalization in isolated systems, interaction quenches in Luttinger liquids and other correlated systems, the role of integrability and conservation laws, many-body localization, open quantum systems, etc.
Special Talks and Sessions. Several special sessions were incorporated into the programme in order to highlight the different communities brought together in this meeting. In the first and second weeks, there were one-hour Symposia providing broad overviews of pump-probe spectroscopy and cold atom experiments, delivered respectively by J. Demsar and D. Weiss, two internationally leading experts. During the second (workshop) week, the institute colloquium (by H.-P. Breuer) addressed dynamics in open quantum systems. During the third week, there was a special session on the role of integrability in non-equilibrium dynamics, featuring an overview talk by F. Essler on quenches in integrable systems and several short talks on other aspects of integrability. The third week also contained a session on short talks by junior physicists.
Summary. The workshop collected and attracted a large number of researchers interested in the rapidly growing field of quantum matter out of equilibrium. The overwhelming interest in attending the programme (many applicants had to be rejected) and the participation of many leading researchers showed that a multi-week event was appropriate and useful. The meeting was characterized by an overall high quality of talks and a lot of discussions and interaction between different communities. We believe that the programme was successful in its goals, and that it will positively stimulate further growth of the field.

Advances in Quantum Chaotic Scattering: From (Non-)Linear Waves to Few-Body-Systems, Workshop
Scientific coordinators: R. Ketzmerick, U. Peschel, K. Richter, P. Schlagheck

This international one-week workshop (9 - 13 September 2013) dealt with wave and particle scattering processes and with the resulting complex dynamics. Those scattering processes play an important role in atomic and molecular systems, in electromagnetic wave propagation, in mesoscopic science, as well as in the dynamics of ultracold atoms. Special emphasis was put on the propagation of coherent light and matter waves in disordered systems, on wave optics and acoustics within complex scattering geometries, on the semiclassical understanding of scattering in mesoscopic systems, as well as on classical and quantum dynamics in chaotic few-body systems featuring a high-dimensional phase space.
The workshop was co-financed by the German Science Foundation Research Unit FOR760 Scattering Systems with Complex Dynamics. This allowed for 100 participants (selected from even more applicants) presenting 24 invited talks, 16 contributed talks, and an amazing number of 58 posters during the week. Both invited and contributed talks were of very high standard, scientifically and in their way of presentation. Among the contributed talks a platform was given to young scientists on the quest for permanent positions. The large number of posters, which were presented in two lively poster sessions,

demonstrated the timeliness of the topic of the workshop. Among the high-ranking speakers of the workshop the experimental talks by H.-J. Stöckmann, M. Fink (colloquium), and M. Oberthaler were particularly fascinating and well presented for the audience.
The workshop provided a detailed account on the state of the art in the different branches of the field of quantum chaotic scattering. Moreover, it showed a clear trend to go beyond fundamental research and to address questions and topics related to technologically relevant applications in very diverse fields like random lasers, optical microcavities, acoustic wave phenomena, or the analysis of vibrational waves in cars. This trend may be an indication as to where the field of quantum chaotic scattering is going to evolve in the years to come.
It was a great pleasure for the organizers and the participants to have the professional support of the visitors program, in particular of Katrin Lantsch, and to use the superb facilities of the mpi**pks**.

Topology and Nonequilibrium in Low-Dimensional Electronic Systems, Workshop
Scientific coordinators: A. Mirlin, F.v. Oppen

Topological phenomena have emerged as a central theme in condensed matter physics. With topological insulators and superconductors as well as quantum Hall systems, a broad set of topological phases in electronic systems are now accessible in the laboratory. Moreover, there exist close relations with the Dirac fermion physics in graphene. At present, this field is rapidly evolving both theoretically and experimentally. The Workshop "Topology and nonequilibrium in low-dimensional electronic systems" involved a balanced participation of theorists and experimentalists, with 100 participants in total, and managed to collect many of the key participants in the field. The focus was put on the fundamental physics exhibited by novel systems, with a particular emphasis of non-equilibrium phenomena.
The central topics of the Workshop and the corresponding key speakers were:

- Topological insulators and related topological states of matter: M.Z. Hasan (Princeton), C. Kane (U of Pennsylvania), J. Moore (UC Berkley), A. Ludwig (UC Santa Barbara), X. Qi (Stanford), R. Moessner (MPI Dresden), E. Demler (Harvard)
- Topological superconductors, realizations and manifestations of Majorana fermions: R.-R. Du (Rice), A. Yazdani (Princeton), C. Marcus (Copenhagen), L. Glazman (Yale), P. Brouwer (FU Berlin), K. Flensberg (Copenhagen), R. Egger (Düsseldorf)
- Quantum dynamics, many-body quantum coherence: N. Gedik (MIT), X. Xu (U of Washington), M. Fisher (UC Santa Barbara)
- Integer and fractional edge states in quantum Hall systems and topological insulators: Y. Gefen (Weizmann Inst), M. Heiblum (Weizmann Inst), J. Smet (Stuttgart), A. Stern (Weizmann Inst), Y. Oreg (Weizmann Inst), B. Trauzettel (Würzburg), D. Zumbühl (Basel)
- Kinetics, transport and tunneling spectroscopy of surface states: C. Brüne (Würzburg), N.P. Ong (Princeton), M. Morgenstern (Aachen)
- Dirac fermion physics of graphene: F. Koppens (Barcelona), L. Levitov (MIT), A. Morpurgo (Geneva), E. Andrei (Rutgers), M. Potemski (Grenoble), I. Gornyi (Karlsruhe), C. Dean (New York), P. Jarillo-Herrero (MIT)

One of the highlights of the conference was the MPI Colloquium talk on coherence and controlled dephasing in quantum Hall interferometers given by M. Heiblum (Weizmann Inst.) whose pioneering works have determined the development of this field.
In addition to 35 invited talks, the conference program included 11 contributed talks as well as 45 posters presented at two poster sessions. Almost all posters and contributed talks were presented by young scientists who had an excellent opportunity to discuss their results with world-leading experts in the field. In particular, excellent talks were given by young researchers J. Dufouleur (Dresden), T. Karzig (Caltech), T. Oka (Tokyo), I. Protopopov (Karlsruhe), D. Bagrets (Cologne), D. Abanin (Perimeter Inst), A. Mitra (New York U), A. Levchenko (Michigan State U), M. Titov (Nijmegen), O. Zilberberg (ETH), E. Hankiewicz (Würzburg).
The Workshop was a highly successful event which gave a possibility of very fruitful discussions of the recent progress in the field and future perspectives and triggered new collaborations. The feedback which we got from the participants also indicates that this was a very stimulating event. The organizational support by the Institute Staff, in particular Mandy Lochar, was outstanding as usual.

Korrelationstage 2013, Workshop
Scientific coordinators: H. Fehske, C. Pfleiderer, F. Pollmann

The Korrelationstage are workshops on the physics of strongly correlated electron systems. The meetings have a long tradition and represent an important platform for the scientific exchange and promotion of young scientist in the community. The focus and format is constantly adjusted to capture the novel developments in the field and the interest of the participants. The Korrelationstage 2013 introduced a number of new concepts and ideas to stimulate discussions between the about 100 participants. In addition to about 60 oral presentations and two poster sessions with more than 60 contributions, the program was enriched with focus and overview sessions. The workshop started with a reception on Sunday, September 22nd and ended on Friday, September 27th.
The Korrelationstage 2013 focussed on four topics: *Phenomenology*, *Integrable systems*, *Topology and Entanglement*, and *Nonequilibrium and Transport*. These are timely and rapidly developing fields in which the interplay between experiments and theory is particularly fruitful. The talks and discussions to these topics were very lively. The poster sessions, which gave in particular young researchers the chance to present their results, were well attended and discussion in front of the posters lasted until late in the night.
In the field of *Phenomenology*, recent advances in the understanding of charge and spin excitations in correlated materials were discussed. A focus in the *Integrable systems* sessions were newly developed methods for the calculation of static and dynamic correlation functions that allow for direct comparison with experiments. Major advances in the numerical simulation of systems out of equilibrium and breakthroughs in optical lattice experiments have been reported in sessions on *Nonequilibrium and Transport*. In sessions focussing on *Topology and Entanglement*, a number of conceptually new quantum phases have been predicted theoretically and new materials were discussed which potentially realize these phases. As one of the highlights of the workshop, focus sessions were held on the four topics. Each session was opened by a short introduction after which young researchers had the opportunity to give short oral presentations about the contents of their poster contributions. The short presentations helped to start discussions among the participants. Each of the focus sessions was then summarized by experts of the respective fields. The summaries by the experts were very successful as they provided a very comprehensive overview of the new developments and state of the art.
Another highlight was a session in which representatives from a number of Sonderforschungsbereiche (SFB) and Forschergruppen (FOR) reported recent progress. This session gave a broad overview about some of current research funded by the Deutsche Forschungsgemeinschaft (DFG).
Prof. Naoto Nagaosa accepted our invitation as the distinct speaker of the public colloquium in which he gave a talk on "Topological particle in magnets". His very inspiring talk highlighted many of the recent theoretical advances in the understanding of topological phenomena in condensed matter physics and their relevance for experiments.

Synergetic Approaches to Complexity, Focus Workshop
Scientific coordinators: H. Haken, J. Peinke, G. Radons

Main focus of the conference. It is still one of the big challenges to understand the macroscopic behavior of complex systems composed of many interacting subsystems driven into nonequilibrium situations. In this focus workshop the latest developments in understanding complex systems with the help of tools and concepts from Synergetics were presented and discussed. In particular, the contributions showed newest concepts for handling complex systems by the use of stochastic concepts. Furthermore applications to time-series analysis and anomalous transport as well as to spontaneous structure formation and to the problem of turbulence were presented. The contributions of this workshop were grouped in the following session:

- Pattern Formation
- Time Series Analysis
- Turbulence
- Anomalous Transport

The unique contribution of Rudolf Friedrich to this field bridging pure theory with experimental and technical applications was emphasized during this workshop.
Most important participants. E. Barkai (Israel), M. Bestehorn (Germany), E. Bodenschatz (Germany),

E. Govekar (Slovenia), R. Hilfer (Germany), H. Kantz (Germany), R. Metzler (Germany), J.-F. Pinton (France), A. Pumir (France) U. Thiele (UK), R.R. Tabar (Iran), M. Wilczek (USA), N. Zabusky (Isreal) Besides the 23 main talks there was one general colloquium by Hermann Haken on Reminiscences on the early days of synergetics.
How scientific newcomers presented themselves. In the organization of this workshop we paid special attention to young researchers in this field in order to give them the opportunity to present their work either by a talk or by a poster. The time to discuss the scientific content of the posters was given in a special Poster Session in the evening. We experienced a vivid and long lasting discussion.
Scientific results of the conference in the broader sense. The general interest in the conference's topic became obvious by the participation of more than 50 researchers. It became clear that the synergetic approach to complex systems is still a challenging one and that many new physical aspects of this approach were recently discovered. Most interestingly this research field gets more and more interdisciplinary and new advanced methods are developed. The participants went home with new insights and new contacts for their further work.
As organizers we are happy that this conference was successful. In particular we and all participant appreciated the inspiring atmosphere as well as the perfect local organization of the Max-Planck-Institut für Physik komplexer Systeme.

Astrophysical Turbulance: From Galaxies to Planet, Workshop
Scientific coordinators: E. Bodenschatz, U. Christensen, S. Dreizler

Scope and scientific topics. Fluid dynamics is a unifying physical process which connects the largest down to the smallest scales in astrophysics. Formation and evolution of the largest structure in the universe, the physics in the interstellar medium, and the formation of planets are some examples. Magnetic field generation in planets, stars, and galaxies is another unifying aspect. The aim of the workshop was to provide the environment for bringing scientists from different communities together under this umbrella. The large diversity of astrophysical topics addressed was certainly a challenge. The first half of the workshop was therefore organized as school, with the intention to have a broad and also comprehensive introduction to the various aspects covered within the workshop. In these intensive two days, all length scales have been addressed and a common ground for the upcoming contributed talks and posters has been laid.
While the range of astrophysical topics was broad, the many contributions involved numerical simulations which provided another unifying aspect. Interestingly, laboratory experiments can also provide important insights for understanding astrophysical processes. The workshop hence also covered a wide range of methods for studying turbulent processes in astrophysics.
Participants. Due to the structure of the workshop, there was a good mixture of senior experts, mainly covering the introductory lectures on the various aspects of astrophysical turbulence, and young scientists. The latter took advantage of the opportunity to present their results to experts in different fields, discussing it in a broader physical context, and receiving input from a broad community. The young participants contributed a large part to intense and lively discussions.
Conclusion and outlook. The workshop has been highly successful to impart an understanding that turbulent processes in different astrophysical systems and at very different scales are often governed by the same physical principles and can be studied using similar methods. The arrangement within the Max Planck Institute for Physics of Complex Systems has been very favorable for achieving this goal. It combines the advantages of a secluded setting for the workshop with the benefits of a lively city. This workshop could be the first in a series of similar ones organized in the same way.

Small Systems far from Equilibrium: Order, Coorelations, and Fluctuations, Workshop
Scientific coordinators: M. Henkel, D. Mukamel, M. Pleimling, G.M. Schütz

The workshop has been focused on the following main topics: fluctuation and work theorems and their implications for the understanding of non-equilibrium entropy-production in small systems, the theory of large deviations, dynamically generated long-range correlations far from equilibrium, and emerging cooperative phenomena and their relation to microscopic dynamics. While these topics are certainly theoretically motivated, several talks provided a detailed comparison with state-of-the-art experiments in this field.
The workshop has been attended by some of the leading scientists in the field, as for example Udo Seifert

(Stuttgart) and Sergio Ciliberto (Lyon) on fluctuation theorems , Bernard Derrida (Paris), Christian Maes (Leuven), and Hyunggyu Park (Seoul) on large deviations, Satya Majumdar (Orsay), Stefano Ruffo (Florence), and Kazumasa Takeuchi (Tokyo) on long-range correlations, Deepak Dhar (Tata Institute), Sid Redner (Boston), and Erwin Frey (München) on cooperative phenomena.
The workshop provided an opportunity for quite a large number of students and young scientists to present their work through oral and poster contributions which we found of very high quality. We are very pleased with their active participation, both during their presentations and in the general discussion. Our workshop was received with enthusiastic response by the community as demonstrated by the large number of high quality applications. In the workshop we had 24 invited speakers and 20 further participants selected out of 60 applicants. In addition, a considerable number of the researchers at the Max-Plank-Institut attended the different presentations.
The workshop provided an opportunity for researchers from various subfields of this broad and fast developing research area to intensively interact and exchange ideas. In particular, the current state of the art of the fluctuation theorems and their intricate relationship to non-equilibrium entropy production was presented and discussed in detail. The intensive discussions have resulted in a number of new collaborations.

From Dynamics to Statistical Physics and Back, Focus Workshop
Scientific coordinators: H. Kantz, A. Politi

Main focus. This short focus workshop dealt with recent progresses in the understanding of the dynamics and statistics of systems with many degrees of freedom, the realm of statistical physics. As it turns out, many non-equilibrium phenomena are much better accessible if dynamical features of the systems are taken into account. In the converse, many dynamical systems can be characterised in the terminology of statistical physics. Concepts from dynamical systems theory such as bifurcations and Lyapunov exponents meet concepts from statistical physics such as phase transitions and localization. A broad range of systems, ranging from fluids over spin systems to biological and even economic systems, was discussed during the meeting.
Senior participants. The invited speakers as listed on the conference announcement represent a subset of the most influential and active researchers in this field.
Young scientists. Being a focus workshop with a very dense program (29 invited talks of 30 minutes each), the organizers decided not to provide time for contributed talks. Younger researchers instead were encouraged to present their work on posters during the poster session on the first evening (18 posters), which led to very lively discussions.
Main scientific results. The workshop succeeded to provide an excellent exchange of knowledge between more dynamically oriented researchers and more statistical physics oriented work. In addition, it demonstrated how the same set of concepts and methods finds applications in very diverse applications.
A couple of talks related to neuro-science emphasised the role of criticality in such out-of-equilibrium systems as the brain, but also the role of synchronization among neurons. Other biology-related talks showed that statistical tools in gene expression might help to find personalised treatment for cancer, and how molecular motors are relevant for all kinds of biophysical processes. Here, conformation dynamics is closely linked with the thermodynamics of small systems. Indeed, as an outstanding experimental result, the verification of Landauer's principle in an optical tweezer experiment was highly appreciated and lively discussed.
On the more fundamental side, recent achievements in the treatment of interacting particle systems were presented, such as mixed order phase transitions or the role of Lyapunov exponents in mechanical models of fluids. Another prominent issue were finite size corrections and the way how to approach the thermodynamic limit in computer simulations, exemplified for the problem of heat conduction. While the analytical treatment of physical problems usually involve some approximations, numerical simulations suffer from both finite systems size and potentially lack of convergence in time, so that the comparison of analytical and numerical results remains a challenge. Rough interfaces such as described by the KPZ equation turned out to be a paradigm which occurs unexpectedly in many physical contexts that range from transport problems in one-dimensional systems to the spreading of infections.
A few talks gave an outstanding outline of the historical development of some still unsolved issues, such as the FPU paradox or the problem of heat conduction where some recent theoretical progress is still partially challenged by direct numerical simulations. A major achievement of this workshop, in addition to these numerous specific scientific results, has been to stimulate the exchange of concepts and ideas and

to allow for new approaches to long standing problems in the realm of complex many particle dynamics.

Weak Chaos and Weak Turbulence, Workshop
Scientific coordinators: E. Kartashova, A. Pikovsky, D. Shepelyansky

Main focus of the workshop. In organizing this workshop we intended to find an overlap between theoretical, computational, experimental, and mathematical studies in the fields of weakly nonlinear Hamiltonian systems close to integrable ones, and of wave (weak) turbulence. Albeit of several cancellations, such an overlap was indeed achieved. Invited talks and contributed presentations gave a good overview both of fundamentals of the envisaged directions and of the recent achievements. Many participants expressed the opinion, that such an exchange of expertise was very useful for their future work.
Most important participants. To the highlights of the presentations at the workshop belong:

- A colloquium talk by Prof. Turitsyn (Aston) who gave a nice introduction in the field of complex regimes in fiber lasers, with both fundamental and applied aspects.
- Prof. Flach (Auckland) in his talk gave a comprehensive review of recent results in the field of disordered weakly nonlinear lattices.
- Prof. Nasarenko (Warwick) reported on the progress in studies in wave interactions.
- Prof. Wang (Paris-Sud) presented a variant of KAM-like theorem for the nonlinear Schrödinger equation.
- Prof. Dhar (Tata) reported on the studies of head conduction in weakly nonlinear lattices.

Presentation of scientific newcomers. In contributed oral talks and poster presentations young scientists had an opportunity to report on their studies. All of them were on a high scientific level. We would like to mention especially the contributions of A. Frishman, T. Grafke, F. Onken, and M. Sala.
Scientific results in a broader sense. Complex nonlinear systems, in spite of enormous activity in this field, remain a challenging problem of modern science. This workshop confirmed once more that the best progress can be achieved if the efforts of theoreticians, experimentalists, mathematicians, and specialists in computations are combined.

Recent Progress and Perspectives in Scaling, Multifractality, Interactions, and Topological Effects Near Anderson Transitions, Focus Workshop
Scientific coordinators: F. Evers, I. Gruzberg, V. Kagalovsky

The main focus of the meeting. The focus of the meeting has been on the Anderson transitions and the associated scaling behavior. A small, but very distinguished group of experimentalists has presented an overview and most recent results on effects of disorder and critical behavior in quantum Hall systems (Morgenstern, Pan), topological insulators (Morgenstern), and semiconductors (Pan, Pudalov). Most notably, an intriguing overview about ongoing activities and perspectives on studies of localization in systems of cold atoms was given (Aspect). On the theory side, the spectrum of systems that have been discussed was very wide including graphene-type matter, disordered semi-conductors, superconductors (with Mayorana fermions), Kondo systems, and topological insultators. All these topics were held together by the common theme of localization and criticality.
The most important attendees.
Experiment: A. Aspect, M. Morgenstern, Wei Pan, V. Pudalov.
Theory: J. Chalker, A. Finkelstein, Y. Fyodorov, V. Kravtsov, A. Mirlin, T. Ohtsuki, K. Slevin, F. Wegner, M. Zirnbauer.
Scientific newcomers and how they presented themselves. Anderson localization is still a very active research topic that offers difficult challenges, beautiful theoretical concepts and relevant applications to the young generation. For this reason the community keeps attracting excellent young scientists. To give them an opportunity to present their research to the community, the meeting had invited talks (40 min) given by junior professors and research group leaders, (Bardarson, Bettelheim, Burmistrov, Foster, Gornyi, Ivanov, Narayanan, Obuse, Oganesyan, Ostrovsky, Scardicchio, Titov, Wan). Moreover, several highly promising postdocs presented their recent work in 20 minute talks (Bagrets, Bondesan, Schwiete).
Scientific results in a broader sense. The meeting presented a forum where several very recent and important developments have been discussed intensively. We mention some of them:

- Pure scaling observables at metal-insulator transitions and implications for the scaling analysis (Obuse, Zirnbauer; discussions Evers, Gruzberg, Mirlin, Ohtsuki, Römer, Slevin, Wan, and others).

- Many-body localization, numerical results (Bardarson, Oganesyan, Scardicchio: discussions Chalker).
- Multifractality and interactions (Burmistrov, Foster, Gornyi, Kettemann, Kravtsov, Slevin).
- Disordered Dirac fermions and graphene (Foster, Gornyi, Mirlin, Ostrovsky, Titov)
- Disorder effects in flat bands (Aoki, Chalker).

A broader perspective, contacts and collaborations. In our application, we have stated that "Now is a good time to bring together selected experimentalists and theorists to discuss and share the excitement of their latest research. We stress that experimental realization of Anderson localization include acoustics, optics, and cold atomic gases. We hope that the participants in the workshop will be able to forge a unified view of the recent developments in the field of Anderson transition with the focus on critical scaling, including subleading exponents, their high accuracy determination, multifractal wave functions, and interaction and topological effects".
We believe that all our goals have been achieved. Many participants have told us that they learned a lot. In particular, new contacts have been forming (Aspect/Finkelstein, Evers/Lugan) that may well become a basis for future collaborations.

Brownian Motion in Confined Geometries, Workshop
Scientific coordinators: S.M. Bezrukov, L. Schimansky-Geier, G. Schmid

Main focus of the workshop. The symposium concentrated on both the theory and experiment of mass and charge transport in artificial and natural micro- and nano-structures, with the goal to deepen current understanding of the diffusive mechanisms in confined geometries. Restricting the volume of the phase space available to the diffusing particles by means of confining boundaries, or obstacles, brings remarkable entropic effects. Driven transport of charged particles across bottlenecks, such as ion transport through artificial nanopores or biological channels, represents a ubiquitous situation, where diffusion is effectively controlled by geometrical restrictions.
The theoretical findings come along with new experimental observations in biological channels, porous materials, and — newly — artificial nanopores with tuned particle-pore interactions. Manipulation of the dynamics by hydrodynamic flow fields and the direct observation of the diffusing particle inside the channel enable investigation of the escape times of the individual polymers or other structured particles from cavity-forming reservoirs through narrow bottlenecks.
Format of the workshop. The scientific program started Monday morning, 17 March, and continued until Friday noon, 21 March. It accommodated 29 invited lectures, 10 contributed talks, and 27 posters. A one-hour colloquium talk was given on Monday late afternoon.
Remarkable talks and participants, newcomers. The most applauded talks included those given by Ulrich Keyser (University of Cambridge), Murugappan Muthukumar (University of Massachusetts), Sidney Redner (Boston University), Igor Sokolov (Humboldt-Universität zu Berlin), Clemens Bechinger (University of Stuttgart), Hartmut Löwen (University of Düsseldorf), Peter Hänggi (University of Augsburg), Ralf Metzler (University of Potsdam), and Fabio Marchesoni (Universita' di Camerino). Importantly, the newcomers included both bright theoreticians (e.g., Drs S. Martens, J. Dzubiella, R. Voituriez) and superb experimentalists (e.g., Drs S. Lemay, S. Pagliara).
General outcome, perspectives. Among the main achievements of the workshop was to bridge the existing gap between the scientists who work on the theory of Brownian motion of confined particles and those who perform experimental work on transport of polymers, such as proteins, DNA, and RNA in confining media and on transport in model systems. As witnessed by a great number of responses received by the workshop organizers, the participants from both theory and experiment have found the meeting truly rewarding and constructively different from large-format conferences. A lot of questions were asked by younger participants, suggesting that the atmosphere of the workshop was friendly and conducive to general discussions.
The high interest in the workshop suggests that it was timely, thus reflecting the growth of the field. The participants went home with new insights and new contacts for their future work.

Topological Matter Out of Equilibrium, Focus Workshop
Scientific coordinators: R. Moessner, S. Parameswaran

The **mpipks** workshop "Topological Matter Out of Equilibrium" was held from March 27-29, 2014. The goal of the workshop was to bring together two extremely active areas of present research, namely, out-of-equilibrium phenomena in quantum many-particle systems, and the study of topological phases of

matter. Thus far, much of the work on nonequilibrium statistical mechanics has relied on the notion of a local order parameter, absent in topological phases. Conversely, studies of topological phenomena have focused on equilibrium and ground-state properties.
The intersection of these fields remains largely uncharted territory.
This workshop brought together theorists from both groups, as well as experimentalists studying dynamical phenomena in a variety of systems, covering topics such as topological phenomena in driven systems, hydrodynamic descriptions of phases with emergent gauge fields, ultrafast and inelastic spectral probes of quantum matter, the development of numerical methods, and finally potential experiments in the solid state and ultracold atomic gases.
The talks were organized around the following main themes:

- theoretical description of out-of-equilibrium systems and phases with unconventional dynamics in a diverse variety of contexts, ranging from non-Fermi liquid states of matter to many-body-localized systems
- proposed experimental probes of a variety of non-equilibrium phenomena
- the possibility to engineer new states of matter in driven systems, such as in photonic systems or through "Floquet band structures"
- experimental results on real materials

The organizers attempted to have a wide representation of participants from different fields. These included many of the key workers in the theory of topological phases and disordered quantum systems (Prof. E. Altman, Prof. D. Pekker, Prof. V. Oganesyan, Prof. A. Bernevig, Prof. M. Foster, Dr. S. Bhattacharjee, Dr. A. Chandran); in the theoretical experimental study of such phases in cold atomic gases (Prof. A. Paramekanti), in photonic materials (Prof. A. Szameit) and in solid-state systems (Prof. N. Gedik, Prof. B. Gaulin, Prof. J. Orenstein, Prof. C. Pfleiderer, Prof. C. Broholm); the participants also included a high-energy physicist (Prof. S. Hartnoll) describing techniques to understand non-Fermi liquid transport using methods and insights from string theory.
Younger participants. As both the central topics are relatively young, much of our participation was from PhD/Masters student, postdocs and junior faculty. Indeed, several interesting talks were given by students, postdoctoral fellows and junior faculty: Prof. M. Foster, Prof. D. Pekker, Mr. Knolle, Dr. S. Bhattacharjee, Dr. A. Chandran). We also had an excellent selection of posters (both by junior and senior participants); indeed, from the poster submissions a handful were selected for oral presentations.
Summary. The workshop substantially achieved its stated goal of bringing together a diverse range of participants actively engaged in research on a wider variety of topics within the umbrella of non-equilibrium aspects of topological phases. There were several fruitful interactions across the different subtopics represented at the workshop; hopefully these will stimulate further work and collaborative research in new directions. Participants particularly appreciated the abundant time for discussions that were an integral part of the program.

Circle Meeting on Biological Physics, Focus Workshop
Scientific coordinators: G. Salbreux, F. Jülicher

The meeting was part of an annual workshop bringing together members from 5 institutes in Europe at the leading edge of research in experimental and theoretical biological physics: the European Laboratory of Molecular Biology in Heidelberg, the Institut Curie in Paris, the AMOLF in Amsterdam, the University of Saarbrücken, and the **mpipks** in Dresden. In addition, members of the MPI-CBG in Dresden joined the meeting this year. The meeting aims at discussing research topics at the interface between physics and biology and at fostering interactions between key institutions playing a role in this quickly growing field. Participants are primarily PhD students and postdoctoral fellows, who can benefit from the meeting to present their research and learn about state-of-the-art developments in the field. The circle meeting happened for the first time in 2009 in Dresden, and then went to Amsterdam, Saarbrücken, Paris and Heidelberg, before coming back to Dresden in 2014.
62 participants and 5 scientific coordinators joined the meeting this year, and 22 talks were given by PhD students and postdocs selected from all the participating institutes. The speakers discussed a range of subject from the molecular and cellular scale to the tissue level in biology. More specifically, the topics covered included the mechanics of microtubules in the spindle during cell division, the properties of actomyosin network in the cell, cell rheology, the motion of bacteria, lipid membrane mechanical properties

and its interaction with the cytoskeleton, mechanisms of transcription by RNA polymerase, the circadian clock and developmental processes at the scale of the embryo in several model organisms. Talks displayed a high level of quality and triggered exciting scientific discussions. This stimulating environment will most certainly have helped establishing new fruitful collaborations between participants. In addition, two poster sessions with 33 presented posters allowed for further interactions between participants.
Overall, the meeting was highly successful and confirmed the key role of the circle meeting in allowing for students and postdocs in physical biology to meet and exchange on their research. A following online survey revealed a overwhelming positive feedback of participants, with 90% of the answers positively evaluating the opportunities of discussion with other participants and the format of the meeting. This result clearly shows that this meeting was a crucial event to promote interaction and scientific exchanges in physical biology in Europe.

DNA-Based Nanotechnology: Digital Chemistry, Workshop
Scientific coordinators: M. Mertig, C. Richert, H. Yan

Building intricate functional nanoscale structures is one of the most important challenges for science and technology. Top-down methods, such as lithography, are being pushed to their limits in today's manufacturing processes, making it ever more important to develop bottom-up methods that produce structure well beyond the traditional scale of molecules. Among the bottom-up methods, DNA nanotechnology stands out as the most rapidly growing, and perhaps most promising field. Due to the programmability of DNA duplexes, their well-defined geometry, their mechanical properties, and the ability to combine duplexes with branching elements, such as Holliday junctions or turns, a structural diversity is achievable that is unrivalled by other techniques. At the same time, the ready availability of synthetic oligonucleotides and long single-stranded templates has opened the door to the fabrication of structures up to several hundred nanometers in size with predictable location of every single atom in the mega-Dalton arrangement. While single-stranded DNA tile assembly has been known for more than two decades, DNA origami constitutes a more recent development.
The workshop was the second of its kind in Dresden. While the first DNATEC meeting, in 2009, had focused on new structures, this year's conference was focused on function. One hot topic that appeared in numerous presentations was nanophotonics. The ability to place colloidal nanoparticles on DNA scaffolds opened the door to forays into structures acting as antennae at optical wavelengths, materials with negative refractive index, or opto-electronic circuits. Another topic that was hotly debated was dynamic systems. Results presented ranged from controlled oscillating or evolving systems to nanorobots. In some instances, the motion of DNA walker-assemblies or of enzymatic machinery on DNA origami tracks can now be observed in real time, using fast-scan atomic force microscopy, as presented in a very impressive way by Hiroshi Sugiyama from Kyoto University. Anyone proposing ten years ago that individual functional molecules would be observed spectroscopically in real time and in their programmed movement along a surface would have met with scepticism. Today, this is a reality. Yet another area in which great progress has been made is the interfacing of artificial DNA structures and living cells. Several talks showed, how the field of synthetic biology is beginning to merge with DNA nanotechnology to produce biomimetic cell assemblies with new properties. Protocells can be designed, their membranes modelled through structural DNA origami, and their porosity tunes by artificial nanopores. Few fields can boast such an impressive synergy between physics, chemistry, and biology. Only the collaboration between these fields then produces the technological advances that were proudly displayed at the meeting.
It would be near impossible, if not unfair, to single out individual contributors to this meeting. It is noteworthy, though, that the participants included Nadrian Seeman, who pioneered the field of DNA nanotechnology in the 1980s, and most of the leaders of the field as it is perceived today. Speakers hailed from all parts of the scientific world, including the East and the West Coast of the USA, Japan, India, the UK and many other European countries. In addition, the meeting attracted many young researchers, working in the field of DNA nanotechnology today. The presentation format left time for in-depth discussions that were supplemented by the poster sessions and the countless exchanges during breaks and meals. The mpi**pks** provided a perfect setting for a truly interdisciplinary conference on a fast developing topic that has moved from a curiosity to a structuring technique to an avant-garde method for assembling functional machines. Plans for the next DNATEC meeting are already being talked about!

ETW Program: Nonlinear Physics at the Nanoscale: A Cross-Fertilization on Stochastic Methods, Workshop
Scientific coordinators: J. Brand, S. Flach, P. Schwerdtfeger

In 2014, the mpi**pks** has launched a joint workshop program together with the recently founded New Zealand Institute for Advanced Study (NZIAS) in Auckland, New Zealand.

NZIAS aspires to become a leading centre for theoretical research and intellectual inquiry in the sciences and to build a reference space for creative and strong interacting workshops and seminars. Within its broad spectrum of research activities, an active centre of theoretical chemistry and physics with about 30 members (including five faculty members) shows interesting overlap potential with research parts conducted at mpi**pks**.

The joint program between NZIAS and mpi**pks** is projected for four years (2014-2017) and comprises exploratory workshops and seminars in Auckland and Dresden on current topics in the field of Nonlinear Physics at the Nanoscale.

The program will host two tandem events, each of which consists of one workshop at mpi**pks** and one at NZIAS. The larger scale mpi**pks** workshop addresses a question on the boundary of two fields of research within the general field of Nonlinear Physics At the Nanoscale. In the course, of this workshop new ideas and bridges are identified, one of which is then to be focussed in the subsequent NZIAS meeting.

The first kickoff meeting (coordinators: Peter Schwerdtfeger, Joachim Brand, Sergej Flach) took place in Dresden 12-16 May 2014 on *Nonlinear Physics at the Nanoscale: A Cross-Fertilization on Stochastic Methods*. It brought together 60 researchers from all over the world, with five participants from New Zealand, and four from Australia. It was a planned but also unexpected success with many excellent talks and a huge potential for further cross-fertilization. We enjoyed 6 keynotes lectures, 24 invited talks, 9 contributed talks, and 21 poster presentations. The topics ranged from various techniques to simulate quantum matter with temporal noise, to many body quantum interactions in the presence of spatial noise (disorder). The seemingly different subareas are closely connected in physics, mathematics, and computational methods. Peter Schwerdtfeger delivered a splendid Public Evening Lecture to an audience of more than 150 scientifically interested members of the Dresden community. The topic of the lecture was *At The Edge Of The Periodic Table: The Chemistry Of Superheavy Elements*. Further highlights of the meeting were an excursion into the heart of the old Dresden city, which included a pipe organ concert in the Church of the Court, and a subsequent excellent conference dinner at the Saxonian parliament on the banks of the Elbe river.

Many meeting participants from both hemispheres expressed their strong interest in joining the return meeting, which took place in early 2015 in Rotorua, New Zealand, and was followed by a one-week seminar at NZIAS in Auckland.

Causality, Information Transfer and Dynamical Networks, Seminar and Workshop
Scientific coordinators: J. Davidsen, P. Grassberger, B. Schelter

Inferring cause-effect relationships from observations is one of the fundamental challenges in natural sciences and beyond. Due to the technological advances over the last decade, the amount of observations and data available to characterize complex systems and their dynamics has increased substantially, making scientists face this challenge in many different areas. One specific example is the brain for which one can make multivariate recordings of its activity on many different levels, ranging from single neurons to extended brain regions. Another important example is the identification of genes that interact to control cellular processes by transcriptional activation of a set of target genes – identifying their interactions is an essential task for network reverse engineering in modern systems biology. Several analysis techniques from information theory, statistics and related disciplines exist to estimate causal influences, interactions and connectivity from general multivariate recordings under certain assumptions. The connectivity is often of particular importance since it allows one to describe the dynamics of a given system in the modern language of complex network theory and to tackle questions related to structure and functionality.
CIDNET targeted various fundamental issues and open questions that remained. These included but are not restricted to: 1. Suitable choice of a network definition in terms of nodes for a given system. 2. Scale-dependent properties of the networks. 3. Role of nonlinearities in extracting causal influences and interactions. 4. Distinguishing between direct and indirect interactions. 5. Feedback between dynamics and interactions. 6. Unobserved processes. 7. Observational noise and non-stationarities.
CIDNET invited 32 outstanding experts in this area of research from all over the world. To name only a

few of the key attendees, who contributed to the big success of CIDNET by triggering and facilitating discussions and new collaborations, we list: (a) Celso Grebogi (University of Aberdeen): Multi-layered networks and emergence of spatiotemporal order in ecological systems, (b) Klaus Lehnertz (University of Bonn): Measuring directed interactions in the human brain, (c) Dante Chialvo (University of the Balearic Islands & UCLA): Emergent complex neural dynamics, neuronal avalanches and the critical brain, and (d) Michal Zochowski (University of Michigan): From network structure to brain function and back. Key contributions from local participants - Holger Kantz (mpi**pks**): Direction of coupling from phases of interacting oscillators: A permutation information approach and Stefan Kiebel (TU Dresden and MPI for Human Cognitive and Brain Sciences): Dynamic models for brain function and neuroimaging data analysis - completed the CIDNET seminar and workshop programme.
In particular, young investigators and researcher from related disciplines were given the chance to present their work during the seminar programme and additionally posters during the workshop phase. Several discussions and new collaboration were facilitated through this. Overview talks in the various areas were given by experts that led to extremely fruitful discussions during which scientific newcomers could gain and increase their knowledge in the important research field of CIDNET.
The key scientific result of CIDNET in most certainly the various novel collaborations that emerged from the in depth discussions during the seminar and workshop phase of the CIDNET programme. These collaborations will result in various publications and research grant triggered by CIDNET. Already during the seminar phase, researchers that hadn't worked together joint forces to tackle some of the challenges mentioned above.

Topology and Entanglement in Correlated Quantum Systems, Seminar and Workshop
Scientific coordinators: E. Berg, N. Cooper, F. Pollmann, X.-G. Wen

The combined workshop and seminar program was held from 14 July - 08 August 2014. The main goal was to bring together scientists working on topological phenomena in condensed matter systems, with an emphasis of such phenomena which arise due to inter-particle interactions. As the field of topological phases in correlated quantum system is a very young one, many of the participants and speakers were young scientists — either faculty before tenure, postdocs, or even graduate students.
Important progress was reported on several topics:

- Classification of topological phases in the presence of interactions. Major progress on the classification of interacting topological phases have been reported by several of the speakers including Lukasz Fidkowski (Stony Brook University), Titus Neupert (Princeton University), Michael Levin (University of Chicago), Andrew Essin (California Institute of Technology), and Fiona Burnell (University of Minnesota).
- Significant new developments on the field of symmetry protected topological phases has been presented by several speakers including by Shinsei Ryu (University of Illinois at Urbana-Champaign), Michael Levin (University of Chicago), Fiona Burnell (University of Minnesota), Masaki Oshikawa (University of Tokyo), Michael Zaletel (University of California, Berkeley), Keisuke Totsuka (Kyoto University), and Shigeki Onoda (RIKEN).
- New discoveries on how topologically ordered states could be realized in cold atom systems or be in newly designed materials. Key contributors included Gunnar Möller (University of Cambridge), Moty Heiblum (The Weizmann Institute of Science), Loren Aycock and Mohammad Hafezi (both from the University of Maryland).
- Non-abelian excitations in topologically ordered systems — which might be the basis for fault tolerant quantum computing. Contribution by Johannes Knolle (mpi**pks**), Roger Mong (California Institute of Technology), Kirill Shtengel (University of California), Adiel Stern (The Weizmann Institute of Science), Seyyed Mir Abolhassan Vaezi (Cornell University), Jason Alicrea (Caltech), and Yidun Wan (Perimeter Institute for Theoretical Physics).
- Progress on the fractional quantum Hall effect and fractional topological insulators. Bulk-Edge correspondence in topologically ordered states was discussed in talks by Bernd Rosenow (Universität Leipzig), Andrea Young (Massachussetts Institute of Technology), Victor Gurarie (University of Colorado), Nicolas Regnault (École Normale Supérieure de Paris), and Steve Simon (University of Oxford).
- Entanglement and Many-Body Localization was covered in talks by Gil Refael (California Institute of Technology), Jens H Bardarson (mpi**pks**), Dmitry Abanin (Perimeter Institute), and Ehud Altman

(The Weizmann Institute of Science).

A very pedagogical introduction to "Topological Order" for non-specialists was given in a colloquium by Steve Simon (University of Oxford).
To summarize, the combined workshop and seminar program achieved its goal of bringing together a wide range of leading scientist. Active discussions (especially during the seminar weeks) stimulated further work and collaborative research in new directions.

Quantum Spin Dynamics: From Exotic Excitation to Novel Transport and Non-Equilibrium Phenomena, Seminar and Workshop
Scientific coordinators: W. Brenig, A.L. Chernyshev, M. Zhitomirsky

The goal of QSD14 was to bring together different communities of theorists and experimentalists working on quantum magnets, transport in magnetic materials and models, and on the non-equilibrium dynamics of correlated systems. This selection of topics for the workshop and seminar aimed at attracting key researchers in fields that are closely related regarding their techniques, theoretical approaches, and the challenges they face, but are conventionally confined to more specialized conferences, which limits potentially useful cross-fertilization of ideas.
The main unifying theme was the physics of unconventional excitations and their impact on the transport and non-equilibrium properties of strongly-correlated and spin systems. These themes are paradigmatic to low-dimensional and frustrated quantum magnets and have recently become hot topics in the traditionally more classical field of magnonics as well as in skyrmion matter and topological systems in general. The latter research areas share a lot of common ideas and employ similar analytical and numerical methods, as well as experimental approaches.
From a broader perspective, the study of collective and dynamical properties of spin systems is not only a timely area of basic research in solid state physics, but new insights from this field may induce progress in future applied sciences of a wide variety. These include spintronics, quantum computing and information, thermal management for device design, as well as data storage. Therefore, a spin-off into other scientific or technological disciplines could be envisioned, such as information technology, electrical engineering, functional material synthesis, and active device design.
Along these central ideas, the program of QSD14 was set up to comprise a carefully balanced blend of excellent talks, covering a wide range of topics during the workshop week, provoking lively discussions and extensive exchange of ideas and expertise. Moreover, ample time was allotted during the seminar week to pursue individual as well as collaborative research, benefiting from the excellent resources and environment provided by the mpi**pks**. Some of the existing collaborations among the attendees have received additional momentum and some new collaborations were initiated with the other visiting seminar attendees.
A total of 80 participants from several European countries, from the USA, Japan, India, Australia, and Canada have contributed to the success of the event. Key presentations included talks by internationally renowned researchers like Prof. Ian Affleck (UCB), Prof. Federico Becca (SISSA), Prof. Leon Balents (UCSB), Prof. Andrey Chubukov (UMN), and Prof. Roderich Moessner (mpi**pks**).
The QSD14 workshop and seminar attracted many young researchers with substantial contributions to the event were made by the PhD/Masters students, postdocs, and junior faculty. This included several interesting talks e.g. by Prof. Adrian Feiguin, PD. Dr. Markus Garst, Dr. Christian Hess, and Mr. Johannes Knolle. In addition, there was also an excellent selection of posters comprising very relevant contributions not only from senior, but especially from junior participants.

Echoes in Complex Systems, Workshop
Scientific coordinators: A. Goussev, R. Jalabert, D. Wisniacki

This one-week workshop (22 - 26 September 2014) addressed recent advances in a broad area of physics concerned with echoes in complex media. Disordered systems, as well as classically chaotic and quantum many-body systems, are sufficiently complex to impregnate the echo response with the signature of their characteristic physical parameters. Systems of each of these three types were extensively discussed during the workshop. Special emphasis was put on the many-body case, in particular, on understanding alternative definitions of the echo, stemming from different experimental scenarios and strategies for a quantitative investigation of the concept.
A particularly important development treated in the workshop was the link between two kinds of echoes:

those in which a quantum state is reversed in time (Loschmidt echo) and those in which a wave propagating in a complex medium is recorded and re-injected back into the system (time-reversal mirrors). The potentiality of echoes to characterize seemingly disconnected problems (such as criticality close to a quantum phase-transition, nonequilibrium work statistics, and parametric correlations of eigen-levels) emerged as one of the most interesting aspects of the meeting. The theoretical aspects of the Loschmidt echo, concerning the applicability of different semiclassical approaches, is an important question for the Quantum Chaos community and has been discussed thoroughly.
The workshop was markedly interdisciplinary. The subject of echoes concerns various physics communities, as well as those of chemists working in nuclear magnetic resonance. It was also an international meeting with participants from all over the world, including China, Japan, the United States, Mexico, Brazil, Argentina, and many European countries. The main scientific leaders of the field were present, and a special place was reserved for young participants, allowing them to present their research work. A very lively poster session took place on Thursday evening. The Monday colloquium was given by one of the organizers, who presented an overview of the field to the large community of Dresden physicists. On Tuesday, a special session entitled "Echoes in Magnetic Resonance" took place honoring one of the pioneers of in the field, the late Prof. Patricia Levstein. Leading experts of Nuclear Magnetic Resonance reviewed her scientific work, crucially important in triggering the interest for echoes in complex systems. The success of the conference would not have been what it was without the precious help from the institute's administration, especially that of Ms. Mandy Lochar, to whom the organizers are particularly indebted.

New States of Matter and their Excitations, Workshop
Scientific coordinators: J.H. Bardarson, F. Pollmann

The workshop was held from September 29 - October 2, 2014. The workshop's main goal was to bring together scientists researching collective behavior of condensed matter systems. The program consisted of two days of tutorials and two days of research talks including a poster session.
The eight tutorials were mainly aimed at junior researchers and covered both theoretical and experimental topics. On the experimental side, two excellent tutorials, presented by Bella Lake (Helmholtz Zentrum Berlin) and Christian Pfleiderer (Technische Universität München), introduced the basics and recent developments in Neutron Scattering techniques. A very interesting tutorial on the application of photoemission to topological systems was given by Oliver Rader (Helmholtz Zentrum Berlin). John Mydosh (Leiden University) gave an outstanding tutorial about the history of the Kondo effect and spin glasses. On the theory side, Piet Brouwer (Freie Universität Berlin) gave a marvelous pedagogical introduction to Majorana physics in one dimensional wires. Jens H. Bardarson (mpi**pks** Dresden) covered the recent developments in the field of many-body localization and gave a very accessible introduction to this emerging field. An enlightening tutorial on quantum quenches and integrable models was given by Fabian Essler (Oxford University), and Kai Philipp Schmidt (TU Dortmund) gave a lucid overview on topological quantum order and its breakdown.
All tutorial session were well attended and lively discussions enriched the sessions. Many of the local students from the mpi**pks**, the Technische Universität Dresden, and the neighboring institutes participated in the tutorial sessions.
The fourteen research talks focused mainly on the recent progress made by the various groups and partners constituting Helmholtz Virtual Institute:

- Progress on the topic frustrated magnetism and spin-liquids was reported on by several speakers including John Chalker (Oxford University), Matthias Vojta (TU Dresden), Roderich Moessner (mpi**pks** Dresden), Diana Quintero Castro (Helmholtz Zentrum Berlin), and Alan Tennant (Oak Ridge National Laboratory).
- Significant new developments on many-body localization were discussed in the talks by Shivaji Sondhi (Princeton University) and Gil Refael (California Institute of Technology).
- New discoveries in the field of topological phenomena in condensed matter physics were presented by Markus Morgenstern (RWTH Aachen), Alessandro Romito (FU Berlin), Bjoern Sbierski (FU Berlin), and Leonid Pryadko (University of California, Riverside).
- Progress on the understanding of dynamics in spin-systems was reported in the presentations of Claudio Castelnovo (University of Cambridge) and Salvatore Manmana (University of Göttingen).

To summarize, the combined workshop and tutorial program achieved its goal of bringing together a wide

range of leading scientist. In particular during the tutorial program, clear and pedagogical lectures helped young scientists to learn about recent developments in the field. Active discussions, especially during the poster session, stimulated new collaborative research.

Pressure and Strain Effects in Correlated Electron Materials, Workshop
Scientific coordinators: J.P. Attfield, J. Hamlin, P. Hirschfeld, R. Valenti

Main focus of the meeting. The aim of this workshop was to bring together and stimulate a dialog between the best experimentalists synthesizing and characterizing strongly correlated systems under pressure/strain and theorists working on modeling as well as first-principles descriptions of correlated systems under pressure/strain. The workshop was held over four days with a total of 57 participants (29 from Germany, 10 from Europe besides Germany, 12 from North America, and 6 from Asia, with 10 female participants). The workshop included roughly eight presentations per day and two evening poster sessions. The presentations for many of the talks have been made available on the mpi**pks** website.
Important participants and scientific newcomers. Presentations at the conference can be broken into the following categories:

- Ultra-high pressure studies of elemental solids (Eremets, Loa, and Schilling)
- Mott criticality in organic conductors (Kanoda and Lang)
- Complex oxides and synthesis under high pressure (Attfield, Azuma, Khomskii, Ovshinnikov, Saha-Dasgupta, Shimikawa, and Stummer)
- Strain effects in oxide thin films and heterostructures (Dörr, Del Genio, Hwang, Kopp, von Löhneysen, and Zabeleta)
- Novel phase diagrams and quantum phase transitions (Batista, Cooper, Friedemann, Grosche, Haase, Julian, Mazin, and Pfeiderer)
- Iron-based superconductors (Bud'ko, Felser, Fernandes, Meingast, Putzke, Schmalian, and Tomić)

The presentations of both the senior and more junior researchers were of a high caliber. In addition, there were a number of interesting posters that stimulated fruitful discussions between senior and junior researchers.
Scientific results of the conference. Strongly correlated materials hold great promise for technological applications. These materials are frequently highly sensitive to pressure and strain. Thus both theorists and experimentalists studying strongly correlated materials often examine the effects of pressure or strain. Within this broad community, there are several subgroups, including those studying the effects of hydrostatic pressure on bulk materials and those examining the effects of strain (e.g. epitaxial) on thin films. Because of differences in techniques, these communities do not interact as closely as it might be hoped. Both experimental approaches, combined with insight from theory, will likely be necessary to realize the goal of being able to control and predict the properties of strongly correlated materials. PSECEM14 furthered this goal by helping to foster a dialog between the various experimental communities and the theoretical community that is attempting to explain the properties of strongly correlated materials under pressure/strain.

Atomic Physics 2014, Workshop
Scientific coordinators: J.-M. Rost, T. Pfeifer

Main focus of the workshop. The meeting brought together international leaders and experts in the field of strong-field light-matter interaction, in particular concerning atoms, molecules and clusters/nanoparticles in intense or high-energy light/laser fields. The main focus theme was "Slow electrons and short light pulses". The interest in this topic was born several years ago, where the so-called low-energy structure in strong-field (tunneling-/multiphoton-) photoemission spectra was found to be the result of the interaction of an electron with the spatially extended potential of its parent ion. Since then, a number of further benchmark results, and low-energy "fine structure" have been obtained by continuous progress in experiments (enhanced resolution of detectors, improved control over laser fields and better statistics) as well as in theory (improved quasi-classical models and analysis). Slow electrons occur also in a range of other scenarios (e.g. harder photons, clusters, Rydberg atoms) outside the special topic of low-energy (fine) structure. The main goal of this workshop was to create and convey a comprehensive picture of the various physics processes that lead to slow-electron creation, and to disentangle and/or unify these mechanisms.

Key topics and corresponding speakers. To approach the main focus topic under a variety of perspectives, to obtain new insight and to create impact for other fields-speakers covering a broad variety of related fields in their talks were invited to the workshop:

- Quantum Control: Esa Räsänen, Matthias Wollenhaupt, Stefanie Gräfe
- Molecules: Eberhard Gross, Jamal Berakdar, Hans Jakob Wörner, Itzik Ben-Itzhak, Francoise Remacle
- Clusters, Nanoparticles, Solids: Thomas Fennel, Frank Stienkemeier, Thomas Möller, Matthias Kling, Thomas Brabec, Bernd Schütte
- Quantum Statistics: Andreas Buchleitner, Peter Lambropoulos, Hossein Sadeghpour
- Strong x-rays/FEL: Markus Drescher, Robin Santra, Georg Schmid, Agapi Emmanouilidou
- Rydberg systems, trapped atoms and ions: Georg Raithel, Alejandro Saenz, Robert Jones
- Few-body systems: Anthony Starace, Nirit Dudovich, Reinhard Dörner, Boris Bergues, Dieter Bauer, Ursula Keller, Enderalp Yakaboylu, Olga Smirnova, Cosmin Blaga, Ulf Saalmann, Christian Ott, Zenghu Chang, Chii-Dong Lin, Manfred Lein, Koudai Toyota, Jens Biegert, Lutz Fechner

General scientific outcome and perspectives. While being counterintuitive at first, strong fields typically create fast electrons by strong acceleration forces the observation and analysis of slow electrons allows to focus on and to understand the challenging physics beyond the strong-field approximation, where atomic potential and laser field govern the strong-field dynamics on equal footing.
Participants of the Workshop who study apparently different processes shared their most recent results. Throughout the presentations, several connections and interfaces opened up showing that similar experimental observations and theoretical concepts are present across areas. In particular, slow electrons occur in free and bound states (e.g. Rydberg atoms), can be created and controlled with laser frequencies ranging from the THz to the x-ray domain, emerge by quantum and classical processes in few-body as well as in complex systems.
This experience widened the scope for all participants, allowing them to think about their problems in a broader sense and approaching them with new tools and ideas. Cooperations among participants were fostered and forged. Very importantly, younger researchers were able to make contacts to experts, helped by stimulating discussions at their excellently prepared posters.

Many-body Dynamics out of Equilibrium, Workshop
Scientific coordinators: J.H. Bardarson, S. Parameswaran, F. Pollmann

The mpi**pks** workshop "Many Body Dynamics Out of Equilibrium" was held from March 11-14, 2015. The goal of the workshop was to bring together theorists and experimentalists working at the interface of two of the most complex issues in quantum science: non-equilibrium dynamics and strongly interacting many-body systems.
The talks were organized around the following main themes:

- The theory of many-body localization and related questions of ergodicity breaking
- Realizing many-body localization in experiments
- Floquet dynamics of periodically driven systems
- Basic issues of non-equilibrium dynamics and thermalization

The organizers attempted to have a wide representation of participants from different fields. These included many of the key workers in the theory of many-body localization systems (Prof. D. Abanin, Dr. B. Bauer, Dr. A Chandran, Prof. F. Huveneers, Dr. J.A. Kjäll, Prof. C.R. Laumann, Prof. A. Mirlin, Prof. V. Oganesyan, Prof. D. Pekker, Prof. A. Scardicchio, Dr. M. Serbyn, Prof. S. Sondhi, Dr. R. Vasseur) and driven systems (Dr. A.G. Grushin, Prof. A. Mitra and Prof. M. Rudner); in the theoretical and experimental study of such phases in cold atomic gases (Prof. I. Bloch, Prof. M. Lukin, Prof. D. Weld); experts in the field of thermalization and non-equilibrium dynamics (Prof. L.F. Cugliandolo, Dr. F. Heidrich-Meisner, Prof. F. Marquardt, Prof. S. Miyashita, Prof. M. Rigol, Prof. K. Sengupta); and on issues of adiabaticity and quantum optimization (Prof. A. Green, as well as Profs. Laumann and Scardicchio). The workshop was truly international, with participants representing several countries in Europe, the United States, Japan, and India. The main scientific program was preceded by tutorial sessions led by Profs. I. Bloch, A. Green, and S. Sondhi, and concluded with a day of discussions.

Younger Participants. As the central topics are relatively young, much of our participation was from PhD/Masters student, postdocs and junior faculty. Indeed, several nice talks were given by postdoctoral fellows and junior faculty: Dr. B. Bauer, Dr. A. Chandran, Prof. A. Das, Prof. D. Weld, Dr. A.G. Grushin, Dr. J. Kjäll, Prof. M. Rudner, and Dr. R. Vasseur. We also had an excellent selection of posters (both by junior and senior participants).
Summary. The workshop substantially achieved its stated goal of bringing together a diverse range of participants actively engaged in research on a wider variety of topics within the umbrella of non-equilibrium aspects of many-body systems. There were several fruitful interactions across the different subtopics represented at the workshop; hopefully these will stimulate further work and collaborative research in new directions. Participants particularly appreciated the abundant time for discussions that were an integral part of the program, and the tutorials that preceded the scientific program.

Activity meets Biology, Focus Workshop
Scientific coordinators: S. Grill, G. Salbreux, V. Zaburdaev

The international Workshop on occasion of Frank Jülicher's 50th birthday "Activity Meets Biology" became a highlight for the biophysical community of Dresden in spring of 2015.
In a two-day workshop with a very dense scientific program, 14 experts in the fields of biological and theoretical physics presented their most recent results. United by scientific interests, collaboration with Frank Jülicher, by previous research stays in Dresden and resulting historical connections, the speakers created an exceptional atmosphere of this event. Natural interaction of the speakers during the talks melted communication barriers and allowed all participants to get the maximum from asking questions, initiating discussions in question times, and continuing them during the coffee breaks.
We should especially mention an exceptionally high attendance of this workshop by young researchers of the Dresden bio-physical community. Students, postdocs, and group leaders from BIOTEC, MPI-CBG, B-CUBE became active participants of the workshop. For two days the lecture hall was completely full with sitting and standing listeners. Many students used the chance to discuss their work and ask for advice from the world-leading experts in their fields. For others it was an opportunity to update the status of ongoing collaborative projects. We believe that not a minute of these two days was lost and instead was fully used for fruitful scientific discussions.
It is truly difficult to select the most significant contributions of the workshop. However, we could follow how the excellence of already established experts, who were supervisors or senior colleagues of Frank Jülicher in the past, through the work of Frank himself, now shines in the new generation of young scientist. We should note the talks by two great representatives of the French school of soft-matter and biological physics, professors Jaques Prost and Jean-Francois Joanny on hydrodynamics of active fluids and physics of epithelial tissue. Anthony Hyman, currently a director of the MPI-CBG, presented a very recent work on phase separating fluids as a new way on looking on the cytoplasm of the cell. Prof. Erwin Frey gave an excellent talk overviewing the scaling laws in polymer theory. Finishing of the workshop was in hands of Ewa Paluch and Iva Tolić representing the younger generation, who now have their own groups in London and Zagreb.
We think that this short workshop clearly demonstrated how dynamic and active the field of quantitative bio-physics is. Now already several generations of scientist contributed to its growth and development but at the same time it is still very young so that representatives of all generations are still networked and are working together. The role of the **mpipks** is central in this development as it continues to cultivate the culture of close interaction between theory and experiment through its daily work, but also through the organization of the conferences like this one, where activity met biology again in March 2015.

Criticality in Biology: A Critical Assessment, Seminar and Workshop
Scientific coordinators: H. Chaté, M.A. Muñoz

This event consisted in a one-week workshop (7-10 April 2015) followed by a one-week Seminar (13-17 April 2015).
The end of the twentieth century saw a wave of interest in understanding why different natural phenomena exhibit "critical features" such as diverging spatio-temporal correlations, huge response to perturbations, highly complex structures and variability, etc. This apparent critical behavior emerges spontaneously, in a self-organized way, without any apparent need for parameter fine tuning. Even if a general theory of self-organized criticality is still missing, a lot of theoretical understanding and experimental progress were

achieved.
In the last few years, empirical evidence has accumulated that some biological systems also exhibit critical features. Examples range from gene expression patterns, to optimal cell growth, bacterial clustering, bird flocks, insect-colony foraging, and spontaneous brain activity. At variance with inanimate matter, criticality in living systems can be hypothesized to be the outcome of some adaptive or evolutionary process, which, for reasons to be understood, selects for it. A conjecture – borrowed from computer science – claims that information-processing biological systems can perform complex computations only if they operate at criticality, i.e. at the borderline between a disordered phase in which noise propagates unboundedly – thereby corrupting information processing and storage – and ordered phase in which perturbations readily fade away, hindering the ability to react and constraining computing capabilities. Critical dynamics provides a delicate compromise between these two conflicting tendencies, and has been claimed to entail functional advantages such as optimal transmission and storage of information, computational capabilities, and maximal sensitivity to stimuli. Despite its thrilling implications, the criticality hypothesis is still in its infancy and elicits some skepticism.
It was the goal of this workshop and seminar to provide a critical assessment of the "criticality hypothesis" in the presence of the main players involved. It is fair to say that this goal was reached. Important progress was made, especially in (i) discussing criteria for assessing the validity and significance of power law fits, (ii) debating different modeling approaches to brain complex dynamics, (iii) debating on the possible functional advantages of critical or quasi-critical dynamics, (iv) discussing the possible evolutionary origin of dynamics at criticality, (v) comparing aspects of criticality in neural dynamics, gene regulatory networks, and other biological systems. Intense, illuminating, and sometimes heated discussions took place both during the workshop and along the seminar week, as well as during the interesting poster session. One general important conclusion is that more data is needed to put order in the somewhat chaotic state of the theoretical debate.
The event was international, markedly interdisciplinary, with physicists, mathematicians, biologists, and neuroscientists, both theoreticians and experimentalists. Some of the most important participants were: Lucilla De Arcangelis, University of Naples (Italy), John Beggs, Indiana University (USA), Andrea Cavagna, Universita di Roma (Italy), Dante Chialvo, CONICET Buenos Aires (Argentina), Alain Destexhe, Laboratory for Computational Neuroscience, CNRS (France) Peter Grassberger, Forschungszentrum Jülich (Germany), Claudius Gros, University of Frankfurt, (Germany), Frank Jülicher, mpi**pks**, Dresden (Germany), Kunihiko Kaneko, University of Tokio (Japan), Marcelo Magnasco, Rockefeller University, New York (USA), Matteo Marsili, ICTO Trieste (Italy), Dietmar Plenz, NIMH, Bethesda (MD, USA), Ilya Shmulevich, Systems Biology, Seattle, (USA), Yuhai Tu, IBM Yorktown Heights, New York (USA). A few remarkable young participants emerged as well, notably I. Mastromatteo, PK Mohanty, V. Priesemann, J. Soriano, Qianyuan Tang. Summing up, the combined workshop and seminar achieved their goal of bringing together a wide range of leading scientists. The success of the conference would not have been what it was without the precious and nice help from the Visitors Program staff, especially that of Maria Pätzold to whom the scientific coordinators are enormously indebted.

Novel Light Sources from Laser-Plasma Interaction, Workshop
Scientific coordinators: M. Bussmann, M. Grech, E. Siminos

The last decade has witnessed an explosion of activity in the development of novel radiation sources based on laser-plasma interaction (LPI), fueled by the wide availability of high-power lasers, with many promising applications. The workshop Novel Light Sources from Laser-Plasma Interaction (NLIGHT15) brought together theorists and experimentalists working across a wide range of topics in this area.
The workshop aimed at triggering exchanges among experts on different subjects. To achieve this goal the workshop program was centered around seven main topics and an 1h30 overview talk (including 30 minutes of discussion) was given by a senior scientist for each topic. The first day of the workshop was devoted to X-ray and X-FEL sources from LPI and an overview talk was given by Prof. W. Leemans (Berkeley). The overview talk provided an introduction to Laser Wakefield Acceleration and its use to drive free electron lasers and Thomson-based γ-ray sources. The second day morning session was devoted to parametric amplification of short pulses. Prof. N. Fisch (Princeton) gave a tutorial talk that covered the topic of Raman amplification as a route towards extreme light intensities. In the afternoon session Prof. Luis Silva (Lisbon) covered the topic of γ-ray sources and QED processes with an emphasis on computational modeling of such processes. The third day of the workshop was devoted to pump-probe experiments and applications of LPI sources and took place at the Helmholtz Zentrum Dresden

Rossendorf (HZDR). Prof. H. Chapman (Hamburg) gave an introduction on the imaging of molecules with X-ray free-electron laser pulses, covering the latest advances on femtosecond crystallography. A tour of the facilities of HZDR followed the morning session. The next day of the workshop was devoted mainly to XUV & attosecond pulse sources from LPI. Dr. F. Quéré (Paris) gave a tutorial talk on plasma mirrors as sources of attosecond pulses through laser-driven high-harmonic generation, covering both theoretical and experimental aspects. On the last day of the workshop the topics of filamentation and THz generation were visited. Prof. S. L. Chin (Laval) gave an overview talk of filamentation science and its applications, exposing the many facets of filamentation in air and its use in light sources. In addition to these tutorial talks, the institute's colloquium was given by Prof. J. Meyer-ter-Vehn (Garching), covering in a pedagogical manner the multiple light generation mechanisms from relativistic laser-plasma interactions. Moreover, during the last day of the workshop a public evening lecture was delivered by Prof. J. Meyer-ter-Vehn, attracting around 150 participants of all ages.
In addition to the invited tutorial talks, a total of 29 contributed and invited talks of 25 minute duration (+5 min questions) were given by senior and junior scientists and PhD students. Particular attention was given to assigning talks to postdocs and PhD students in order to provide them an opportunity to introduce themselves to the community. Moreover, 27 poster presentations were given by young scientists. Two sessions (Monday and Tuesday) were allocated in order to maximize the available time for interaction among poster presenters and participants. The format of the workshop was met with great enthusiasm by the participants. The pedagogical and in-depth introductions of the main topics through tutorial talks triggered lively discussions. At the same time the contributed talks and poster presentations provided a wider coverage of the different topics. The workshop was attended by 69 participants with 21 different nationalities and participation was balanced between junior and senior researchers. Moreover, some of the participants came from different communities (e.g. atomic physics, laser physics) and greatly benefited from the tutorial talks, while they also provided valuable insights to the laser-plasma community. Based on the enthusiastic input from participants and the extended discussions during the workshop, we believe that our goal of facilitating interactions between scientists working on different areas of laser-plasmas interactions and even in different fields of physics was met with great success. We believe that the unique characteristic of mpi**pks** to host the workshop and accommodate the participants in-house contributed significantly to creating a friendly atmosphere that helped trigger interactions and forge a sense of community.
The scientific organizers would like to thank the Max Planck Society for making the workshop possible by providing financial support and the required facilities and HZDR for providing additional financial support. We are indebted to the visitors program of mpi**pks** for providing flawless organization.

Random Walks and Nonlinear Dynamics in the Life of Cells, Workshop
Scientific coordinators: S. Denisov, L. Manning, V. Zaburdaev

While the meetings on random walks, anomalous diffusion and their applications has become a tradition for the mpi**pks** and were always attracting world leading experts in the field, it was the intention of the organizers to make a step in a new direction. A biophysical community of Dresden is one of the characteristic examples of how rapidly the field of molecular and cell biology and theoretical physics approach each other. A growing amount of collaboration between scientists in those fields lead to a number of definitive breakthroughs. Stochastic processes and nonlinear phenomena are ubiquitous in biology, but only recently, due to significant advances in the experimental techniques, they were detected at the level of individual cells. Therefore it was the purpose of the workshop to emphasize the intersection of theory and newest of experiments with the hallmarks of random walks and non-linear dynamics and their role in the life of cells.
By putting together the program of this workshop we could achieve a good balance of theory and experiment but with a smooth transition through the speakers who are actively working in both. Interestingly even by selecting an apparently narrow theme of the conference, a very diverse set of topics could be covered. Major discussion lines of the conference were on the mechanisms of individual cell motility, bacterial colonies, mechano-chemistry of cell organization and patterning, and anomalous diffusion. As usual for a conference with so many outstanding speakers it is hard to highlight the most noticeable contributions. The talks by Tony Hyman (MPI-CBG, Dresden) and Stephan Grill (TU Dresden) showed most recent developments in our biophysical understanding of protein organization in the cytoplasm and mechano-chemical processes governing the early embryonic development. Paul Janmey (University of Pennsylvania, USA) and Gijsje Koenderink (AMOLF, Amsterdam) discussed a highly non-trivial dynam-

ics of cytoskeletal networks in the living cells. Berenike Maier (University of Köln) and Gerard Wong (UCLA, USA) reported their work on bacterial colonies - biofilms - a very extensively growing field of interdisciplinary research with a tight connection to applications in medicine and bio-engineering. It was our feeling that despite the variety of topics the participants were really communicating on the "same language" as the problems of non-linear dynamics and random walks were bridging their research. We are certain that many more great collaborations will develop from the interactions started on the workshop. In the proposal to the conference we put a special emphasis on younger participants. Out of 33 talks, 8 were delivered by young researchers who were at the stage of starting their own group or being a senior postdoc. It should be noted that we had many more good candidates for the short talk presentations than we had slots. Two poster sessions were very actively attended on both days and served the main platform for after-talks discussions (along with the excursion and conference dinner). A colloquium talk by Jane Kondev (co-author of the book on Physical Biology of the Cell) deserves a special mention. As anticipated it was a highly pedagogical account of basics and recent developments in our understanding of the physics of chromatin. It was given on a very accessible level and ended with a very intensive discussion involving the participants of the conference, members of the institute and listeners from local institutions in Dresden.
The event was truly international with 60 workshop participants from 23 countries, including UK, USA, India, Ukraine, Sweden, Israel, Poland, Italy, Russia, China and South Africa. By advertising the workshop in Dresden we were happy to see many attendees (students and group leaders) from the MPI-CBG, B-Cube, and BIOTEC. We also enjoyed the flawless, effective and supportive work of the Visitors Program of the **mpipks** (Mandy Lochar) and provided facilities. We hope that soon there will another opportunity to organize the next scientific event in Dresden.

Dynamics of Multi-Level Systems, Seminar and Workshop
Scientific coordinators: F. Atay, K. Lindgren, E. Olbrich

The workshop was attended by 67 participants and brought together scientists working in multiple disciplines as diverse as mathematics, physics, neuroscience, computer science, cognitive sciences, social sciences, and economics. The workshop was preceded by a two-week summer school that provided the theoretical background in the field of dynamical systems, information theory, and specific application areas including neuroscience and atmospheric physics. The school included sessions where the young participants could present their work in talks and posters. All feedback from the school participants indicate that the school was of very high quality and extremely useful for making a bridge to the workshop week.
The main goal of the workshop was to advance the understanding of multilevel systems by discussing recent developments of the mathematical and computational formalisms as well as their validation on real world applications. Major topics were mathematical concepts for the description of hierarchies (N. Ay, J. Johnson) and its applications (T. Vicsek, C. Huepe) which are closely related to concepts for level identification (J. Jost, M. Nilsson-Jacobi) and the use of information theoretic concepts (S. Amari, J. Jost, O. Pfante, M. Hilbert, D. Wolpert). A prominent topic both at the school and the workshop was the dynamics of slowfast systems (F. Verhulst, C. Kühn, T. Bellsky). S. Havlins talk provided the connection to the currently very active field of multilayer networks.
A second group of talks presented the current understanding of the dynamics of multilevel systems in specific applications areas such as the foundations of quantum mechanics (P. Blanchard), stochastic thermodynamics (H. Kantz), neuroscience (O. Faugeras, L. van Hemmen), economics (M. Gallegati), cognitive science (P. Gärdenfors, M. Warglien), and swarm behavior (K. Tunstrøm) which also provided challenges for the further development of the theoretical foundations and mathematical concepts.
One of the invited speakers, Tamas Vicsek, gave an Institute's Colloquium talk on the first day of the Workshop on the topic *Quantitative Approaches to Hierarchy*, thereby providing an early link from the workshop theme to several other areas of complex systems.
The main results of DYMULT15 can be summarized in two parts: First, several existing theoretical tools from different scientific fields were interpreted within the context of multilevel systems and it was discussed how they can be used in a synergetic way for addressing multilevel problems and applications. Second, recent developments and new approaches specifically conceived for multilevel systems were presented. The high level of participation, the congenial and enthusiastic atmosphere at the school and workshop, and prolonged discussions among the renowned experts as well as younger scientists indicate that the event has been successful in achieving its goals.

Quantum Correlated Matter and Chaos - A Workshop in Honor of the Life and Work of Richard Prange, Workshop
Scientific coordinators: S.M. Anlage, S. Fishman, G. Radons

This one-week workshop (21 - 26 June, 2015) addressed recent advances in a broad area of physics concerned with quantum correlated matter, Anderson localization with interactions, quantum chaos, random matrix theory, and econophysics. The Workshop explored areas of overlap in emerging problems in nonlinear dynamics, condensed matter and atomic physics. This combination was inspired by the work of Richard Prange (a Gutzwiller Fellow at the mpi**pks** in 2001), as exchanging ideas between these fields resulted in substantial progress in the past. The key topics discussed include quantum / wave chaos, correlated materials, topological states of matter, Majorana Fermions, Anderson localization, quantum phase transitions, random matrix theory, nonlinear dynamics, mesoscopic physics, and econophysics.
The workshop was markedly interdisciplinary. The subject concerns various physics communities, as well as those working in mathematics and quantitative finance. It was also an international meeting, with participants from all over the world, including China, Japan, India, the United States, Israel, Colombia, Brazil, and many European countries. There was also strong representation from the mpi**pks**, and the Technical Universities in Dresden, Illmenau and Chemnitz. The main scientific leaders of the field were present, and a special place was reserved for young participants, allowing them to present their research work. A very lively poster session, with 36 contributions, took place over the course of three evenings. The Monday colloquium was given by Carlo Beenakker (Univ. of Leiden, NL), who presented an overview of Majorana modes in condensed matter to the large community of Dresden physicists. On Monday evening, a special talk entitled "Richard Prange and his Physics" was delivered by Sankar Das Sarma (Univ. of Maryland, USA). Two panel discussions on hot topics in Quantum Correlated Matter and Chaos were organized on Tuesday and Thursday evenings. The first was on the topic of "Field Theory and Quantum Chaos", moderated by Italo Guarnari (Univ. of Insubria, IT) and the second on "Many-Body Localization", moderated by Sankar Das Sarma. Both panels included lively discussion, were well-attended by the participants, and were considered of great scientific value for ongoing research.
Overview talks on major topics covered in the workshop were given by I. Aleiner, A. Altland, B. Altshuler, G. Casati, S. Das Sarma, D. Delande, V. Galitski, F. Haake, R. Ketzmerick, U. Smilanski, V. Yakoveko.A number of remarkable younger researchers also gave oral contributions, including D. Abanin, E. Altman, R. Band, J. Bardarson, Y. Bar Lev, R. Chicireanu, O. Giraud, B. Gutkin, V. Josse, U. Kuhl, G. Lemarié, N. Lindner, T. Micklitz, M. Rechtsman, A. Sawicki, S. Sodin, K. Sun, and S. Wimberger.
The scientific coordinators received generous external support from ONR Global to cover the travel costs for more than half of the participants. The success of the conference would not have been what it was without the precious help from the institute's administration, especially that of Ms. Maria Pätzold, to whom the organizers are particularly indebted.

Charge Transfer meets Circuit Quantum Electrodynamics, Workshop
Scientific coordinators: M. Blencowe, B. Huard, B. Kubala

We are glad to report on this successful workshop that addressed the rapidly growing field of nonlinear mesoscopic devices strongly coupled to quantum resonators. The workshop gathered for the first time most of the main players in this emerging field of research, as well as interested newcomers. Almost all invited speakers accepted to come right away, even the busiest ones, showing how timely the event seemed to be. At the forefront of research in this new direction, we had talks from the main actors of four types of mesoscopic devices that one can now couple to well-controlled electromagnetic modes: tunnel junctions (Ankerhold, Clerk, Hofheinz, Nazarov, Portier, Rimberg, etc.), single charges or spin (Flindt, Kontos, Petta, Samuelsson, Wallraff, etc.), Andreev states (Bouchiat, Goffman, etc.) and mechanical oscillators (Sillanpää, Steele, etc.). We also had talks from leading researchers in related fields, such as Astafiev, Delsing, Devoret, Hakonen, Leek, etc.
The newcomers were either senior researchers who work on related fields and were interested to learn about this new topic, or junior researchers who appear to have benefited a lot from attending the workshop. There were many questions during the talks and the participants benefited from the social events to foster new collaborations. Besides, the participants appreciated the environment of MPIKS, and in particular the wonderful organization by Ms. Katrin Lantsch very much.
The workshop has decisively bolstered this interesting and emerging field. We hope that the newcomers

will benefit from what they have learned and will start new projects in this direction. It is now evident that well-controlled microwave modes in the quantum regime offer a new tool to explore mescoscopic physics in a variety of regimes and systems.

3.4 Collaboration with Experimental Groups

- *Building an artificial, transcriptionally active nucleus to study the coupling between mechanics and gene expression* with J. Guck, BIOTEC (Dresden, Germany)
- *Eye development* with M. Ader, CRTD (Dresden, Germany)
- *Comparative genomics* with M. Brand, CRTD (Dresden, Germany)
- *Non-coding RNAs* with F. Calegari, CRTD (Dresden, Germany)
- *Cis-regulation* with E. Tanaka, CRTD (Dresden, Germany)
- *Ultrasound studies on frustrated magnets* with S. Zherlitsyn and J. Wosnitza, Helmholtz Center Dresden-Rossendorf (Dresden, Germany)
- *Correlated materials* with B. Buechner, S. Wuhrmehl, IFW (Dresden, Germany)
- *Quantum transport in topological insulator nanowires* with R. Giraud and J. Dufouleur, IFW (Dresden, Germany)
- *Physical properties of cytoplasm* with S. Alberti, MPI-CBG (Dresden, Germany)
- *Mechanics of Drosophila wing disc development* with S. Eaton, MPI-CBG (Dresden, Germany)
- *Mechanisms of spindle orientation during zebrafish development* with J. Huisken, MPI-CBG (Dresden, Germany)
- *Genomic analysis* with W. Huttner, MPI-CBG (Dresden, Germany)
- *Phase separation in living cells* with A. Hyman, MPI-CBG (Dresden, Germany)
- *Mechanics of interkinetic nuclear migration in the zebrafish embryonic retina* with C. Norden, MPI-CBG (Dresden, Germany)
- *Spindle scaling during early embryogenesis* with C. Norden, MPI-CBG (Dresden, Germany)
- *Planarian transcriptomics and genomics* with J. Rink, MPI-CBG (Dresden, Germany)
- *Chromosome alignment in meiosis of fission yeast* with I. Tolić, MPI-CBG (Dresden, Germany)/Ruđer Bošković Institute (Zagreb, Croatia)
- *Drosophila gene expression* with P. Tomancak, MPI-CBG (Dresden, Germany)
- *Maternal to zygotic transition in zebrafish embryos* with N. Vastenhouw, MPI-CBG (Dresden, Germany)
- *Weyl semimetals* with C. Felser and B. Yan, MPI-CPfS (Dresden, Germany)
- *Arsenic bond fluctuations in zirconium arsenide selenides* with R. Kniep, F. Steglich, MPI-CPfS (Dresden, Germany); T. Cichorek, Institute of Low Temperature and Structure Research, Polish Academy of Sciences (Wroclaw, Poland); R. Niewa, Institute of Inorganic Chemistry, University of Stuttgart (Germany)
- *Unconventional quantum criticality* with F. Steglich, MPI-CPfS (Dresden, Germany)
- *Scanning tunneling spectroscopy on heavy fermion compounds* with S. Wirth, MPI-CPfS (Dresden, Germany)
- *Mammalian phenotypes* with H. Stuckas, Senckenberg Naturhistorische Sammlungen (Dresden, Germany)
- *Ultraconserved elements* with F. Buchholz, TU Dresden (Germany)
- *Tissue modelling of cell competition* with C. Dahmann, TU Dresden (Germany)
- *Molecular motors* with S. Diez, TU Dresden (Germany)
- *Actin alignment in the actin cortex* with S. Grill, TU Dresden (Germany)
- *Novel superconductors* with H.- H. Klauss, TU Dresden (Germany)
- *Ionization with XUV Pulses* with M. Richter, Helmholtz Center (Berlin, Germany)
- *Superradiance in large Xenon Cluster at FLASH* with T. Möller, TU Berlin (Germany)
- *PTCDA monolayers on dielectric surfaces, superradiance* with M. Sokolowski, University of Bonn (Germany)
- *Spectroscopy of molecules in helium nano-droplets and on neon clusters* with F. Stienkemeier, University of Freiburg (Germany)

- *Molecular alignment* with J. Küpper, Center for Free-Electron Laser Science, University of Hamburg (Germany)
- *XFEL experiments at the FLASH free-electron laser* with D. Rolles, DESY (Hamburg, Germany)
- *Stimulated RIXS in the gas phase* with M. Meyer, European XFEL (Hamburg, Germany)
- *Engineering spin-waves in a high-spin ultracold Fermi gas* with C. Becker and K. Sengstock, University of Hamburg (Germany)
- *Giant spin oscillations in an ultracold Fermi sea* with C. Becker and K. Sengstock, University of Hamburg (Germany)
- *Relaxation dynamics of an isolated large-spin Fermi Gas far from equilibrium* with C. Becker and K. Sengstock, University of Hamburg (Germany)
- *Spin-waves of large-spin Fermi gas* with C. Becker and K. Sengstock, University of Hamburg (Germany)
- *Engineering artificial gauge fields in triangular optical lattice* with J. Simonet and K. Sengstock, University of Hamburg (Germany)
- *Engineering Ising-XY spin models in a triangular lattice via tunable artificial gauge fields* with J. Simonet and K. Sengstock, University of Hamburg (Germany)
- *Multiphoton excitations of quantum gases in driven optical lattices* with J. Simonet and K. Sengstock, University of Hamburg (Germany)
- *High-resolution spectroscopy of stimulated EUV emission of krypton and Xenon at the FLASH FEL* with J. C. Lopez-Urrutia, MPI for Nuclear Physics (Heidelberg, Germany)
- *Observation of Poincarè-Birkhoff scenario in cold atom gases* with M. Oberthaler, University of Heidelberg (Germany)
- *Monitoring of transport of Rydberg excitation using electromagnetically induced transparency* with S. Whitlock, University of Heidelberg (Germany)
- *Comparative genomics* with M. Platzer, Leibniz Institute for Age Research (Jena, Germany)
- *Electron wakefield acceleration* with M. Kaluza, University of Jena (Germany)
- *Spatio-temporal pulse shaping* with S. Nolte, University of Jena (Germany)
- *Time-resolved EUV spectroscopy at the FLASH free-electron laser* with A. Ehresmann, University of Kassel (Germany)
- *Resonant-assisted tunneling in microwave cavities* with U. Kuhl, Nice University (France) and H. J. Stöckmann, Marburg University (Germany)
- *Cyst formation in the Drosophila wing disc* with A. Classen, LMU München (Germany)
- *Actin cortex formation in vesicle* with A. Bausch, TU München (Germany)
- *Cell oscillations in dorsal closure* with J. Solon, Center for Genomic Regulation (Barcelona, Spain)
- *X-ray imaging of living cells* with T. Pfohl, University of Basel (Switzerland)
- *Ion pumps* with F. Tadini-Buoninsegni, University of Florence (Italy)
- *Electron wakefield acceleration* with S. Mangles, Imperial College (London, UK)
- *Physics of cell migration* with E. Paluch, UCL (London, UK)
- *Experiments and data analysis of nonequilibrium fluctuations of a nano-device* with S. Ciliberto, ENS (Lyon, France)
- *High-resolution spectroscopy in stimulated RIXS* with J.-E. Rubensson and J. Nordgren, Uppsala University (Sweden)
- *Mechanics of zebrafish epiboly* with C. P. Heisenberg, Institute of Science and Technology (Vienna, Austria)
- *Thermoelectric transport* with S. Buehler-Paschen, TU Wien (Austria)
- *Spectroscopy of organic dye aggregates* with J. Hauer, TU Wien (Austria)
- *HHG spectroscopy of coherent electronic wave packets in NO* with H. J. Wörner, ETH (Zürich, Switzerland)
- *Transport through strongly correlated quantum devices* with G. Scott, Quantum Systems Research (Alcatel-Lucent, USA)
- *Imaging of large xenon clusters in conjunction with superradiance experiments at FLASH* with C. Bostedt, Argonne National Laboratory (USA)
- *Inner-shell atomic x-ray lasers* with J. J. Rocca, Colorado State University (Fort Collins, USA)
- *X-ray lasers and x-ray spectroscopy* with R. A. London and G. Brown, Lawrence Livermore National Laboratory (USA)
- *Stimulated x-ray emission of transition-metal complexes* with U. Bergman, LCLS, SLAC National Accelerator Laboratory (USA)

- *Electron removal from fullerenes and fullerene negative ions* with N. Berrah, Storrs Center (Mansfield, USA)
- *Distinct magnetic phase transition at the surface of an antiferromagnet* with the experimental groups of S. Langridge, ISIS Facility, STFC Rutherford Appleton Laboratory and D. Gibbs, Brookhaven National Laboratory (New York, USA)
- *Non-equilibrium behaviour in spin ice* with S. Grigera, UNLP-Conicet (La Plata, Argentina)
- *Spin liquids* with S. Nagler, A. Tennant, Oak Ridge National Laboratory (USA)
- *Functional protein tests* with C. H. Kang, Washington State University (USA)
- *Dynamics of N. gonorrhoeae bacterial colonies* with N. Biais, Brooklyn College, City University of New York (USA)
- *Spatial dynamics of coupled myosin motors* with A.-M. Lauzon, McGill University Health Centre (Montreal, Canada)

3.5 Externally Funded Research and Relations to Industry

3.5.1 DFG Projects

- Gottfried Wilhelm Leibniz-Preis 2013, Prof. R. Moessner
- Collaborative Research Center *Correlated magnetism: from frustration to topology*, Prof. R. Moessner, Dr. F. Pollmann
- Research Training Group *Itinerant magnetism and superconductivity in intermetallic compounds*, Prof. R. Moessner

Individual Projects

- *Kontrolle der epithelialen Zellschichtausbreitung im Zebrafish*, Dr. S. Grill, Dr. G. Salbreux
- *Microswimmers - from single particle motion to collective behavior*, Dr. B. Friedrich

3.5.2 EU Funding

- ERC Starting Grant *Emergent active mechanical behavior of the actomyosin cell cortex*, Dr. S. Grill
- EU-FP7 *Hybrid architecture for quantum information using Rydberg ensembles and superconductors*, Prof. J.-M. Rost, Dr. T. Pohl
- EU-FP7 *Quantum integral light matter interface*, Prof. J.-M. Rost, Dr. T. Pohl
- EU-FP7 *Systems biology of mitosis*, Prof. F. Jülicher
- EU-FP7 *Topological effects in matter with strong spin-orbit coupling*, Prof. R. Moessner
- EU Marie Curie actions - networks for initial training *Cooperativity in highly excited Rydberg ensembles - control and entanglement*, Prof. J.-M. Rost, Dr. T. Pohl
- EU Marie Curie actions - networks for initial training *Correlated multielectron dynamics in intense light fields*, Prof. J.-M. Rost
- EU Horizon 2020 *Chemistry with ultrashort pulses and free-electron lasers: looking for control strategies through exact computations*, Prof. U. Saalmann
- EU Horizon 2020 *Rydberg quantum simulators*, Prof. J.-M. Rost, Dr. T. Pohl

3.5.3 Additional External Funding

- BMBF Grant *Collective organization of cells and tissues: systems biology of tissue size and shape*, Prof. F. Jülicher
- European Project Center *Chemical information technology*, Prof. F. Jülicher
- European Research Network *European network in systems biology*, Prof. F. Jülicher
- Helmholtz Association *Helmholtz virtual institute new states of matter and their excitations*, Prof. R. Moessner
- The Royal Society *Newton fellow: singularimetry in light-matter interaction*, Dr. J. Goette

- Volkswagen Foundation *Propagation of extreme events in spatially extended excitable systems*, Prof. H. Kantz
- Volkswagen Foundation *Recurrent extreme events in spatially extended excitable systems: mechanism of their generation and termination*, Prof. H. Kantz
- Volkswagen Foundation *Towards molecular engines: cooperative coupling of molecular motors in engineered environments*, Prof. F. Jülicher
- HFSP *Human frontiers science program career development award*, Dr. J. Brugues
- John Templeton Foundation *Quantum Hardness*, Prof. R. Moessner

3.5.4 Scholarships

- Benoit, Vincenti; Univ. Lyon Internship
- Beiran, Manuel; DAAD Internship
- Chung, Ming-Chiang; National Chung Hsing University
- Deluca Silberberg, Anna; Institute for Catalan Studies, St. Jordi Award
- Dikande, Alain Moise; AvH Research Fellowship
- Morr, Dirk; AvH Research Fellowship
- Kaiser, Vojtech; ESN Lyon/TU Dresden
- Kajtoch, Dariusz; Erasmus Programm
- Langari, Abdollah; AvH Research Fellowship
- Leitao, Jorge; Erasmus Programm
- Moudgalya, Sanjay; DAAD WISE Scholarship
- Petrova, Olga; AvH Research Fellowship
- Politi, Paolo; AvH Research Fellowship
- Ramaswamy, Rajesh; AvH Research Fellowship
- Rodriguez, Javier; Ministry of Economy and Competitiveness of Spain, Predoctoral Research Grant
- Rodrigues Pereira, Afranio; DAAD
- Sondhi, Shivaji; AvH Research Award
- Trallero-Giener, Carlos; AvH Research Fellowship
- van der Wuff, Erik; ESF Short Visit Grant

3.5.5 Cooperations with Industry

- *Participation in BASF advanced research initiative at Harvard*, Dr. Vasily Zaburdaev

3.5.6 External Cofunding of Workshops and Seminars

2013

- Focus workshop *Flat bands: design, topology, and correlations*
  (6% of budget)
- School and workshop *Ultracold Rydberg physics*
  (90% of budget)
- Workshop *Advances in quantum chaotic scattering: from (non-)linear waves to few-body systems*
  (27% of budget)

2014

- Focus workshop *Topological matter out of equilibrium*
  (9% of budget)
- Workshop *DNA-based nanotechnology: digital chemistry*
  (16% of budget)
- Focus workshop *Physical origins of correlated extreme events*
  (57% of budget)

- Seminar and workshop *Topology and entanglement in correlated quantum systems*
  (6% of budget)
- Workshop *Arbeitstreffen Rydbergphysik*
  (71% of budget)
- Focus workshop *New states of matter and their excitations*
  (67% of budget)

2015

- Focus workshop *Many-body dynamics out of equilibrium*
  (23% of budget)
- School and seminar *Dynamics of multi-level systems*
  (38% of budget)
- Focus workshop *Quantum hardness*
  (100% of budget)
- Workshop *Quantum correlated matter and chaos: a workshop in honor of the life and work of Richard Prange*
  (34% of budget)

3.6 Teaching and Education

3.6.1 Lectures at Universities

Wintersemester 12/13

- *Nonlinear dynamics*, Prof. H. Kantz, TU Dresden
- *Studium integrale: Zeit aus Raum*, Prof. J. M. Rost, TU Dresden
- *Ultracold atoms in optical lattices*, Dr. A. Eckardt, TU Dresden

Sommersemester 2013

- *Biophysik III: theoretical biophysics* Prof. F. Jülicher, Dr. S. Grill, TU Dresden
- *Introduction to statistical inference* Dr. V. Zaburdaev, TU Dresden
- *Non-linear optical spectroscopy* Dr. A. Eisfeld, TU Dresden
- *Topology and new kinds of order in condensed matter physics* Dr. S. Kirchner, TU Dresden

Wintersemester 2013/2014

- *Biological hydrodynamics* Prof. S. Grill, Dr. G. Salbreux, TU Dresden
- *Complex networks* Prof. H. Kantz, Dr. E. Altmann, TU Dresden
- *Discrete algorithms for computational biology* Dr. M. Hiller, TU Dresden
- *Structure of matter* Prof. S. Skupin, FU Jena

Sommersemester 2014

- *Biophysik III: Theoretical biophysics* Prof. F. Jülicher, Prof. S. Grill, TU Dresden
- *Computational many-body physics* Dr. F. Pollmann, Dr. J. Bardarson, TU Dresden
- *Studium Integrale: ist Komplexität ein physikalisches Problem?* Prof. J. M. Rost, TU Dresden
- *The primary steps of photosynthesis* Dr. A. Eisfeld, TU Dresden

Wintersemester 2014/2015

- *Biological hydrodynamics* Prof. S. Grill, Dr. G. Salbreux, TU Dresden
- *Discrete algorithms for computational biology* Dr. M. Hiller, TU Dresden
- *Kinematics of noisy motion* Dr. B. Friedrich, TU Dresden
- *Levy stable distributions in atomic/molecular gases* Dr. A. Eisfeld, TU Dresden

- *Many-body dynamics in ultracold quantum gases* Dr. A. Eckardt, Dr. M. Haque, TU Dresden
- *Networks, function and genomics* Dr. M. Hiller, TU Dresden
- *Stochastische Prozesse* Prof. H. Kantz, TU Dresden
- *Synchronization: embryonic development to electronic networks* Dr. L. Wetzel, Dr. D. J. Jörg, TU Dresden
- *Theory of open quantum systems* Dr. A. Eisfeld, TU Dresden
- *Theoretische Physik B für Studierende des Lehramtes* Dr. N. Rohringer, Uni Hamburg
- *Übungen zur theoretischen Physik B für Studierende des Lehramtes* Dr. N. Rohringer, Uni Hamburg

Sommersemester 2015

- *Biological hydrodynamics* Dr. J. Brugues, TU Dresden
- *Biophysik III: Theoretical biophysics* Prof. F. Jülicher, Prof. S. Grill, TU Dresden
- *Continuum mechanics for biological physics* Dr. B. Friedrich, Biotec
- *Einführung in die Theorie nichtlinearer optischer Prozesse* Dr. N. Rohringer, Uni Hamburg
- *Fourier transform spectroscopy* Dr. A. Eisfeld, TU Dresden
- *Timely topics of atomic and molecular physics with femtosecond x-ray free-electron laser sources* Dr. N. Rohringer, Uni Hamburg

3.6.2 Professional skills training

Block seminars

- January 2013, one-day seminar on *Scientific writing*
  Dr. C. Schütte, ProSciencia
  Topics: Structuring of data; story drafting; scientific writing.
- October 2013, two-day seminar on *Scientific publishing*
  Dr. T. Pattard, senior assistant editor at Physical Review A
  Topics: Scientific writing; editorial processes and communication with editors; refereeing.
- December 2014, two-day seminar on *Presentation skills*
  K. K. Meyer-Ross, HTW Dresden
  Topics: Preparation of slides; visual aids and technical equipment; dealing with interruptions; time management; strategies against stage fright.

Talk series on professional skills topics (since December 2014)

- *A few thoughts on the art giving a talk*
  Dr. J. Bardarson, group leader at mpi**pks**
- *A few things to keep in mind when applying for a postdoc position*
  Dr. L. Do, head of the visitors program, mpi**pks**
- *High performance computing in the real world*
  Dr. N. Henkel, mpi**pks** alumnus, now at GNS Systems GmbH
- *Scientific writing*
  Prof. C. Timm, IMPRS faculty member
- *Customized software for life insurance*
  Dr. A. Pernice, mpi**pks** alumnus, now at msg life AG
- *Industry: a transition from unconventional superconductivity into conventional magnetism*
  Dr. H. Vieyra, mpi**pks** alumnus, now at VACUUMSCHMELZE GmbH & Co. KG
- *Founding, Start-Ups and Industry - a theoretical physicists point of view*
  Prof. M. Abel, founder and CEO of Ambrosys GmbH

3.6.3 Degrees

Habilitation

- Grill, S.: *Morphogenetische Funktionen des Aktomyosin-Zytoskeletts.* Dresden, 2013

Dissertations

- Aliee, M.: *Dynamics and mechanics of compartment boundaries in developing tissues.* Dresden, 2013
- Bannasch, G.: *Relaxationsprozesse in stark gekoppelten ultrakalten Plasmen.* Dresden, 2013
- Böhme, G. A.: *Emergence and persistence of diversity in complex networks.* Dresden, 2013
- Demirel, G.: *Moment-Closure approximations for contact processes in adaptive networks.* Dresden, 2013
- Gharakhani, J.: *Cell cytoplasm compartmentalization.* Dresden, 2013
- Henkel, N.: *Rydberg-dressed Bose-Einstein condensates.* Dresden, 2013
- Laptyeva, T. V.: *Nonlinear waves in random lattices.* Dresden, 2013
- Maucher, F.: *Nonlinear waves in nonlocal media.* Dresden, 2013
- Rajasekaran, B.: *Analysis of movement of cellular oscillators in the pre-somitic mesoderm of the zebrafish embryo.* Dresden, 2013
- Siegert, S.: *Rank statistics of forecast ensembles.* Dresden, 2013
- Wulffen, A. K. von: *A bridge between short-range and seasonal forecasts.* Dresden, 2013
- Zwicker, D.: *Physical description of centrosomes as active droplets.* Dresden, 2013

- Aufderheide, H.: *Implications of eigenvector localization for the dynamics of complex networks.* Dresden, 2014
- Di Cintio, P. F.: *Dynamics of heterogeneous clusters under intense laser fields.* Dresden, 2014
- Fruth, F.: *Spontaneous otoacoustic emissions in an active nonlinear time domain model of the cochlea.* Dresden, 2014
- Jörg, D.: *Genetic oscillations and vertebrate embryonic development.* Dresden, 2014
- Kaiser, V.: *The Wien Effect in electric and magnetic coulomb systems : from electrolytes to spin ice.* Dresden and Lyon, 2014
- Knolle, J.: *Dynamics of a quantum spin liquid.* Dresden, 2014
- Merkel, M.: *From cells to tissues: remodeling and polarity reorientation in epithelial tissues.* Dresden, 2014
- Mukherjee, R.: *Strong interactions in alkaline-earth Rydberg ensembles.* Dresden, 2014

- Möbius, S.: *Intertwining exciton dynamics and nuclear motion in Rydberg aggregates.* Dresden, 2015
- Ritschel, G.: *Energietransfer und Absorption molekularer Aggregate bei endlicher Temperatur.* Dresden, 2015
- Sartori, P.: *Effect of curvature and normal forces on motor regulation of cilia.* Dresden, 2015

Master

- Belohlavy, S.: *Competition between nucleosomes and transcriptional machinery determines the timing of genome activation in the zebrafish embryo.* Dresden, 2015

Diploma

- Ehrlich, C.: *Sequence dependent modelling of backtracking dynamics during DNA transcription.* Dresden, 2013
- Hubatsch, L.: *Fast kinetics of DNA repair.* Dresden, 2013

3.6.4 Appointments and Awards

Appointments

- Prof. N. Goehring accepted the offer for a professorship at the *London Research Institute*.
- Prof. S. Grill accepted the offer for a professorship at the *Technical University Dresden*.
- Prof. A. Jannasch accepted the offer for a assistant professorship at the *University of Tübingen*.

- Prof. S. Kirchner accepted the offer for a professorship at the *Zhejiang University in Hangzhou*.
- Dr. G. Salbreux accepted the offer for a group leader position at the *Francis Crick Institute in London*.
- Prof. S. Skupin accepted the offer for a research position at the *CNRS Centre Lasers Intenses et Applications in Bordeaux*.

Awards

- Grill, S.: *Binder-Innovationspreis 2013*
- Hiller, M.: *German Life Science Award 2013*
- Jülicher, F.: *Ordentliches Mitglied der Akademie der Wissenschaften und der Literatur, since 2013*
- Lange, S.: *Ehrenfried-Walter-von-Tschirnhaus-Urkunde (TU Dresden) 2013*
- Moessner, R.: *Gottfried Wilhelm Leibniz-Preis (DFG) 2013*
- Vorberg, D.: *Lohrmann-Medaille (TU Dresden) 2013*

- Berndt, F.: *Ehrenfried-Walter-von-Tschirnhaus-Urkunde (TU Dresden) 2014*
- Brugues, J.: *Career Development Award (Human Frontiers Science Program) 2014*
- Fulde, P.: *Ehrenbürger der Provinz Gyeong buk in Korea 2014*
- Karschau, J.: *Springer Thesis Award 2014*
- Mertig, N.: *Georg-Helm-Prize (TU Dresden) 2014*
- Midtvedt, D.: *Best PhD thesis award (Chalmers University) 2014*

- Bardarson, J.: *APS Outstanding Referee 2015*
- Berndt, F.: *Professor-Schwabe-Prize (TU Dresden) 2015*
- Eckardt, A.: *TUD Young Investigator (TU Dresden) 2015*
- Garzon-Coral, C.: *Springboard to postdoc fellowship award 2015*
- Knolle, J.: *Dissertationspreis der Sektion kondensierte Materie der DPG 2015*
- Pollmann, F.: *Walter-Schottky Preis 2015*

3.7 Public Relations

3.7.1 Long Night of the Sciences

Over the last three years, the institute has participated in the annual *Long Night of the Sciences*. Jointly with the Technische Universität Dresden and many other research institutes in Dresden, we opened our doors for the general public from 6pm to midnight. The members of our institute conveyed the importance and fascination of their research to a broad audience with various talks, shows, a science cinema, posters and a lot of different presentations of their work. The resonance was very good, with about 3000 visitors counted at each event.

Impressions of the Long Night of the Sciences and Science in the City Hall

3.7.2 Science in the City Hall

The **mpipks**, the Technische Universität Dresden and the City of Dresden run a series of public lectures by leading scientists who explain their field of research to a lay audience. Since 2011, when the City Hall, the original venue, was closed for renovation, the three annual lectures have taken place in the "Kleines Haus" of Dresden's State Theater.

2013

- *Darf es in der fortgeschrittenen Moderne überhaupt noch Katastrophen geben?*
  Prof. W.-R. Dombrowsky, Steinbeis University Berlin (about 200 participants)
- *BEE-onik, was die Technik von Bienen lernen kann*
  Prof. J. Tautz, Julius Maximilian University of Würzburg (about 320 participants)
- *Ist Leben konstruierbar? Auf dem Weg zur künstlichen Zelle*
  Prof. P. Schwille, Max Planck Institute of Biochemistry (about 300 participants)

2014

- *Mathematik zum Anfassen*
  Prof. A. Beutelspacher, Justus Liebig University Giessen (about 350 participants)
- *Geschüttelt, nicht gerührt! James Bond im Visier der Physik*
  Prof. M. Tolan, TU Dortmund University (about 370 participants)
- *Heisse Quellen in der Tiefsee: Oasen des Lebens*
  Prof. N. Dubilier, Max Planck Institute for Marine Microbiology (about 250 participants)

2015

- *Die Evolution des Denkens*
  Prof. O. Güntürkun, Ruhr-University Bochum (about 250 participants)

3.7.3 mpipks School Contact Program

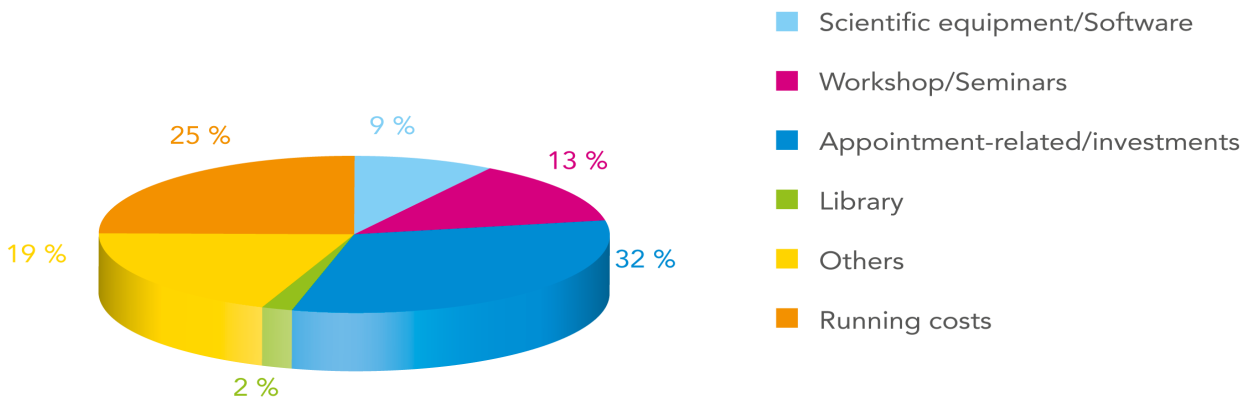
Public lecture for Junior Doctors

The **mpipks** offers high school classes the opportunity to catch a glimpse of the day-to-day life of a scientist. Every year, about fifteen classes visit us to attend a lecture by a junior member of the institute, who presents his field of research and answers questions about studying the sciences, pursuing a PhD, etc. A list of available lecture topics is published on our webpages and sent to high school teachers upon request.

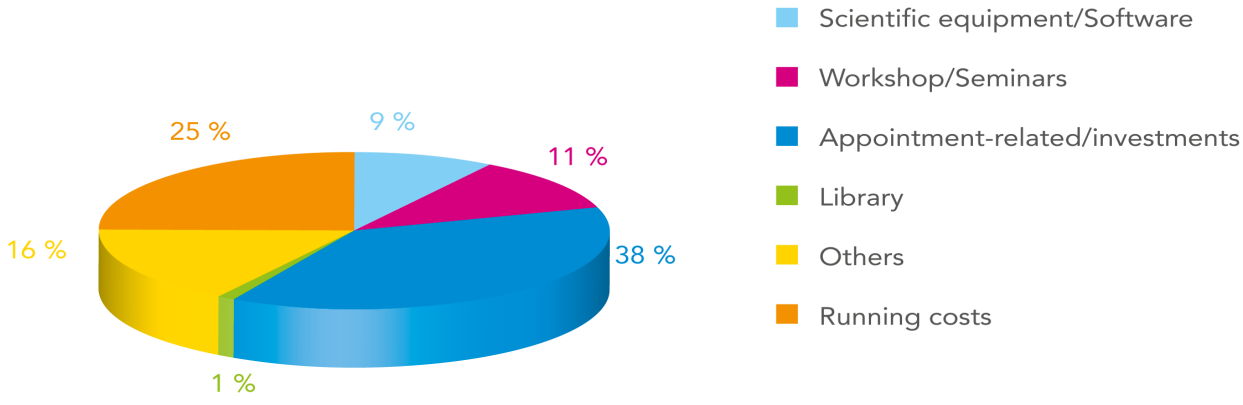
In addition, the institute participates in the program *Junior Doctor* organized by the network *Dresden - Stadt der Wissenschaft*. The participating research institutes offer a variety of lectures for children, who are awarded a "Junior Doctor degree" when attending a stated number of talks. Each school year, the **mpipks** contributes to the curriculum with six lectures for students from the 3rd grade onwards.

3.8 Budget of the Institute

Research Budget 2013

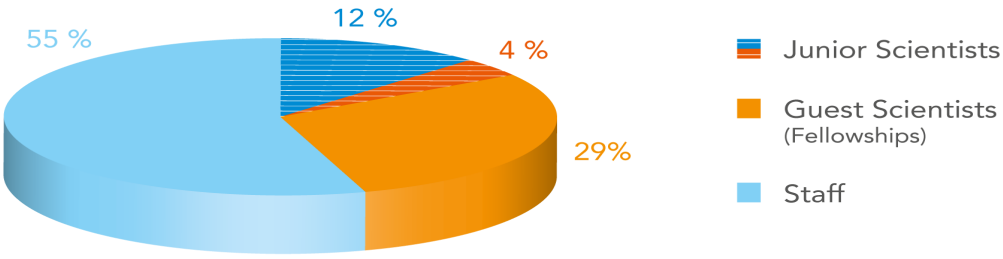


Research Budget 2014

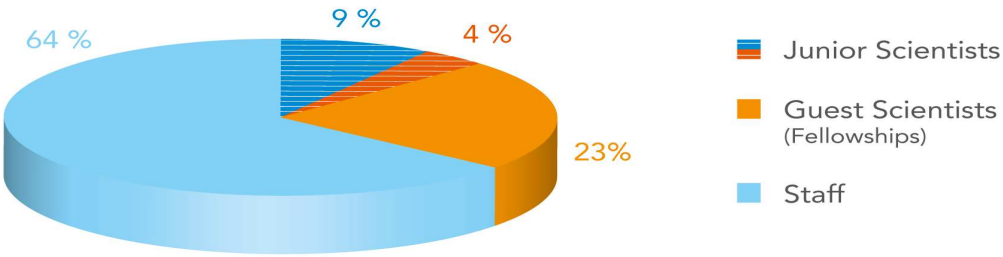


Research budget during the past two years

Personnel Budget 2013



Personnel Budget 2014



Budget for personnel

3.9 Equipment and Premises

3.9.1 Computing Facilities

The wide variety of methods employed by our scientists for doing their research work implies a relatively broad spectrum of hard- and software which is maintained by our computer department. Thus, compute nodes of very different size are available on site for numerical calculations. Presently, our computing facilities are homogeneous in the sense that both the hardware architecture (x86) and the operating system (Linux) are the same throughout our cluster.

The close past has seen a slight increase in the requirements for graphics, partly due to activities in our Biological Physics division but also driven by the fact that visualization of results has become more important.

About one third of our offices are equipped with Thin Clients while the majority of our scientists use workstations. Presently the institute hosts approximately 550 servers with a total of approximately 12000 CPU cores on site and, since 2010, a compute cluster located in Garching with additional 1500 CPU cores which is best suited for applications that are highly parallelized.

Our computers have up to 64 CPU cores and a maximum of 3 Terabytes of main memory and a maximum of 50 Terabytes of local disk space. A few nodes with powerful GPUs are available for our scientists. We run 10 Gigabit and Gigabit Ethernet as a local area network interconnect. 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 PCs in our institute, running a Windows operating system, mainly for office applications. We also offer about 100 laptops for our scientists in order to provide them the possibility to continue their work while travelling. Furthermore, we run a Windows Terminalserver in our network to offer access to a Windows environment from every desktop. Cloud services, VPN access, Wifi and other services are also available for our scientists. For numerical and analytical calculations there are various software packages available. During the last few years we have noticed a tendency towards integrated software environments while fewer people are writing their own programs using programming languages like C++ or Fortran 90. In many cases a lot of the ongoing software development is done and driven by free software, e.g. in the Biological Physics department, though proprietary software also plays an important role at our institute.

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 Thin Clients 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 300 MBit/s. Redundancy is achieved by automatic failover to a second line to our neighboring institute (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, Mac OS and cloud services, hardware and web, network and Windows, general user support. In addition to those five people we employ four trainees and one student of the Berufsakademie Dresden. Small to medium sized programming tasks are done by our staff and trainees. The development of large software applications, like a new database system for our visitors program or a refresh of our webpages, usually has 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 AIX might only come into play if particularly fast hardware becomes available that is not supported by Linux. So far the highly specialized GPUs are not well accepted by our scientists since the effort for adapting programs to this architecture is relatively high while the overall speedup in most cases is only moderate. There are tendencies that both restrictions may fall, meaning that GPUs might play a bigger role in the future. Our cluster in Garching, presently being shared with the Fritz Haber Institute (Berlin) will be replaced in autumn 2015. This new

cluster will be shared between the Fritz Haber Institute, the MPI for the Structure and Dynamics of Matter (Hamburg) and our institute.

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. By the end of 2013, the era of Intel's IA64 based systems ended at our institute and we were back to a homogeneous infrastructure, this time based on Linux, running on x86 systems. 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	nodes	main memory (TB)	disk space (TB)
1996	33	0.01	0.5
1998	66	0.06	2.0
2000	95	0.3	8
2002	162	0.6	22
2004	327	2.6	90
2006	345	5.5	190
2008	360	15	510
2010	400	22	560
2012	370	75	770
2014	560	116	1500

3.9.2 Library

The library of the mpi**pks** is a service unit with a wide range of duties. Most evidently, it provides a large stock of scientific books and journals for the use of all members of the mpi**pks** including workshops participants. The library rooms are accessible 24 hours per day and provide scientists with printed media and scientific information in many forms. The automatic check out system permits institute employees to borrow books at any time. A modern Book2net machine and Xerox machine allow printing, scanning and copying. Those who find the libraray atmosphere inspiring for their work or who simpy need a desk for their literature search find quiet workplaces on the second floor of the library building. The library may also be used by scientists from outside the institute, but for practical reasons their access is restricted to office hours of the librarian.

Currently, our library stock consists of about 5,200 monographs, about 16,800 bound journal volumes and 42 scientific journal subscriptions in print, which can be easily located through the online catalogue. Readers can propose to purchase particular books which they need through a web form, which is one way how our book holdings are systematically complemented.

Via the library homepage, mpi**pks** users, identified through the IP address of their computer, have access to about 52,000 online journals and 540,000 e-books, as well as numerous literature and factual databases, online encyclopedias, dictionaries, MPG Resource Navigator, the e-Doc Server, international catalogues

etc. The new discovery system VuFind simplifies the access to various information ressources such as the new library online catalogue.

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 **mpipks**, e.g., for the yearbook of the Max Planck Society or the institute's scientific reports. Also the demands of Open Access are related to these 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 **mpipks** publications' metadata by the librarian.

A library steering committee of scientists representing the divisions and groups of the **mpipks** makes sure that the needs of scientists are optimally served by the library. In quarterly meetings decisions such as new journal subscriptions are made.

The library used to be on the ground floor of the main building. In autumn 2012, it was relocated into the newly built guesthouse 4. In the new facilities, books and journals can be found on the four floors of an open-plan room flooded with light. in addition, there is a reading room 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 and informal access.

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. The massive extension of online access to journal articles makes it foreseeable that print issues of journals might be fully replaced by online access in a few years. Most of our online access is organized by the central Max Planck Digital Library MPDL in Munich, who also guarantees the unlimited access to back-issues. In the future, 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 new library in guest house 4

3.9.3 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.

Guest house 4

Guest house 1 has 20 single and five 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 ten one-bedroom apartments with kitchen, and three two-bedroom apartments with living room, bathroom and kitchen for up to three persons (e.g. families). One of the larger 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 to all guests.

Guest house 3 allows to accommodate guests in five two-bedroom apartments similarly equipped to those in guest house 2. On the first floor, two apartments have been converted into offices, which are used by short term guest scientists.

Since November 2012, the newly built guest house 4 additionally offers 14 single and eight 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.

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. If needed, the family apartement is used for child daycare, which can be arranged for workshop participants.

3.10 Committees

3.10.1 Scientific Advisory Board

According to the rules of the Max Planck Society, the mpi**pks** has a Scientific Advisory Board. The members of the Board advise the board of directors concerning the research at the institute. The Board assesses the research direction of the institute, the scientific relevance and likelihood of 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:

Cugliandolo, 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
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80333 München

Ivanov, M.
Professor Dr.

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Grossbritannien

Kurths, J.
Professor Dr.

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14473 Potsdam

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Professor Dr.

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3.10.2 Board of Trustees

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3.11 Members of the mpipks

(as of June 2015)

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 22

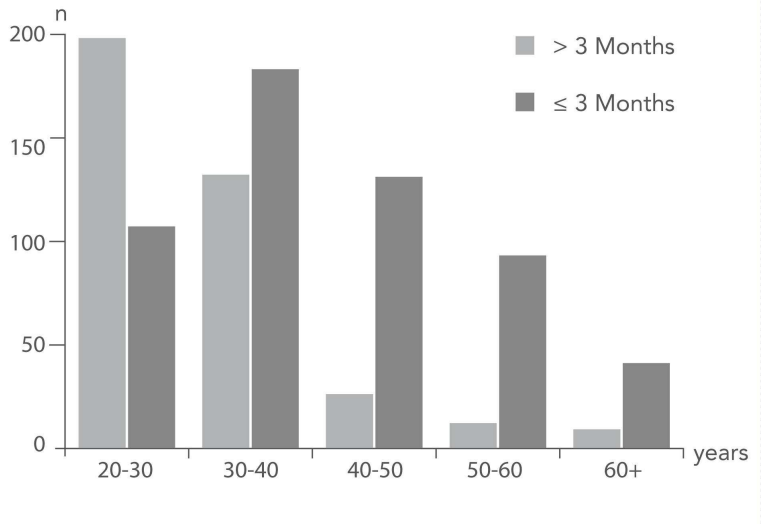
2. **Externally funded research staff** — **11**

3. **PhD students** — **76**

   - PhD students with internal supervision 61
     German PhD students *35*
     Foreign PhD students *26*
   - PhD students with external supervision 15
     PhD students with external funding *5*
     IMPRS PhD students with external supervision *10*

4. **Guest scientists** — **70**

   - German guest scientists 24
   - Foreign guest scientists 46



Age distribution

The structure of the mpi**pks** with its large visitors program and its focus on the development of junior scientists means that research positions are almost exclusively temporary. Beside the directors, the only exceptions are two permanent W2-positions.

Chapter 4

Publications

4.1 Atomic and Molecular Structure

2013

Bilodeau, R.C., N.D. Gibson, C.W. Walter, D.A. Esteves-Macaluso, S. Schippers, A. Müller, R.A. Phaneuf, A. Aguilar, M. Hoener, J.M. Rost and N. Berrah: Single-Photon Multiple Detachment in Fullerene Negative Ions: Absolute Ionization Cross Sections and the Role of the Extra Electron. Physical Review Letters **111**, 043003 (2013).

Cioslowski, J.: The weak-correlation limits of few-electron harmonium atoms. The Journal of Chemical Physics **139**, 224108 (2013).

Mikhailov, A.I., A.V. Nefiodov and G. Plunien: Electron correlations in cross sections for ionization of heliumlike ions by high-energy particle impact. Physical Review A **87**, 032705 (2013).

Rodrigues, J.N.B., P.A.D. Goncalves, J.E. Santos and A.H. Castro Neto: Thermodynamics of a Potts-like model for a reconstructed zigzag edge in graphene nanoribbons. Physical Review B **87**, 134204 (2013).

Vorberger, J. and D.O. Gericke: Effective ion-ion potentials in warm dense matter. High Energy Density Physics **9**, 178-186 (2013).

2014

Cioslowski, J.: Note on the asymptotic isomer count of large fullerenes. Journal of Mathematical Chemistry **52**, 1-5 (2014).

Fratini, F., L. Safari, A.G. Hayrapetyan, K. Jankälä, P. Amaro and J.P. Santos: Quantized form factor shift in the presence of free electron laser radiation. EPL **107**, 13002 (2014).

Macri, T., S. Saccani and F. Cinti: Ground State and Excitation Properties of Soft-Core Bosons. Journal of Low Temperature Physics **177**, 59-71 (2014).

Nefiodov, A.V. and G. Plunien: Ionization with excitation by Compton scattering of high-energy photons from helium-like ions in the metastable $1s2s_1S$ and $1s2s_3S$ states. Physics Letters A **378**, 1022-1024 (2014).

Ovchinnikov, Y.N., A. Halder and V.V. Kresin: Flat Thomas-Fermi artificial atoms. EPL **107**, 37001 (2014).

Vorberger, J. and D.O. Gericke: Comparison of electron-ion energy transfer in dense plasmas obtained from numerical simulations and quantum kinetic theory. High Energy Density Physics **10**, 1-8 (2014).

Zhang, S.B., X.Y. Li, J.G. Wang, JY.Z. Qu and X.J. Chen: Multicenter distorted-wave method for fast-electron-impact single ionization of molecules. Physical Review A **89**, 052711 (2014).

Zoubi, H.: Collective interactions in an array of atoms coupled to a nanophotonic waveguide. Physical Review A **89**, 043831 (2014).

2015

Bramanti, A.P., A. Santana-Bonilla and R. Rinaldi: Quantum-dot Cellular Automata: Computation with Real-world Molecules. International Journal of Unconventional Computing **11**, 63-82 (2015).

Cioslowski, J.: The Coulomb, exchange, and correlation components of the electron-electron repulsion in harmonium atoms **142**, 114105 (2015).

Cioslowski, J.: One-electron reduced density matrices of strongly correlated harmonium atoms. Journal of Chemical Physics **142**, 114104 (2015).

Kraus, D., J. Vorberger, J. Helfrich, D.O. Gericke, B. Bachmann, V. Bagnoud, B. Barbrel, A. Blažević, D.C. Carroll, W. Cayzac et. al.: The complex ion structure of warm dense carbon measured by spectrally resolved x-ray scattering. Physics of Plasmas **22**, 056307 (2015).

Sträter, C. and A. Eckardt: Orbital-driven melting of a bosonic Mott insulator in a shaken optical lattice. Physical Review A **91**, 053602 (2015).

Zoubi, H.: Dark bogolon-excitons in a linear atomic super-lattice. New Journal of Physics **17**, 023053 (2015).

4.2 Deterministic Dynamics

2013

Altmann, E.G., J.S.E. Portela and T. Tél: Chaotic Systems with Absorption. Physical Review Letters **111**, 144101 (2013).

Altmann, E.G., J.S.E. Portela and T. Tél: Leaking chaotic systems. Reviews of Modern Physics **85**, 869-918 (2013).

Aufderheide, H., L. Rudolf, T. Gross and K.D. Lafferty: How to predict community responses to perturbations in the face of imperfect knowledge and network complexity. Proceedings of the Royal Society B **280**, 20132355 (2013).

Bodai, T., E.G. Altmann and A. Endler: Stochastic perturbations in open chaotic systems: Random versus noisy maps. Physical Review E **87**, 042902 (2013).

Bodai, T., G. Karolyi and T. Tel: Driving a conceptual model climate by different processes: Snapshot attractors and extreme events. Physical Review E **87**, 022822 (2013).

Botha, A.E., Yu.M. Shukrinov and M.R. Kolahchi: Onset of chaos in intrinsic Josephson junctions. Chaos, Solitons & Fractals **48**, 32-37 (2013).

Briggs, J.S. and A. Eisfeld: Quantum dynamics simulation with classical oscillators. Physical Review A **88**, 062104 (2013).

Chotorlishvili, L., R. Khomeriki, A. Sukhov, S. Ruffo and J. Berakdar: Dynamics of Localized Modes in a Composite Multiferroic Chain. Physical Review Letters **111**, 117202 (2013).

Di Cintio, PF., L. Ciotti and C. Nipoti: Relaxation of *N*-body systems with additive $r_{-\alpha}$ interparticle forces. Monthly Notices of the Royal Astronomical Society **431**, 3177-3188 (2013).

Epperlein, J., A.L. Do, T. Gross, T. and S. Siegmund: Meso-scale obstructions to stability of 1D center manifolds for networks of coupled differential equations with symmetric Jacobian. Physica D **261**, 1-7 (2013).

Gnutzmann, S., H. Schanz and U. Smilansky: Topological Resonances in Scattering on Networks (Graphs). Physical Review Letters **110**, 094101 (2013).

Gori, G., T. Macri and A. Trombettoni: Modulational instabilities in lattices with power-law hoppings and interactions. Physical Review E **87**, 032905 (2013).

Hennig, D., C. Mulhern and A.D. Burbanks: From strong chaos via weak chaos to regular behaviour: Optimal interplay between chaos and order. Physica D **253**, 102-110 (2013).

Kantz, H., G. Radons and H. Yang: The problem of spurious Lyapunov exponents in time series analysis and its solution by covariant Lyapunov vectors. Journal of Physics A **46**, 254009 (2013).

Kolahchia, M.R., Yu.M. Shukrinovb, M. Hamdipoura, A.E. Bothad and M. Suzukie: Some chaotic features of intrinsically coupled Josephson junctions. Physica C **491**, 63–65 (2013).

Kuehn, C., S. Siegmund and T. Gross: Dynamical analysis of evolution equations in generalized models. IMA Journal of Applied Mathematics **78**, 1051-1077 (2013).

Leitao, J.C., J.M. Viana Parente Lopes and E.G. Altmann: Monte Carlo Sampling in Fractal Landscapes. Physical Review Letters **110**, 220601(2013).

Manchein, C., A. Celestino and M.W. Beims: Temperature Resistant Optimal Ratchet Transport. Physical Review Letters **110**, 114102 (2013).

Maucher, F., E. Siminos, W. Krolikowski and S. Skupin: Quasiperiodic oscillations and homoclinic orbits in the nonlinear nonlocal Schrodinger equation. New Journal of Physics **15**, 083055 (2013).

Ovchinnikov, Y.N.: Families of solutions to the generalized Ginzburg-Landau equation and structural transitions between them. Journal of Experimental and Theoretical Physics **117**, 480-486 (2013).

Ovchinnikov, Y.N. and V.Z. Kresin: Networks of Josephson junctions and their synchronization. Physical Review B **88**, 214504 (2013).

Rayanov, K., G. Radons and S. Flach: Decohering localized waves. Physical Review E **88**, 012901 (2013).

Shukrinov, Y.M., I.R. Rahmonov and K.V. Kulikov: Double resonance in the system of coupled Josephson junctions. JETP Letters **96**, 588-595 (2013).

Uriu, K., S. Ares, A.C. Oates and L.G. Morelli: Dynamics of mobile coupled phase oscillators. Physical Review E **87**, 032911 (2013).

Vitanov, N.K., Z.I. Dimitrova and H. Kantz: Application of the method of simplest equation for obtaining exact traveling-wave solutions for the extended Korteweg-de Vries equation and generalized Camassa-Holm equation. Applied Mathematics and Computation **219**, 7480-7492 (2013).

Zschaler, G. and T. Gross: Largenet2: an object-oriented programming library for simulating large adaptive networks. Bioinformatics **29**, 277-278 (2013).

2014

Abdulack, S.A., W.T. Strunz and M.W. Beims: Finite kicked environments and the fluctuation-dissipation relation. Physical Review E **89**, 042141 (2014).

Adamashvili, G.T., D.J. Kaup and A. Knorr: Dissipative solitons of self-induced transparency. Physical Review A **90**, 053835 (2014).

Brison, O.J. and J.A.C. Gallas: What is the effective impact of the explosive orbital growth in discrete-time one-dimensional polynomial dynamical systems? Physica A **410**, 313-318 (2014).

Carbajal L., R.O. Dendy, S.C. Chapman and J.W.S. Cook: Linear and nonlinear physics of the magnetoacoustic cyclotron instability of fusion-born ions in relation to ion cyclotron emission. Physics of Plasmas **21**, 012106 (2014).

Galiceanu, M., M.W. Beims and W.T. Strunz: Quantum energy and coherence exchange with discrete baths. Physica A **415**, 294-306 (2014).

Gallas, M.R. and J.A.C. Gallas: Distribution of chaos and periodic spikes in a three-cell population model of cancer. European Physical Journal-Special Topics **223**, 2131-2144 (2014).

Hennig, D. and C. Mulhern: Nonlinear chains inside walls. Physica D **283**, 29-36 (2014).

Hennig, D., C. Mulhern, A.D. Burbanks and L. Schimansky-Geier: Nonlinear response of a linear chain to weak driving. Physical Review E **89**, 012906 (2014).

Kubo, K. and T. Shimada: Periodic orbit theory revisited in the anisotropic Kepler problem. Progress of Theoretical and Experimental Physics **3**, 023A06 (2014).

Kullig, J., C. Löbner, N. Mertig, A. Bäcker and R. Ketzmerick: Integrable approximation of regular regions with a nonlinear resonance chain. Physical Review E **90**, 052906 (2014).

Lange, S., M. Richter, F. Onken, A. Bäcker and R. Ketzmerick: Global structure of regular tori in a generic 4D symplectic map. Chaos **24**, 024409 (2014).

Lazarides, A., A. Das and R. Moessner: Equilibrium states of generic quantum systems subject to periodic driving. Physical Review E **90**, 012110 (2014).

Lazarides, A., A. Das and R. Moessner: Periodic Thermodynamics of Isolated Quantum Systems. Physical Review Letters **89**, 150401 (2014).

Manchein, C., M.W. Beims and J.M. Rost: Characterizing weak chaos in nonintegrable Hamiltonian systems: The fundamental role of stickiness and initial conditions. Physica A **400**, 186-193 (2014).

Mulansky, M.: Scaling of chaos in strongly nonlinear lattices. Chaos **24**, 024401 (2014).

Nag, T., S. Roy, A. Dutta and D. Sen: Dynamical localization in a chain of hard core bosons under periodic driving. Physical Review B **89**, 165425 (2014).

Ngo, S., A. Peshkov, I.S. Aranson, E. Bertin, F. Ginelli and H. Chaté: Large-Scale Chaos and Fluctuations in Active Nematics. Physical Review Letters **113**, 038302 (2014).

Richter, M., S. Lange, A. Bäcker and R. Ketzmerick: Visualization and comparison of classical structures and quantum states of four-dimensional maps. Physical Review E **89** 022902 (2014).

Sethia, G.C. and A. Sen: Chimera States: The Existence Criteria Revisited. Physical Review Letters **112**, 144101 (2014).

Shi, X.Q., H. Chaté and Y.Q. Ma: Instabilities and chaos in a kinetic equation for active nematics. New Journal of Physics **16**, 035003 (2014).

Taillefumier, M., J. Robert, C.L. Henley, R. Moessner and B. Canals: Semiclassical spin dynamics of the antiferromagnetic Heisenberg model on the kagome lattice. Physical Review B **90**, 064419 (2014).

Tieleman, O., C. Skokos and A. Lazarides: Chaoticity without thermalisation in disordered lattices. EPL **105**, 20001 (2014).

Vitanov, N.K. and Z.I. Dimitrova: Solitary wave solutions for nonlinear partial differential equations that contain monomials of odd and even grades with respect to participating derivatives. Applied Mathematics and Computation **247**, 213-217 (2014).

Zagoya, C., L.S. Schulman and F. Grossmann: Interference nature of quantum breather oscillation. Journal of Physics A **47**, 165102 (2014).

Zaletel, M.P., R.S.K. Mong and F. Pollmann: Flux insertion, entanglement, and quantized responses. Journal of Statistical Mechanics, P10007 (2014).

2015

Altmann, E.G., J.S.E. Portela and T. Tel: Chaotic explosions. EPL **109**, 30003 (2015).

Beims, M.W., M. Schlesinger, C. Manchein, A. Celestino, A. Pernice and W.T. Strunz: Quantum-classical transition and quantum activation of ratchet currents in the parameter space. Physical Review E **91**, 052908 (2015).

Bradley, E. and H. Kantz: Nonlinear time-series analysis revisited. Chaos **25**, 097610 (2015).

Budanur, N.B., P. Cvitanovic, R.L. Davidchack and E. Siminos: Reduction of SO(2) Symmetry for Spatially Extended Dynamical Systems. Physical Review Letters **114**, 084102 (2015).

Da Silva, R.M., C. Manchein, M.W. Beims and E.G. Altmann: Characterizing weak chaos using time series of Lyapunov exponents. Physical Review E **91**, 062907 (2015).

Jörg, D.J.: Nonlinear transient waves in coupled phase oscillators with inertia. Chaos **25**, 053106 (2015).

Junges, L. and J.A.C. Gallas: Stability diagrams for continuous wide-range control of two mutually delay-coupled semiconductor lasers. New Journal of Physics **17**, 053038 (2015).

Mulhern, C., S. Bialonski and H. Kantz: Extreme events due to localization of energy. Physical Review E **91**, 012918 (2015).

Sala, M. and R. Artuso: Oseledets' splitting of standard-like maps. Chaos **25**, 023113 (2015).

4.3 Dynamics in Nanoscale Systems

2013

Bird, J., R. Kaiser, I. Rotter and G. Wunner: Special Issue: Quantum Physics with non-Hermitian Operators: Theory and Experiment. Fortschritte der Physik/ Progress of Physics **61**, 51–419 (2013).

Eleuch, H., A. Prasad and I. Rotter: Enhancement of photon intensity in forced coupled quantum wells inside a semiconductor microcavity. Physical Review E **87**, 022916 (2013).

Hafermann, H., P. Werner and E. Gull: Efficient implementation of the continuous-time hybridization expansion quantum impurity solver. Computer Physics Communications **184**, 1280-1286 (2013).

Herbut, I.F.: Majorana mass, time reversal symmetry, and the dimension of space. Physical Review D **87**, 085002 (2013).

Lee, S.-Y. and Y. Chung: Charge stability of a triple quantum dot with a finite tunnel coupling. Physical Review B **87**, 045302 (2013).

Munárriz, J., C. Gaul, A.V. Malyshev, P.A. Orellana, C.A. Müller and F. Domínguez-Adame: Strong spin-dependent negative differential resistance in composite graphene superlattices. Physical Review B **88**, 155423 (2013).

Munoz, E., C.J. Bolech and S. Kirchner: Universal Out-of-Equilibrium Transport in Kondo-Correlated Quantum Dots: Renormalized Dual Fermions on the Keldysh Contour. Physical Review Letters **110**, 016601 (2013).

Nisoli, C., R. Moessner and P. Schiffer: Colloquium: Artificial spin ice: Designing and imaging magnetic frustration. Review of Modern Physics **85**, 1473-1490 (2013).

Poghossian, A., M. Weil, A.G. Cherstvy and M.J. Schöning: Electrical monitoring of polyelectrolyte multilayer formation by means of capacitive field-effect devices. Analytical and Bioanalytical Chemistry **405**, 6425-6436 (2013).

Popkov, V. and M. Salerno: Anomalous currents in a driven XXZ chain with boundary twisting at weak coupling or weak driving. Journal of Statistical Mechanics, P02040 (2013).

Rotter, I.: Dynamical stabilization and time in open quantum systems. Fortschritte der Physik/ Progress of Physics **61**, 178-193 (2013).

Saikin, S.K., A. Eisfeld, S. Valleau and A. Aspuru-Guzik: Photonics meets excitonics: natural and artificial molecular aggregates. Nanophotonics **2**, 21–38 (2013).

Scott, G.D., D. Natelson, S. Kirchner and E. Muñoz: Transport characterization of Kondo-correlated single-molecule devices. Physical Review B **87**, 241104 (2013).

Sethia, G.C., A. Sen and G.L. Johnston: Amplitude-mediated chimera states. Physical Review E **88**, 042917 (2013).

Toldin, F.P., M. Tröndle and S. Dietrich: Critical Casimir forces between homogeneous and chemically striped surfaces. Physical Review E **88**, 052110 (2013).

2014

Abdussalam, W. and P. Machnikowski: Superradiance and enhanced luminescence from ensembles of a few self-assembled quantum dots. Physical Review B **90**, 125307 (2014).

Bonilla, A.S., R. Gutierrez, L.M. Sandonas, D. Nozaki, A.P. Bramanti and G. Cuniberti: Structural distortions in molecular-based quantum cellular automata: a minimal model based study. Physical Chemistry Chemical Physics **16**, 17777-17785 (2014).

Brown, C.R.D., D.O. Gericke, M. Cammarata, B.I. Cho, T. Döppner, K. Engelhorn, E. Förster, C. Fortmann, D. Fritz, E. Galtier, S.H. Glenzer, M. Harmand, P. Heimann, N.L. Kugland, D.Q. Lamb, H.J. Lee, R.W. Lee, H. Lemke, M. Makita, A. Moinard, C.D. Murphy, B. Nagler, P. Neumayer, K.U. Plagemann, R. Redmer, D. Riley, F.B. Rosmej, P. Sperling, S. Toleikis, S.M. Vinko, J. Vorberger et.al.: Evidence for a glassy state in strongly driven carbon. Scientific Report **4**, 5214 (2014).

Cinti, F., M. Boninsegni and T. Pohl: Exchange-induced crystallization of soft-core bosons. New Journal of Physics **16**, 033038 (2014).

Cinti, F., T. Macri, W. Lechner, G. Pupillo and T. Pohl: Defect-induced supersolidity with soft-core bosons. Nature Communications **5**, 3235 (2014).

Daoud, M., R.A. Laamara and H. El Hadfi: Pairwise quantum and classical correlations in multi-qubits states via linear relative entropy. Internation Journal of Quantum Information **12**, 1450035 (2014).

Díaz, E., K. Miralles, F. Domínguez-Adame and C. Gaul: Spin-dependent terahertz oscillator based on hybrid graphene superlattices. Applied Physics Letters **105**, 103109 (2014).

Fletcher, L.B., A.L. Kritcher, A. Pak, T. Ma, T. Doppner, C. Fortmann, L. Divol, O.S. Jones, O.L. Landen, H.A. Scott, J. Vorberger, D.A. Chapman, D.O. Gericke, B.A. Mattern, G.T. Seidler, G. Gregori, R.W. Falcone and S.H. Glenzer: Observations of Continuum Depression in Warm Dense Matter with X-Ray Thomson Scattering. Physical Review Letters **112**, 145004 (2014).

Forchheimer, D., S.S. Borysov, D. Platz and D.B. Haviland: Determining surface properties with bimodal and multimodal AFM. Nanotechnology **25**, 485708 (2014).

Gaul, C., F. Domínguez-Adame, F. Sols and I. Zapata: Feshbach-type resonances for two-particle scattering in graphene. Physical Review B **89**, 045420 (2014).

Guo, A.M., E. Díaz, C. Gaul, R. Gutierrez, F. Domínguez-Adame, G. Cuniberti and Q.F. Sun: Contact effects in spin transport along double-helical molecules. Physical Review B **89** 205434 (2014).

Hentschel, M. and G. Röder: The mesoscopic X-ray edge problem: Boundary effects enhance photoabsorption in quantum dots. European Physical Journal B **87**, 12 (2014).

Kutschan, B., K. Morawetz and S. Thoms: Dynamical mechanism of antifreeze proteins to prevent ice growth. Physical Review E **90**, 022711 (2014).

Lucas, F. and K. Hornberger: Incoherent control of the retinal isomerization in rhodopsin. Physical Review Letters **113**, 058301 (2014).

Midtvedt, D., A. Isacsson and A. Croy: Nonlinear phononics using atomically thin membranes. Nature Communications **5**, 4838 (2014).

Milovanov, A.V. and A. Iomin: Topological approximation of the nonlinear Anderson model. Physical Review E **89**, 062921 (2014).

Papanikolaou, S., D. Charrier and E. Fradkin: Ising nematic fluid phase of hard-core dimers on the square lattice. Physical Review B **89**, 035128 (2014).

Ritschel, G. and A. Eisfeld: Analytic representations of bath correlation functions for ohmic and superohmic spectral densities using simple poles. Journal of Chemical Physics **141**, 094101 (2014).

Takabatake T., K. Suekuni, T. Nakayama, and E. Kaneshita: Phonon-glass electron-crystal thermoelectric clathrates: Experiments and theory. Reviews of Modern Physics **86** 669-716 (2014).

Vlaming, S.M. and A. Eisfeld: Tunable superradiance in porphyrin chains on insulating surfaces. Journal of Physics D **47**, 305301 (2014).

Wirth, S., Y. Prots, M. Wedel, S. Ernst, S. Kirchner, Z. Fisk, J.D. Thompson, F. Steglich and Y. Grin: Structural Investigations of $CeIrIn_5$ and $CeCoIn_5$ on Macroscopic and Atomic Length Scales. Journal of the Physical Society of Japan **83**, 061009 (2014).

Yan, B.H., A.K. Paul, S. Kanungo, M. Reehuis, A. Hoser, D.M. Töebbens, W. Schnelle, R.C. Williams,T. Lancaster, F. Xiao, J.S. Moller, S.J. Blundell, W. Hayes, C. Felser and M. Jansen: Lattice-Site-Specific Spin Dynamics in Double Perovskite Sr_2CoOsO_6. Physical Review Letters **112**, 147202 (2014).

2015

Kou, L.Z., F.M. Hu, B.H. Yan, T. Wehling, C. Felser, T. Frauenheim and C.F. Chen: Proximity enhanced quantum spin Hall state in graphene. Carbon **87**, 418-423 (2015).

Lim, L.K., J.N. Fuchs and G. Montambaux: Geometric phase in Stuckelberg interferometry. Physical Review A **91**, 042119 (2015).

Popkov, V., M. Salerno and R. Livi: Full decoherence induced by local fields in open spin chains with strong boundary couplings. New Journal of Physics **17**, 023066 (2015).

Schönleber, D.W., A.Croy and A. Eisfeld: Pseudomodes and the corresponding transformation of the temperature-dependent bath correlation function. Physical Review A **91**, 052108 (2015).

4.4 Electronic Structure

2013

Antipov, A.E., P. Ribeiro, J. Kroha and S. Kirchner: Identifying Kondo orbitals through spatially resolved STS. Physica Status Solidi B **250**, 562-567 (2013).

Cioslowski, J. and J. Albin: Asymptotic equivalence of the shell-model and local-density descriptions of Coulombic systems confined by radially symmetric potentials in two and three dimensions. Journal of Chemical Physics **139**, 114109 (2013).

Cornaton, Y., A. Stoyanova, H.J.A. Jensen and E. Fromager: Alternative separation of exchange and correlation energies in range-separated density-functional perturbation theory. Physical Review A **88**, 022516 (2013).

Friedemann, S., S. Paschen, C. Geibel, S. Wirth, F. Steglich, S. Kirchner, E. Abrahams, and Q. Si: Comment on "Zeeman-Driven Lifshitz Transition: A Model for the Experimentally Observed Fermi-Surface Reconstruction in $YbRh_2Si_2$". Physical Review Letters **111**, 139701 (2013).

Ishizuka, H., M. Udagawa and Y. Motome: Polynomial expansion Monte Carlo study of frustrated itinerant electron systems: Application to a spin-ice type Kondo lattice model on a pyrochlore lattice. Computer Physics Communications **184**, 2684-2692 (2013).

Kagalovsky, V. and A.L. Chudnovskiy: Decoherence induced by magnetic impurities in a quantum hall system. Journal of Experimental and Theoretical Physics **116**, 657-662 (2013).

Kou, L., B. Yan, F. Hu, S.C. Wu, T.O. Wehling, C. Felser, C. Chen and T. Frauenheim: Graphene-Based Topological Insulator with an Intrinsic Bulk Band Gap above Room Temperature. Nano Letters **13**, 6251–6255 (2013).

LeBlanc, J.P.F. and J.P. Carbotte: Effect of dynamical screening on single-particle spectral features of uniaxially strained graphene: Tuning the plasmaron ring. Physical Review B **87**, 205407 (2013).

Merker, L., S. Kirchner, E. Munoz and T.A. Costi: Conductance scaling in Kondo-correlated quantum dots: Role of level asymmetry and charging energy. Physical Review B **87**, 165132 (2013).

Morawetz, K.: The effect of electromagnetic fields on a charged catenary. AIP Advances **2**, 022146 (2012).

Morawetz, K.: Terahertz out-of-plane resonances due to sprin-orbit coupling. EPL **104**, 27005 (2013).

Ovchinnikov, Y.N.: Dynamics of an N-vortex state at small distances. Journal of Experimental and Theoretical Physics **116**, 173-179 (2013).

Pouladsaz, D., M. Schreiber and T.G. Gopakumar: DFT study of vibronic properties of d_8 (Ni-, Pd-, and Pt-) phthalocyanines. Journal of Chemical Physics **138**, 014306 (2013).

Rufino, M. J., D.L. Kovrizhin and J.T. Chalker: Solution of a model for the two-channel electronic Mach-Zehnder interferometer. Physical Review B **87**, 045120 (2013).

Salerno, M. and V. Popkov: Optimal transport and von Neumann entropy in a Heisenberg XXZ chain out of equilibrium. Physical Review E **87**, 022108 (2013).

Sticlet, D., B. Dora and J. Cayssol: Persistent currents in Dirac fermion rings. Physical Review B **88**, 205401 (2013).

Sticlet, D. and F. Piechon: Distant-neighbor hopping in graphene and Haldane models. Physical Review B **87**, 115402 (2013).

Stoyanova, A., A.M. Teale, J. Toulouse, T. Helgaker and E. Fromager: Alternative separation of exchange and correlation energies in multi-configuration range-separated density-functional theory. Journal of Chemical Physics **139**, 134113 (2013).

Yan, B., M. Jansen and C. Felser: A large-energy-gap oxide topological insulator based on the superconductor $BaBiO_3$. Nature Physics **9**, 709-711 (2013).

Yushankhai, V. and L. Siurakshina: Analysis of Crystal-Field Multiplets of V3+ Ion in Perovskite Oxides for Resonant Inelastic X-Ray Scattering Spectroscopy. International Journal Of Modern Physics B **27**, 1350185 (2013).

Zhang, D.L., B.H. Yan, S.C. Wu, J. Kübler, G. Kreiner, S.S.P. Parkin and C. Felser: First-principles study of the structural stability of cubic, tetragonal and hexagonal phases in Mn_3Z (Z = Ga, Sn and Ge) Heusler compounds. Journal of Physics - Condensed Matter **25**, 206006 (2013).

2014

Beugeling, W., A. Quelle and C.M. Smith: Nontrivial topological states on a Mobius band. Physical Review B **89**, 235112 (2014).

Craco, L., M.S. Laad and S. Leoni: Normal-state correlated electronic structure of tetragonal FeSe superconductor. In: Journal of Physics Conference Series. VII Brazilian Meeting on Simulational Physics **487**, 012017 (2014).

Deb, O., A. Soori and D. Sen: Edge states of a three-dimensional topological insulator. Journal of Physics-Condensed Matter **26**, 315009 (2014).

Đurić, T., N. Chancellor and I.F. Herbut: Interaction-induced anomalous quantum Hall state on the honeycomb lattice. Physical Review B **89**, 165123 (2014).

Grushin, A.G., A. Gómez-León and T. Neupert: Floquet Fractional Chern Insulators. Physical Review Letters **112**, 156801 (2014).

Hu, S.J., A.M. Turner, K. Penc and F. Pollmann: Berry-Phase-Induced Dimerization in One-Dimensional Quadrupolar Systems. Physical Review Letters **113**, 027202 (2014).

Huang, C.Y., X. Chen and F. Pollmann: Detection of symmetry-enriched topological phases. Physical Review B **90**, 045142 (2014).

Hwang, K., S. Bhattacharjee and Y.B. Kim: Signatures of spin-triplet excitations in optical conductivity of valence bond solids. New Journal of Physics **16**, 123009 (2014).

Kalesaki, E., C. Delerue, C.M. Smith, W. Beugeling, G. Allan and D. Vanmaekelbergh: Dirac Cones, Topological Edge States, and Nontrivial Flat Bands in Two-Dimensional Semiconductors with a Honeycomb Nanogeometry. Physical Review X **4**, 011010 (2014).

Kimberg, V. and C. Miron: Molecular potentials and wave function mapping by high-resolution electron spectroscopy and ab initio calculations. Journal of Electron Spectroscopy and Related Phenomena **195**, 301-306 (2014).

Kobayashi, K., T. Ohtsuki, K.I. Imura and I.F. Herbut: Density of States Scaling at the Semimetal to Metal Transition in Three Dimensional Topological Insulators. Physical Review Letters **112**, 016402 (2014).

Koley, S., M.S. Laad, N.S. Vidhyadhiraja and A. Taraphder: Preformed excitons, orbital selectivity, and charge density wave order in 1T-$TiSe_2$. Physical Review B **90**, 115146 (2014).

Kou, L.Z., F.M. Hu, B.H. Yan, T. Frauenheim and C.F. Chen: Opening a band gap without breaking lattice symmetry: a new route toward robust graphene-based nanoelectronics. Nanoscale **6**, 747-7479 (2014).

Kou, L.Z., S.C. Wu, C. Felser, T. Frauenheim, C.F. Chen and B.H. Yan: Robust 2D Topological Insulators in van der Waals Heterostructures. ACS Nano **8**, 10448-10454 (2014).

Li, C., T. Winzer, A. Walsh, B. Yan, C. Stampfl and A. Soon: Stacking-dependent energetics and electronic structure of ultrathin polymorphic V_2VI_3 topological insulator nanofilms. Physical Review B **90**, 075438 (2014).

McClarty, P.A., A. O'Brien and F. Pollmann: Coulombic charge ice. Physical Review B **89**, 195123 (2014).

Šopík, B., J. Kailasvuori and M. Trushin: Charge transport in two dimensions limited by strong short-range scatterers: Going beyond parabolic dispersion and Born approximation. Physical Review B **89**, 165308 (2014).

Sticlet, D., L. Seabra, F. Pollmann and J. Cayssol: From fractionally charged solitons to Majorana bound states in a one-dimensional interacting model. Physical Review B **89**, 115430 (2014).

Stoyanova, A., A.O. Mitrushchenkov, L. Hozoi, H. Stoll and P. Fulde: Electron correlation effects in diamond: A wave-function quantum-chemistry study of the quasiparticle band structure. Physical Review B **89**, 235121 (2014).

Takabatake, T., K. Suekuni, T. Nakayama and E. Kaneshita: Publisher's Note: Phonon-glass electron-crystal thermoelectric clathrates: Experiments and theory. Review of Modern Physics **86**, 841 (2014).

Tang, P.Z., B.H. Yan, W.D. Cao, S.C. Wu, C. Felser and W.H. Duan: Weak topological insulators induced by the interlayer coupling: A first-principles study of stacked Bi_2TeI. Physical Review B **89**, 041409 (2014).

Wang, G.: Fragmentation of Bloch oscillations in quasiperiodic waveguide arrays. Journal of Optics **16**, 015502 (2014).

Wang, J.R. and G.Z. Liu: Influence of Coulomb interaction on the anisotropic Dirac cone in graphene. Physical Review B **89**, 195404 (2014).

Wendumu, T.B., G. Seifert, T. Lorenz, J.O. Joswig and A. Enyashin: Optical Properties of Triangular Molybdenum Disulfide Nanoflakes. Journal of Physical Chemistry Letters **5**, 3636-3640 (2014).

Wu, S.C., B.H. Yan and C. Felser: Ab initio study of topological surface states of strained HgTe. EPL **107**, 57006 (2014).

Wu, S.C., G.C. Shan and B.H. Yan: Prediction of Near-Room-Temperature Quantum Anomalous Hall Effect on Honeycomb Materials. Physical Review Letters **113**, 256401 (2014).

2015

Anisimovas, E., G. Zlabys, B.M. Anderson, G. Juzeliunas and A. Eckardt: Role of real-space micromotion for bosonic and fermionic Floquet fractional Chern insulators. Physical Review B **91**, 245135 (2015).

Bernard, D., B. Doyon and J. Viti: Non-equilibrium conformal field theories with impurities. Journal of Physics A **48**, 05FT01 (2015).

Grushin, A.G., J. Motruk, M.P. Zaletel and F. Pollmann: Characterization and stability of a fermionic nu=1/3 fractional Chern insulator. Physical Review B **91**, 035136 (2015).

Grushin, A.G., J.W.F. Venderbos and J.H. Bardarson: Coexistence of Fermi arcs with two-dimensional gapless Dirac states. Physical Review B **91**, 121109 (2015).

Gulacsi, M.: Double-exchange mechanism in rare-earth compounds. Annals of Physics **354**, 454-474 (2015).

Gunnarsson, O., T. Schäfer, J.P.F. LeBlanc, E. Gull, J. Merino, G. Sangiovanni, G. Rohringer and A. Toschi: Fluctuation Diagnostics of the Electron Self-Energy: Origin of the Pseudogap Physics. Physical Review Letters **114**, 236402 (2015).

Hartley, N.J., P. Belancourt, D.A. Chapman, T. Döppner, R.P. Drake, D.O. Gericke, S.H. Glenzer, D. Khaghani, S. LePape, T. Ma, P. Neumayer, A. Pak, L. Peters, S. Richardson, J. Vorberger, T.G. White, G. Gregori: Electron-ion temperature equilibration in warm dense tantalum. High Energy Density Physics **14**, 1-5 (2015).

Joswig, J.O., T. Lorenz, T.B. Wendumu, S. Gemming and G. Seifert: Optics, Mechanics, and Energetics of Two-Dimensional MoS_2 Nanostructures from a Theoretical Perspective. Accounts of Chemical Research **48**, 48-55 (2015).

Kanungo, S., B.H. Yan, P. Merz, C. Felser and M. Jansen: Na_4IrO_4: Square-Planar Coordination of a Transition Metal in d_5 Configuration due to Weak On-Site Coulomb Interactions. Angewandte Chemie **54**, 5417-5420 (2015).

Leonhardt, K., N. Peyerimhoff, M. Tautenhahn and I. Veselic: Wegner estimate and localization for alloy-type models with sign-changing exponentially decaying single-site potentials. Reviews in Mathematical Physics **27**, 1550007 (2015).

Mihóková, E. and L.S. Schulman: Low temperature delayed recombination and trap tunneling. Journal of Physics-Condensed Matter **27**, 0775501 (2015).

Roy, S., A. Soori and S. Das: Tunnel magnetoresistance scan of a pristine three-dimensional topological insulator. Physical Review B **91**, 041109 (2015).

Sikora, O., H.W. Chang, C.P. Chou, F. Pollmann and Y.J. Kao: Variational Monte Carlo simulations using tensor-product projected states. Physical Review B **91**, 165113 (2015).

Zhang, S.B., D. Baykusheva, P.M. Kraus, H.J. Wörner and N. Rohringer: Theoretical study of molecular electronic and rotational coherences by high-order-harmonic generation. Physical Review A **91**, 023421 (2015).

4.5 Light-Matter Interaction

2013

Abdallah, J., J. Colgan, and N. Rohringer: Time-dependent calculations of electron energy distribution functions for neon gas in the presence of intense XFEL radiation. Journal of Physics B **46**, 235004 (2013).

Bergé, L., S. Skupin, C. Köhler, I. Babushkin and J. Herrmann: 3D Numerical Simulations of THz Generation by Two-Color Laser Filaments. Physical Review Letters **110**, 073901 (2013).

Birkholz, S., E.T.J. Nibbering, C. Bree, S. Skupin, A. Demircan, G. Genty and G. Steinmeyer: Spatiotemporal Rogue Events in Optical Multiple Filamentation. Physical Review Letters **111**, 243903 (2013).

Carbotte, J.P., J.P.F. LeBlanc and P.E.C. Ashby: Impact of electron-phonon coupling on near-field optical spectra in graphene. Physical Review B **87**, 045405 (2013).

Chapman, D.A., J. Vorberger and D.O. Gericke: Reduced coupled-mode approach to electron-ion energy relaxation. Physical Review E **88**, 013102 (2013).

Dennis, M.R.and J.B. Götte: Beam shifts for pairs of plane waves. Journal of Optics **15**, 014015 (2013).

Di Cintio, PF., U. Saalmann, J.M. Rost: Proton Ejection from Molecular Hydride Clusters Exposed to Strong x-Ray Pulses. Physical Review Letters **111**, 123401 (2013).

El-Ganainy, R., A. Eisfeld, M. Levy and D.N. Christodoulides: On-chip non-reciprocal optical devices based on quantum inspired photonic lattices. Applied Physics Letters **103**, 161105 (2013)

El-Ganainy, R., P. Kumar and M. Levy: On-chip optical isolation based on nonreciprocal resonant delocalization effects. Optics Letters **38**, 61-63 (2013).

Fischer, M., J. Handt, G. Seifert and R. Schmidt: Orientation dependence of energy absorption and relaxation dynamics of C_{60} in fs-laser pulses. Physical Review A **88**, 061403 (2013).

Friou, A., D. Bénisti, L. Gremillet, E. Lefebvre, O. Morice, E. Siminos and D.J. Strozzi: Saturation mechanisms of backward stimulated Raman scattering in a one-dimensional geometry. Physics of Plasmas **20**, 103103 (2013).

Gnodtke, C., U. Saalmann and J.M. Rost: Slow and fast multi-photon ionization of clusters in strong XUV and X-ray pulses. Chemical Physics **414**, 65-68 (2013).

Götte, J.B. and M.R. Dennis: Limits to superweak amplification of beam shifts. Optic Letters **38**, 2295-2297 (2013).

Götte, J.B. and M.R. Dennis: Spin-orbit interactions in vortex singularimetry. Proceedings of SPIE - Sprintronics VI **8813**, 88130Z (2013).

Gorshkov, A.V., R. Nath and T. Pohl: Dissipative Many-Body Quantum Optics in Rydberg Media. Physical Review Letters **110**, 1536 (2013).

Guichard, R., M. Richter, J.M. Rost, U. Saalmann, A.A. Sorokin and K. Tiedtke: Multiple ionization of neon by soft x-rays at ultrahigh intensity. Journal of Physics B **46**, 164025 (2013).

Herrmann, J., M. Weger, R. Locher, M. Sabbar, P. Rivière, U. Saalmann, J.M. Rost, L. Gallmann and U. Keller: Virtual single-photon transition interrupted: Time-gated optical gain and loss. Physical Review A **88**, 043843 (2013).

Khomeriki, R. and J. Leon: All-optical amplification in metallic subwavelength linear waveguides. Physical Review A **87**, 053806 (2013).

Kimberg, V., S. Bin Zhang and N. Rohringer: X-ray lasing in the CO molecule. Journal of Physics B **46**, 164017 (2013).

Kimberg, V. and N. Rohringer: Amplified X-Ray Emission from Core-Ionized Diatomic Molecules. Physical Review Letters **110**, 043901 (2013).

Köhler, C., R. Guichard, E. Lorin, S. Chelkowski, A.D. Bandrauk, L. Bergé and S. Skupin: Saturation of the nonlinear refractive index in atomic gases. Physical Review A **87**, 043811 (2013).

Kraus, D., J. Vorberger, D.O. Gericke, V. Bagnoud, A. Blažević, W. Cayzac, A. Frank, G. Gregori, A. Ortner, A. Otten, F. Roth, G. Schaumann, D. Schumacher, K. Siegenthaler, F. Wagner, F. K. Wünsch and M. Roth: Probing the Complex Ion Structure in Liquid Carbon at 100 GPa. Physical Review Letters **111**, 255501 (2013).

Kraus, P.M., S.B. Zhang, A. Gijsbertsen, R.R. Lucchese, N. Rohringer and H.J. Wörner: High-Harmonic Probing of Electronic Coherence in Dynamically Aligned Molecules. Physical Review Letters **111**, 243005 (2013).

Lucas, F., F. Mintert and A. Buchleitner: Tailoring many-body entanglement through local control. Physical Review A **88**, 032306 (2013).

Macri, T. and A. Trombettoni: Tunneling of polarized fermions in 3D double wells. Laser Physics **23**, 095501 (2013).

Mauger, S., G.C. de Verdière, L. Bergé and S. Skupin: GPU accelerated fully space and time resolved numerical simulations of self-focusing laser beams in SBS-active media. Journal of Computational Physics **235**, 606-625 (2013).

Miri, M.-A., M. Heinrich, R. El-Ganainy and D.N. Christodoulides: Supersymmetric Optical Structures. Physical Review Letters **110**, 233902 (2013).

Möbius, S., M. Genkin, A. Eisfeld, S. Wüster and J.M. Rost: Entangling distant atom clouds through Rydberg dressing. Physical Review A **87**, 051602(R) (2013).

Müller, M., A. Paulheim, A. Eisfeld and M. Sokolowski: Finite size line broadening and superradiance of optical transitions in two dimensional long-range ordered molecular aggregates. Journal of Chemical Physics **139**, 044302 (2013).

Saalmann, U., A. Mikaberidze and J.M. Rost: Spatial Correlations in Finite Samples Revealed by Coulomb Explosion. Physical Review Letters **110**, 133401 (2013).

Saxena, V., I. Kourakis, G. Sanchez-Arriaga and E. Siminos: Interaction of spatially overlapping standing electromagnetic solitons in plasmas. Physics Letters A **377**, 473-477 (2013).

Weninger, C., M. Purvis, D. Ryan, R.A. London, J.D. Bozek, C. Bostedt, A. Graf, G. Brown, J.J. Rocca and N. Rohringer: Stimulated Electronic X-Ray Raman Scattering. Physical Review Letters **111**, 233902 (2013).

Weninger, C. and N. Rohringer: Stimulated resonant x-ray Raman scattering with incoherent radiation. Physical Review A **88**, 053421 (2013).

White, S., G. Nersisyan, B. Kettle, T.W.J. Dzelzainis, K. McKeever, C.L.S. Lewis, A. Otten, K. Siegenthaler, D. Kraus, M. Roth, T. White, G. Gregori, D.O. Gericke, R. Baggott, D.A. Chapmand, K. Wünsch, J. Vorberger and D. Riley: X-ray scattering from warm dense iron. High Energy Density Physics **9**, 573-577 (2013).

Zoubi, H. and H. Ritsch: Excitons and Cavity Polaritons for Optical Lattice Ultracold Atoms. Advances in Atomic, Molecular, and Optical Physics **62**, 171-229 (2013).

2014

Baykusheva, D., P.M. Kraus, S.B. Zhang, N. Rohringer and H.J. Wörner: The sensitivities of high-harmonic generation and strong-field ionization to coupled electronic and nuclear dynamics. Faraday Discussions **171**, 113-132 (2014).

Camacho Garibay, A., U. Saalmann and J.M. Rost: Prevailing Features of X-Ray-Induced Molecular Electron Spectra Revealed with Fullerenes. Physical Review Letters **113**, 083001 (2014).

Chapman, D.A., D. Kraus, A.L. Kritcher, B. Bachmann, G.W. Collins, R.W. Falcone, J.A. Gaffney, D.O. Gericke, S.H. Glenzer, T.M. Guymer, J.A. Hawreliak, O.L. Landen, S. Le Pape, T. Ma, P. Neumayer, J. Nilsen, A. Pak, R. Redmer, D.C. Swift, J. Vorberger and T. Döppner: Simulating x-ray Thomson scattering signals from high-density, millimetre-scale plasmas at the National Ignition Facility. Physics of Plasmas **21**, 082709 (2014).

Chen, B.C., W.R. Legant, K. Wang, L. Shao, D.E. Milkie, M.W. Davidson, C. Janetopoulos, X.F.S. Wu, J.A. Hammer, Z. Liu, B.P. English, Y. Mimori-Kiyosue, D.P. Romero, A.T. Ritter, J. Lippincott-Schwartz, L. Fritz-Laylin, R.D. Mullins, D.M. Mitchell, J.N. Bembenek, A.C. Reymann, R. Böhme, S.W. Grill, J.T. Wang, G. Seydoux, U.S. Tulu, D.P. Kiehart

and E. Betzig: Lattice light-sheet microscopy: Imaging molecules to embryos at high spatiotemporal resolution. Science **346**, 349-351 (2014).

Dahlström, J.M. and E. Lindroth: Study of attosecond delays using perturbation diagrams and exterior complex scaling. Journal of Physics B **47**, 124012 (2014).

Dennis, M.R. and J.B. Götte: Beam shifts to reflected light beams and their axial structure. Proceedings of SPIE **9441**, 94410M (2014).

Dimitrovski, D., J. Maurer, H. Stapelfeldt and L.B. Madsen: Low-Energy Photoelectrons in Strong-Field Ionization by Laser Pulses with Large Ellipticity. Physical Review Letters **113**, 103005 (2014).

Dubček, T., N. Šantic, D. Jukić, D. Aumiler, T. Ban and H. Buljan: Synthetic Lorentz force in classical atomic gases via Doppler effect and radiation pressure. Physical Review A **89**, 063415 (2014).

Gärttner, M., S. Whitlock, D.W. Schönleber and J. Evers: Collective Excitation of Rydberg-Atom Ensembles beyond the Superatom Model. Physical Review Letters **113**, 233002 (2014).

Götte, J.B.: Weak measurements with non-integer orbital angular momentum states.Proceedings of SPIE - Complex Light and Optical Forces VIII **8999**, 899917 (2014).

Götte, J.B., W. Löffler and M.R. Dennis: Eigenpolarizations for Giant Transverse Optical Beam Shifts. Physical Review Letters **112**, 233901 (2014).

Guénot, D., D. Kroon, E. Balogh, E.W. Larsen, M. Kotur, M. Miranda, T. Fordell, P. Johnsson, J. Mauritsson, M. Gisselbrecht, K. Varjù, C.L. Arnold, T. Carette, A.S. Kheifets, E. Lindroth, A. L'Huillier and J.M. Dahlström: Measurements of relative photoemission time delays in noble gas atoms. Journal of Physics B **47**, 245602 (2014).

Jin, C.Y., R. Johne, M.Y. Swinkels, T.B. Hoang, L. Midolo, P.J. van Veldhoven and A. Fiore: Controlling Spontaneous Emission Beyond the Radiative Lifetime. Optics & Photonics News **25**, 44 (2014).

Jin, C.Y., R. Johne, M.Y. Swinkels, T.B. Hoang, L. Midolo, P.J. van Veldhoven and A. Fiore: Ultrafast non-local control of spontaneous emission. Nature Nanotechnology **9**, 886-890 (2014).

Kammel, R., R. Ackermann, J. Thomas, J. Götte, S. Skupin, A. Tünnermann and S. Nolte: Enhancing precision in fs-laser material processing by simultaneous spatial and temporal focusing. Light- Science & Applications **3**, e169 (2014).

Kimberg, V. and N. Rohringer: X-ray lasing in diatomic molecules. Journal of Physics Conference Series: XXVIII International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC) **488**, 032019 (2014).

Kimberg, V., S.B. Zhang and N. Rohringer: X-ray lasing in diatomic molecules. Journal of Physics Conference Series: XXVIII International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC) **488**, 012025 (2014).

LeBlanc, J.P.F. and J.P. Carbotte: Dielectric screening of surface states in a topological insulator. Physical Review B **89**, 035419 (2014).

Pagliano, F., Y.J. Cho, T. Xia, F. van Otten, R. Johne and A. Fiore Dynamically controlling the emission of single excitons in photonic crystal cavities. Nature Communications **5**, 5786 (2014).

Palatchi, C., J.M Dahlström, A.S. Kheifets, I.A. Ivanov, D.M. Canaday, P. Agostini and L.F. DiMauro: Atomic delay in helium, neon, argon and krypton. Journal of Physics B **47**, 245003 (2014).

Rivière, P., S. Iqbal and J.M. Rost: Electronic excitation by short x-ray pulses: from quantum beats to wave peacket revivals. Journal of Physics B **47**, 124039 (2014).

Siminos, E., G. Sánchez-Arriaga, V. Saxena, and I. Kourakis: Modeling relativistic soliton interactions in overdense plasmas: A perturbed nonlinear Schrödinger equation framework. Physical Review E **90**, 063104 (2014).

Weninger, C. and N. Rohringer: Transient-gain photoionization x-ray laser. Physical Review A **90**, 063828 (2014).

Zhang, S.B. and N. Rohringer: Photoemission spectroscopy with high-intensity short-wavelength lasers. Physical Review A **89**, 013407 (2014).

2015

Albert, J., M. Falge, M. Kess, J.G. Wehner, P.P. Zhang, A. Eisfeld and V. Engel: Extended quantum jump description of vibronic two-dimensional spectroscopy. Journal of Chemical Physics **142**, 4919870 (2015).

Cabrera-Granado, E., Y.X. Chen, I. Babushkin, L. Berge and S. Skupin: Spectral self-action of THz emission from ionizing two-color laser pulses in gases.New Journal of Physics **17**, 023060 (2015).

Chapman, D.A., J. Vorberger, L.B. Fletcher, R.A. Baggott, L. Divol, T. Döppner, R.W. Falcone, S.H. Glenzer, G. Gregori, T.M. Guymer, A.L. Kritcher, O.L. Landen, T. Ma, A.E. Pak and D.O. Gericke: Observation of finite-wavelength screening in high-energy-density matter. Nature Communications **6**, 6839 (2015).

Ciappina, M.F., J.A. Perez-Hernandez, A.S. Landsman, T. Zimmermann, M. Lewenstein, L. Roso and F. Krausz: Carrier-Wave Rabi-Flopping Signatures in High-Order Harmonic Generation for Alkali Atoms. Physical Review Letters **114**, 143902 (2015).

Dietrich, C.P., R. Johne, T. Michalsky, C. Sturm, P. Eastham, H. Franke, M. Lange, M. Grundmann and R. Schmidt-Grund: Parametric relaxation in whispering gallery mode exciton-polariton condensates. Physical Review B **91**, 041202 (2015).

Dimitrovski, D. and L.B. Madsen: Theory of low-energy photoelectrons in strong-field ionization by laser pulses with large ellipticity. Physical Review A **91**, 033409 (2015).

Dimitrovski, D., J. Maurer, H. Stapelfeldt and L.B. Madsen: Observation of low-energy electrons in the photoelectron energy distribution from strong-field ionization of naphthalene by circularly polarized pulses. Journal of Physics B **48**, 121001 (2015).

Dumin, Y.V.: Stark effect in the nonuniform field and its influence on the fine structure of Rydberg blockade. Journal of Physics B **48**, 135002 (2015).

Fletcher, L.B., H.J. Lee, T. Döppner, E. Galtier, B. Nagler, P. Heimann, C. Fortmann, S. LePape, T. Ma, M. Millot, A. Pak, D. Turnbull, D.A. Chapman, D.O. Gericke, J. Vorberger, T. White, G. Gregori, M. Wei, B. Barbrel, R.W. Falcone, C.C. Kao, H. Nuhn, J. Welch, U. Zastrau, P. Neumayer, J.B. Hastings and S.H. Glenzer: Ultrabright X-ray laser scattering for dynamic warm dense matter physics. Nature Photonics **9**, 274–279 (2015).

Freethy, S.J., K.G. McClements, S.C. Chapman, R.O. Dendy, W.N. Lai, S.J.P. Pamela, V.F. Shevchenko and R.G.L. Vann: Electron Kinetics Inferred from Observations of Microwave Bursts During Edge Localized Modes in the Mega-Amp Spherical Tokamak. Physical Review Letters **114**, 125004 (2015).

Gamboa, E.J., L.B. Fletcher, H.J. Lee, U. Zastrau, E. Galtier, M.J. MacDonald, M. Gauthier, J. Vorberger, D.O. Gericke, E. Granados, J.B. Hastings and S.H. Glenzer: Single-shot measurements of plasmons in compressed diamond with an x-ray laser. Physics of Plasmas **22**, 056319 (2015).

He, P.L., N. Takemoto and F. He: Photoelectron momentum distributions of atomic and molecular systems in strong circularly or elliptically polarized laser fields. Physical Review A **91**, 063413 (2015).

Johne, R., R. Schutjens, S.F. Poor, C.Y. Jin and A. Fiore: Control of the electromagnetic environment of a quantum emitter by shaping the vacuum field in a coupled-cavity system. Physical Review A **91**, 063807 (2015).

Jukie, D., T. Pohl, and J.B. Goette: Evanescent fields of laser written waveguides. Proceedings of SPIE - Complex Light and Optical Forces IX **8813**, 93790R (2015).

Klaiber, M. and D. Dimitrovski: Survival of Rydberg atoms in intense laser fields and the role of nondipole effects. Physical Review A **91**, 023401 (2015).

Quelle, A., W. Beugeling and C.M. Smith: Topological Floquet states on a Mobius band irradiated by circularly polarised light. Solid State Communications **215**, 27-33 (2015).

Ritschel, G., D. Suess, S. Möbius, W.T. Strunz and A. Eisfeld: Non-Markovian Quantum State Diffusion for temperature-dependent linear spectra of light harvesting aggregates. Journal of Chemical Physics **142**, 034115 (2015).

Sanchez-Arriaga, G., E. Siminos, V. Saxena and I. Kourakis: Relativistic breather-type solitary waves with linear polarization in cold plasmas. Physical Review E **91**, 033102 (2015).

Schönleber, D.W., A. Eisfeld, M. Genkin, S. Whitlock and S. Wüster: Quantum Simulation of Energy Transport with Embedded Rydberg Aggregates. Physical Review Letters **114**, 123005 (2015).

Singh, K.P. and J.M. Rost: Global control of attosecond photoionization of atoms through XUV dispersion. Physical Review A **91**, 013415 (2015).

Van Bijnen, R.M.W., C. Ravensbergen, D.J. Bakker, G.J. Dijk, S.J.J.M.F. Kokkelmans and E.J.D. Vredenbregt: Patterned Rydberg excitation and ionization with a spatial light modulator. New Journal of Physics **17**, 023045 (2015).

Vorberger, J. and D.O. Gericke: Ab initio approach to model x-ray diffraction in warm dense matter. Physical Review E **91**, 033112 (2015).

4.6 Living Matter

2013

Aprea, J., S. Prenninger, M. Dori, T. Ghosh, L.S. Monasor, E. Wessendorf, S. Zocher, S. Massalini, D. Alexopoulou, M. Lesche, A. Dahl, M. Groszer, M. Hiller and F. Calegari: Transcriptome sequencing during mouse brain development identifies long non-coding RNAs functionally involved in neurogenic commitment. The EMBO Journal **32**, 3145-3160 (2013).

Bai, L., T. Widmann, F. Jülicher, C. Dahmann and D.E. Breen: 3D Surface Reconstruction and Visualization of the Drosophila Wing Imaginal Disc at Cellular Resolution. Proceedings SPIE-IS&T Conference on Electronic Imaging **8654**, 86540D (2013).

Belvisi, S. and E. Venturino: An ecoepidemic model with diseased predators and prey group defense. Simulation Modelling practice and theory **34**, 144-155 (2013).

Bonny, M., E. Fischer-Friedrich, M. Loose, P. Schwille and K, Kruse: Membrane Binding of MinE Allows for a Comprehensive Description of Min-Protein Pattern Formation. PLOS Computational Biology **9**, e1003347 (2013).

Buono, C., F. Vazquez, P.A. Macri and L.A. Braunstein: Slow epidemic extinction in populations with heterogeneous infection rates. Physical Review E **88**, 022813 (2013).

Campinho, P., M. Behrndt, J. Ranft, T. Risler, N. Minc and C.P. Heisenberg: Tension-oriented cell divisions limit anisotropic tissue tension in epithelial spreading during zebrafish epiboly. Nature Cell Biology **15**, 1405-1414 (2013).

Cherstvy, A.G. and V.B. Teif: Structure-driven homology pairing of chromatin fibers: the role of electrostatics and protein-induced bridging. Journal of Biological Physics **39**, 363-385 (2013).

Clark, A.G., K. Dierkes and E.K. Paluch: Monitoring Actin Cortex Thickness in Live Cells. Biophysical Journal **105**, 570-580 (2013).

Coelho, M., A. Dereli, A. Haese, S. Kühn, L. Malinovska, M.E. DeSantis, J. Shorter, S. Alberti, T. Gross and I.M. Tolić-Nørrelykke: Fission Yeast Does Not Age under Favorable Conditions, but Does So after Stress. Current Biology **23**, 1844-1852 (2013).

Del Genio, C.I. and T. House: Endemic infections are always possible on regular networks. Physical Review E **88**, 040801 (2013).

Ercsey-Ravasz, M., N.T. Markov, C. Lamy, D.C. Van Essen, K. Knoblauch, Z. Toroczkai and H. Kennedy: A Predictive Network Model of Cerebral Cortical Connectivity Based on a Distance Rule. Neuron **80**, 184-197 (2013).

Erzberger, A., G. Hampp, A.E. Granada, U. Albrecht and H. Herzel: Genetic redundancy strengthens the circadian clock leading to a narrow entrainment range. Journal of the Royal Society Interface **10**, 20130221 (2013).

Fievet, B.T., J. Rodriguez, S. Naganathan, C. Lee, E. Zeiser, T. Ishidate, M. Shirayama, S. Grill and J. Ahringer: Systematic genetic interaction screens uncover cell polarity regulators and functional redundancy. Nature Cell Biology **15**, 103-U229 (2013).

Fürthauer, S., M. Strempel, S.W. Grill and F. Jülicher: Active Chiral Processes in Thin Films. Physical Review Letters **110**, 048103 (2013).

Geyer, V.F., F. Jülicher, J. Howard and B.M. Friedrich: Cell-body rocking is a dominant mechanism for flagellar synchronization in a swimming alga. Proceedings of the National Academy of Sciences of the United States of America **110**, 18058-18063 (2013).

Goehring N.W and S.W. Grill: Cell polarity: mechanochemical patterning. Trends in Cell Biology **23**, 72-80 (2013).

Hiller, M.: Forward Genomics – ein neuer Ansatz der vergleichenden Sequenzanalyse: Vom Phänotyp zum Genotyp. Biologie in unserer Zeit **43**, 34-39 (2013).

Hiller, M., S. Agarwal, J.H. Notwell, R. Parikh, H. Guturu, A.M. Wenger and G. Bejeranoy: Computational methods to detect conserved non-genic elements in hylogenetically isolated genomes: application to zebrafish. Nucleic Acids Research **41**, 15 e151 (2013).

Kalinina, I., A. Nandi, P. Delivani, M.R. Chacon, A.H. Klemm, D. Ramunno-Johnson, A. Krull, B. Lindner, N. Pavin and I.M. Tolic-Norrelykke: Pivoting of microtubules around the spindle pole accelerates kinetochore capture. Nature Cell Biology **15**, 82-87 (2013).

Kücken, M. and C. Champod: Merkel cells and the individuality of friction ridge skin. Journal of Theoretical Biology **317**, 229-237 (2013).

Lee, C.F., C.P. Brangwynne, J. Gharakhani, A.A. Hyman and F. Jülicher: Spatial Organization of the Cell Cytoplasm by Position-Dependent Phase Separation. Physical Review Letters **111**, 088101 (2013).

Markov, N.T., M. Ercsey-Ravasz, D.C. Van Essen, K. Knoblauch, Z. Toroczkai and H. Kennedy: Cortical High-Density Counterstream Architectures. Science **342**, 1238406 (2013).

Meisel, C., E. Olbrich, O. Shriki and P. Achermann: Fading Signatures of Critical Brain Dynamics during Sustained Wakefulness in Humans. Journal of Neuroscience **33**, 17363-17372 (2013).

Nedelcheva-Veleva, M.N., M. Sarov, I. Yanakiev, E. Mihailovska, M.P. Ivanov, G.C. Panova and S.S. Stoynov: The thermodynamic patterns of eukaryotic genes suggest a mechanism for intron-exon recognition. Nature Communications **4**, 2101 (2013).

Polotzek, K. and B.M. Friedrich: A three-sphere swimmer for flagellar synchronization. New Journal of Physics **15**, 045005 (2013).

Reber, S.B., J. Baumgart, P.O. Widlund, A. Pozniakovsky, J. Howard, A.A. Hyman and F. Jülicher: XMAP215 activity sets spindle length by controlling the total mass of spindle microtubules. Nature Cell Biology **15**, 1116-1122 (2013).

Rosandić, M., V. Paar and M. Glunčić: Fundamental role of start/stop regulators in whole DNA and new trinucleotide classification. Gene **531**, 184-190 (2013).

Sartori, P. and S. Pigolotti: Kinetic versus Energetic Discrimination in Biological Copying. Physical Review Letters **110**, 188101 (2013).

Shen, M., S. Bellaousov, M. Hiller, P. de La Grange, T.P. Creamer, O. Malina, R. Sperling, D.H. Mathews, P. Stoilov and S. Stammand: Pyrvinium pamoate changes alternative splicing of the serotonin receptor 2C by influencing its RNA structure. Nucleic Acids Research **41**, 3819-3832 (2013).

Shi, C., C.-H. Huang, P.N. Devreotes and P.A. Iglesias: Interaction of Motility, Directional Sensing, and Polarity Modules Recreates the Behaviors of Chemotaxing Cells. PLoS Computational Biology **9**, e1003122 (2013).

Szalai, R., A. Champneys, M. Homer, D.O. Maoileidigh, H. Kennedy and N. Cooper: Comparison of nonlinear mammalian cochlear-partition models. Journal of the Acoustical Society of America **133**, 323-336 (2013).

Taktikos, J., H. Stark and V. Zaburdaev: How the Motility Pattern of Bacteria Affects Their Dispersal and Chemotaxis. PLoS One **8**, e81936 (2013).

Theves, M., J. Taktikos, V. Zaburdaev, H. Stark and C. Beta: A Bacterial Swimmer with Two Alternating Speeds of Propagation. Biophysical Journal **105**, 1915-1924 (2013).

Wilking, J.N., V. Zaburdaev, M. De Volder, R. Losick, M.P. Brenner and D.A. Weitz: Liquid transport facilitated by channels in Bacillus subtilis biofilms. PNAS **110**, 848-852 (2013).

2014

Alvarez, L., B.M. Friedrich, G. Gompper and U.B. Kaupp: The computational sperm cell. Trends in Cell Biology **24**, 198-207 (2014).

Bajard, L., L.G. Morelli, S. Ares, J. Pécréaux, F. Jülicher and A.C. Oates: Wnt-regulated dynamics of positional information in zebrafish somitogenesis. Development **141**, 1381-1391 (2014).

Baumgart, J. and B.M. Friedrich: Fluid Dynamics Swimming across scales. Nature Physics **10**, 711-712 (2014).

Bormuth, V., J. Barral, J.F. Joanny, F. Jülicher and P. Martin: Transduction channels' gating can control friction on vibrating hair-cell bundles in the ear. Proceedings of the National Academy of Sciences of the United States of America **111**, 7185-7190 (2014).

Bormuth, V., J. Barral, J.F. Joanny, F. Jülicher and P. Martin: Transduction channels' gating can control friction on vibrating hair-cell bundles in the ear. Biophysical Journal **106**, 243A (2014).

Brugués J. and D. Needleman: Physical basis of spindle self-organization. Proceedings of the National Academy of Sciences of the United States of America **111**, 18496-18500 (2014).

Chan, C.J., G. Whyte, L. Boyde, G. Salbreux and J. Guck: Impact of heating on passive and active biomechanics of suspended cells. Interface Focus **4**, 20130069 (2014).

Ciandrini, L., I. Neri, J.C. Walter, O. Dauloudet and A. Parmeggiani: Motor protein traffic regulation by supply-demand balance of resources. Physical Biology **11**, 056006 (2014).

Clark, A.G., O. Wartlick, G. Salbreux and E.K. Paluch: Stresses at the Cell Surface during Animal Cell Morphogenesis. Current Biology **24**, R484-R494 (2014).

Coelho, M., S.J. Lade, S. Alberti, T. Gross and I.M. Tolic: Fusion of Protein Aggregates Facilitates Asymmetric Damage Segregation. PLoS Biology **12**, e1001886 (2014).

Delarue, M., J.F. Joanny, F. Jülicher and J. Prost: Stress distributions and cell flows in a growing cell aggregate. Interface Focus **4**, 20140033 (2014).

Fischer-Friedrich, E., A.A. Hyman, F. Jülicher, D.J. Müller and J. Helenius: Quantification of surface tension and internal pressure generated by single mitotic cells. Scientific Reports **4**, 6213 (2014).

Friedrich, B. and V. Geyer: Grünalgen wackeln sich in den Takt. Physik in unserer Zeit **45**, 113–114 (2014).

Friedrich, B.M. and I.H. Riedel-Kruse: Row with the flow Fluid forces are sufficient to keep flagella beating in synchrony. eLife **3**, UNSP e03804 (2014).

Fruth, F., F. Jülicher and B. Lindner: An Active Oscillator Model Describes the Statistics of Spontaneous Otoacoustic Emissions. Biophysical Journal **107**, 815-824 (2014).

Gonzalez-Gaitan, M. and F. Jülicher: The Role of Endocytosis during Morphogenetic Signaling. Cold Spring Harbor Perspectives in Biology **6**, a016881 (2014).

Jülicher, F.: Dynamic Organization of Developing Epithelia. Biophysical Journal **106**, 13A (2014).

Ma, R., G.S. Klindt, I.H. Riedel-Kruse, F. Jülicher and B.M. Friedrich: Active Phase and Amplitude Fluctuations of Flagellar Beating. Physical Review Letters **113**, 048101 (2014).

Ma, R., L. Laan, M. Dogterom, N. Pavin and F. Jülicher: General theory for the mechanics of confined microtubule asters. New Journal of Physics **16**, 013018 (2014).

Matsa, E., J.E. Dixon, C. Medway, O. Georgiou, M.J. Patel, K. Morgan, P.J. Kemp, A. Staniforth, I. Mellor and C. Denning: Allele-specific RNA interference rescues the long-QT syndrome phenotype in human-induced pluripotency stem cell cardiomyocytes. European Heart Journal **35**, 1078-1087 (2014).

Merkel, M., A. Sagner, F.S. Gruber, R. Etournay, C. Blasse, E. Myers, S. Eaton and J. Jülicher: The Balance of Prickle/Spiny-Legs Isoforms Controls the Amount of Coupling between Core and Fat PCP Systems. Current Biology **24**, 2111-2123 (2014).

Mukundan, V., P. Sartori, V.F. Geyer, F. Jülicher and J. Howard: Motor Regulation Results in Distal Forces that Bend Partially Disintegrated Chlamydomonas Axonemes into Circular Arcs. Biophysical Journal **106**, 2434-2442 (2014).

Naganathan, S.R., S. Fürthauer, M. Nishikawa, F. Jülicher and S.W. Grill : Active torque generation by the actomyosin cell cortex drives left–right symmetry breaking. eLife Sciences **3**, e04165 (2014).

Needleman, D. and J. Brugues: Determining Physical Principles of Subcellular Organization. Developmental Cell **29**, 135-138 (2014).

Ranft, J., M. Aliee, J. Prost, F. Jülicher and J.F. Joanny: Mechanically driven interface propagation in biological tissues. New Journal of Physics **16**, 035002 (2014).

Soroldoni, D., D.J. Jörg, L.G. Morelli, D.L. Richmond, J. Schindelin, F. Jülicher and A.C. Oates: A Doppler effect in embryonic pattern formation. Science **345**, 6193 (2014).

Szafranski, K., C. Fritsch, F. Schumann, L. Siebel, R. Sinha, J. Hampe, M. Hiller, C. Englert, K. Huse and M. Platzer: Physiological state co-regulates thousands of mammalian mRNA splicing events at tandem splice sites and alternative exons. Nucleic Acids Research **42**, 8895-8904 (2014).

Trong, P.K., E.M. Nicola, N.W. Goehring, K.V. Kumar and S.W. Grill: Parameter-space topology of models for cell polarity. New Journal of Physics **16**, 065009 (2014).

Umetsu, D., B. Aigouy, M. Aliee, L.Y. Sui, S. Eaton, F. Jülicher and C. Dahmann: Local Increases in Mechanical Tension Shape Compartment Boundaries by Biasing Cell Intercalations. Current Biology **24**, 1798-1805 (2014).

Walters, Z.B.: Quantum dynamics of the avian compass. Physical Review E **90**, 042710 (2014).

Wartlick, O., F. Jülicher and M. Gonzalez-Gaitan: Growth control by a moving morphogen gradient during Drosophila eye development. Development **141**, 1884-1893 (2014).

Weitkunat, M., A. Kaya-Çopur, S.W. Grill and F. Schnorrer: Tension and Force-Resistant Attachment Are Essential for Myofibrillogenesis in Drosophila Flight Muscle. Current Biology **24**, 705-716 (2014).

Werner, S., J.C. Rink, I.H. Riedel-Kruse and B.M. Friedrich: Shape mode analysis exposes movement patterns in biology: flagella and flatworms as case studies. PloS One **9**, e113083 (2014).

Yarin, Y.M., A.N. Lukashkin, A. A. Poznyakovskiy, H. Meissner, M. Fleischer, J. Baumgart, C. Richter, E. Kuhlisch and T. Zahnert: Tonotopic Morphometry of the Lamina Reticularis of the Guinea Pig Cochlea with Associated Microstructures and Related Mechanical Implications. JARO **15**, 1-11 (2014).

Zaburdaev, V., N. Biais, M. Schmiedeberg, J. Eriksson, A.B. Jonsson, M.P. Sheetz, and D.A. Weitz: Uncovering the Mechanism of Trapping and Cell Orientation during Neisseria gonorrhoeae Twitching Motility. Biophysical Journal **107**, 1523–1531 (2014).

Zwicker, D., M. Decker, S. Jaensch, A.A. Hyman and F. Jülicher: Centrosomes are autocatalytic droplets of pericentriolar material organized by centrioles. Proceedings of the National Academy of Sciences of the Unites States of America **111**, E2636-E2645 (2014).

2015

Aguilar-Hidalgo, D., M.C. Lemos and A. Cordoba: Core regulatory network motif underlies the ocellar complex patterning in Drosophila melanogaster. Physica D **295**, 91-102 (2015).

Alert, R., J. Casademunt, J. Brugues and P. Sens: Model for Probing Membrane-Cortex Adhesion by Micropipette Aspiration and Fluctuation Spectroscopy. Biophysical Journal **108**, 1878-1886 (2015).

Begasse, M.L., M. Leaver, F. Vazquez, S.W. Grill and A.A. Hyman: Temperature Dependence of Cell Division Timing Accounts for a Shift in the Thermal Limits of C. elegans and C. briggsae. Cell Reports **10**, 647-653 (2015).

Bergert, M., A. Erzberger, R.A. Desai, I.M. Aspalter, A.C. Oates, G. Charras, G. Salbreux and E.K. Paluch: Force transmission during adhesion-independent migration. Nature Cell Biology **17**, 524-529 (2015).

Chou, Y.L. and T. Ihle: Active matter beyond mean-field: Ring-kinetic theory for self-propelled particles. Physical Review E **91**, 022103 (2015).

Dahlem, M.A., B. Schmidt, I. Bojak, S. Boie, F. Kneer, N. Hadjikhani and J. Kurths: Cortical hot spots and labyrinths: why cortical neuromodulation for episodic migraine with aura should be personalized. Frontiers in Computational Neuroscience **9**, 00029 (2015).

Etournay, R., M. Popovic, M. Merkel, A. Nandi, C. Blasse, B. Aigouy, H. Brandl, G. Myers, G. Salbreux, F. Jülicher and S. Eaton: Interplay of Cell Dynamics and Epithelial Tension during Morphogenesis of the Drosophila Pupal Wing. ELife **2015**, doi: 10.7554/eLife.07090 (2015).

Geier, C., S. Bialonski, C.E. Elger and K. Lehnertz: How important is the seizure onset zone for seizure dynamics? Seizure **25**, 160-166 (2015).

Gluncic, M., N. Maghelli, A. Krull, V. Krstic, D. Ramunno-Johnson, N. Pavin and I.M. Tolic: Kinesin-8 Motors Improve Nuclear Centering by Promoting Microtubule Catastrophe. Physical Review Letters **114**, 078103 (2015).

Iomin, A.: Maximum therapeutic effect of glioma treatment by radio-frequency electric field. Chaos Solitons & Fractals **71**, 46-54 (2015).

Mentes, A., A.M. Florescu, E. Brunk, J. Wereszczynski, M. Joyeux and I. Andricioaei: Free-Energy Landscape and Characteristic Forces for the Initiation of DNA Unzipping. Biophysical Journal **108**, 1727-1738 (2015).

Otto, O., P. Rosendahl, A. Mietke, S. Golfier, C. Herold, D. Klaue, S. Girardo, S. Pagliara, A. Ekpenyong, A. Jacobi, M. Wobus, N. Toepfner, U.F. Keyser, J. Mansfeld, E. Fischer-Friedrich and J. Guck: Real-time deformability cytometry: on-the-fly cell mechanical phenotyping. Nature Methods **12**, 199-202 (2015).

Prost, J., F. Jülicher and J.F. Joanny: Active gel physics. Nature Physics **11**, 111-117 (2015).

Saias, L., J. Swoger, A. D'Angelo, P. Hayes, J. Colombelli, J. Sharpe, G. Salbreux and J. Solon: Decrease in Cell Volume Generates Contractile Forces Driving Dorsal Closure. Developmental Cell **33**, 611-621 (2015).

Sain, A., M.M. Inamdar and F. Jülicher: Dynamic Force Balances and Cell Shape Changes during Cytokinesis. Physical Review Letters **114**, 048102 (2015).

Seiden, G. and S. Curland: The tongue as an excitable medium. New Journal of Physics **17**, 033049 (2015).

Theves, M., J. Taktikos, V. Zaburdaev, H. Stark and C. Beta: Random walk patterns of a soil bacterium in open and confined environments. EPL **109** 28007 (2015).

Zandt, B.J., B. ten Haken, M.J.A.M. van Putten, M.A. Dahlem: How does spreading depression spread? Physiology and modeling. Reviews in the Neurosciences **26**, 183–198 (2015).

Zwicker, D., A.A. Hyman and F. Jülicher: Suppression of Ostwald Ripening in Active Emulsions. Physical Review E **92**, 012317 (2015).

4.7 Phase Transitions and Critical Phenomena

2013

Assaad, F.F. and I.F. Herbut: Pinning the Order: The Nature of Quantum Criticality in the Hubbard Model on Honeycomb Lattice. Physical Review X **3**, 031010 (2013).

Benhouria, Y., I. Essaoudi, A. Ainane, M. Saber, R. Ahuja, F. Dujardin: Monte Carlo Study of Long-Range Interactions of a Ferroelectric Bilayer with Antiferroelectric Interfacial Coupling. Journal of Superconductivity and Novel Magnetism **26**, 3075-3083 (2013).

Bird, J., R. Kaiser, I. Rotter and G. Wunner: Preface: Quantum Physics with Non-Hermitian Operators: Theory and Experiment. Fortschritte der Physik/ Progress of Physics **61**, 57 - 58 (2013).

Böhme, G. A.: Emergence and persistence of diversity in complex networks. The European Physical Journal Special Topics **222**, 3089-3169 (2013).

Bouhou, S., I. Essaoudi, A. Ainane, M. Saber, R. Ahuja and F. Dujardin: Phase diagrams of diluted transverse Ising nanowire. Jounal of Magnetism and Magnetic Materials **336**, 75-82 (2013).

Bouhou, S., A. Zaim, A. Ainane, M. Kerouad and R. Ahuja: Magnetic properties of a ferromagnetic thin film with four spin interaction: A Monte Carlo simulation study. Journal of Magnetism and Magnetic Materials **339**, 127-132 (2013).

Chen, L., F. Ghanbarnejad, W. Cai, and P. Grassberger: Outbreaks of confections: the critical role of cooperativity. EPL **104**, 50001 (2013).

Eleuch, H. and I. Rotter: Avoided level crossings in open quantum systems. Fortschritte der Physik/ Progress of Physics **61**, 194-204 (2013).

Eleuch, H. and I. Rotter: Width bifurcation and dynamical phase transitions in open quantum systems. Physical Review E **87**, 052136 (2013).

Hsu, B., C.R. Laumann, A.M. Läuchli, R. Moessner and S.L. Sondhi: Approximating random quantum optimization problems. Physical Review A **87**, 062334 (2013).

Huang, C.-Y., X. Chen and F.-L. Lin: Symmetry-protected quantum state renormalization. Physical Review B **88**, 205124 (2013).

Jin, S., A. Sen, W. Guo and A.W. Sandvik: Phase transitions in the frustrated Ising model on the square lattice. Physical Review B **87**, 144406 (2013).

Männel, M., K. Morawetz and P. Lipavský: Coexistence of phase transitions and hysteresis near the onset of Bose-Einstein condensation. Physical Review A **87**, 053617 (2013).

Pixley, J.H., S. Kirchner, K. Ingersent and Q. Si: Quantum criticality in the pseudogap Bose-Fermi Anderson and Kondo models: Interplay between fermion- and boson-induced Kondo destruction. Physical Review B **88**, 245111 (2013).

Popkov, V.: Boundary-driven phase transitions in open driven systems with an umbilic point. European Physical Journal **216**, 139-151 (2013).

Prosen, T., E. Ilievski and V. Popkov: Exterior integrability: Yang-Baxter form of non-equilibrium steady-state density operator. New Journal of Physics **15**, 073051 (2013).

Ribeiro, P., Q. Si and S. Kirchner: Local quantum criticality out of equilibrium: Effective temperatures and scaling in the steady-state regime. EPL **102**, 50001 (2013).

Sen, A., R. Moessner and S.L. Sondhi: Coulomb Phase Diagnostics as a Function of Temperature, Interaction Range, and Disorder. Physical Review Letters **110**, 107202 (2013).

Vorberger, J., D.O. Gericke and W.-D. Kraeft: The equation of state for hydrogen at high densities. High Energy Density Physics **9**, 448-456 (2013).

Wang, H.J., L. Chen, C. Qiu, H.B. Huang and G.X. Qi: Time-delay-induced synchronization in complex networks: Exploring the dynamical mechanism. EPL **101**, 60002 (2013).

Zamani, F., T. Chowdhury, P. Ribeiro, K. Ingersent and S. Kirchner: Quantum criticality in the two-channel pseudogap Anderson model: A test of the non-crossing approximation. Physica Status Solidi B **250**, 547-552 (2013).

2014

Aschwanden, M.J., N.B. Crosby, M. Dimitropoulou, M.K. Georgoulis, S. Hergarten, J. McAteer, A.V. Milovanov, S. Mineshige, L. Morales, N. Nishizuka, G. Pruessner, R. Sanchez, A.S. Sharma, A. Strugarek and V. Uritsky: 25 Years of Self-Organized Criticality: Solar and Astrophysics. Space Science Reviews, DOI 10.1007/s11214-014-0054-6 (2014).

Bastidas, V.M., G. Engelhardt, P. Pérez-Fernández, M. Vogl, and T. Brandes: Critical quasienergy states in driven many-body systems. Physical Review A **90**, 063628 (2014).

Basu U. and P.K. Mohanty: Self-organised criticality in stochastic sandpiles: Connection to directed percolation. EPL **108**, 60002 (2014).

Benhouria, Y., I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin: Dielectric Properties and Hysteresis Loops of a Ferroelectric Nanoparticle System Described by the Transverse Ising Model. Journal of Superconductivity and Novel Magnetism **27**, 2153-2162 (2014).

Benhouria, Y., I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin: The dielectric properties and the hysteresis loops of the spin-1 Ising nanowire system with the effect of a negative core/shell coupling: A Monte Carlo study. Superlattices and Microstructures **73**, 121-135 (2014).

Benhouria, Y., I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin: Thermodynamic properties and hysteresis behaviors of a mixed spin-3/2 and spin-1/2 Ising double walled ferrielectric nanotubes: A Monte Carlo study. Superlattices and Microstructures **75**, 761-774 (2014).

Budkov, Y.A., I.I. Vyalov, A.L. Kolesnikov, N. Georgi, G.N. Chuev and M.G. Kiselev: The local phase transitions of the solvent in the neighborhood of a solvophobic polymer at high pressures. Journal of Chemical Physics **141**, 204904 (2014).

Buerschaper, O., S.C. Morampudi and F. Pollmann: Double semion phase in an exactly solvable quantum dimer model on the kagome lattice. Physical Review B **90**, 195148 (2014).

Chang, J., I. Eremin and J.Z. Zhao: Model of nonadiabatic-to-adiabatic dynamical quantum phase transition in photoexcited systems. Physical Review B **90**, 104305 (2014).

Eleuch, H. and I. Rotter: Exceptional Points in Open and PT-Symmetric Systems. Acta Polytechnica **54**, 106–112 (2014).

Eleuch, H., I. Rotter: Open quantum systems and Dicke superradiance. European Physical Journal D **68**, 74 (2014).

Gross, T., A.L. Do, F. Droste, and C. Meisel: Mechanisms of Self-Organized Criticality in adaptive networks. In: Criticality in Neural Systeme. D. Plenz, E. Niebur, H.G. Schuter (Eds.). Weinheim: Wiley, 2014. 393–402.

Gulacsi, M.: Non-local correlations in the one-dimensional Anderson lattice. Philosophical Magazine Letters **94**, 319-326 (2014).

Hauser, M.J.B. and J.A.C. Gallas: Nonchaos-Mediated Mixed-Mode Oscillations in an Enzyme Reaction System. Journal of Physical Chemistry Letters **23**, 4187-4193 (2014).

Hoening, M., W. Abdussalam, M. Fleischhauer and T. Pohl: Antiferromagnetic long-range order in dissipative Rydberg lattices. Physical Review A **90**, 021603 (2014).

Janssen, L. and I.F. Herbut: Antiferromagnetic critical point on graphene's honeycomb lattice: A functional renormalization group approach. Physical Review B **89**, 205403 (2014).

Li, G., A.E. Antipov, A.N. Rubtsov, S.Kirchner and W. Hanke: Competing phases of the Hubbard model on a triangular lattice: Insights from the entropy. Physical Review B **89**, 161118 (2014).

Morampudi, S.C., C. von Keyserlingk and F. Pollmann: Numerical study of a transition between Z_2 topologically ordered phases. Physical Review B **90**, 035117 (2014).

Si, Q.M., J.H. Pixley, E. Nica, S.J. Yamamoto, P. Goswami, R. Yu and S. Kirchner: Kondo Destruction and Quantum Criticality in Kondo Lattice Systems. Journal of the Physical Society of Japan **83**, 061005 (2014).

Steglich, F., H. Pfau, S. Lausberg, S. Hamann, P.J. Sun, U. Stockert, M. Brando, S. Friedemann, C. Krellner, C. Geibel, S. Wirth, S. Kirchner, E. Abrahams and Q.M. Si: Evidence of a Kondo Destroying Quantum Critical Point in $YbRh_2Si_2$. Journal of the Physical Society of Japan **83**, 061001 (2014).

Wittmann, M. and A.P. Young: Finite-size scaling above the upper critical dimension. Physical Review E **90**, 062137 (2014).

Zhitomirsky, M.E., P.C.W. Holdsworth and R. Moessner: Nature of finite-temperature transition in anisotropic pyrochlore $Er_2Ti_2O_7$. Physical Review B **89**, 140403 (2014).

2015

Bassler, K.E., W. Liu, B. Schmittmann and R.K.P. Zia: Extreme Thouless effect in a minimal model of dynamic social networks. Physical Review E **91**, 042102 (2015).

Bouhou, S., I. Essaoudi, A. Ainane, A. Oubelkacem, R. Ahuja and F. Dujardin: Magnetic Properties of a Transverse Ising Nanoparticle. Journal of Superconductivity and Novel Magnetism **28**, 885-890 (2015).

Chen, L.M., J. Toner and C.F. Lee: Critical phenomenon of the order-disorder transition in incompressible active fluids. New Journal of Physics **17**, 042002 (2015).

Daga, B. and P.K. Mohanty: Phase separation transition of reconstituting k-mers in one dimension. Journal of Statistical Mechanics - Theory and Experiment **2015**, P04004 (2015).

Langari, A., A. Mohammad-Aghaei, and R. Haghshenas: Quantum phase transition as an interplay of Kitaev and Ising interactions. Physical Review B **91**, 024415 (2015).

Oubelkacem, A., I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin: The Magnetic Properties of Multi-surface Transverse Ferroelectric Ising Thin Films. Journal of Superconductivity and Novel Magnetism **28**, 877-883 (2015).

Oubelkacem, A., I. Essaoudi, A. Ainane, F. Dujardin and R. Ahuja: Effect of Seeding Layers on Hysteresis Loops and Phase Transition of the Ferroelectric Thin Film. Ferroelectrics **478**, 1-10 (2015).

Roychowdhury, K. and C.Y. Huang: Tensor renormalization group approach to classical dimer models. Physical Review B **91**, 205418 (2015).

Schauß, P., J. Zeiher, T. Fukuhara, S. Hild, M. Cheneau, T. Macrì, T. Pohl, I. Bloch and C. Gross: Crystallization in Ising quantum magnets. Science **347**, 1455-1458 (2015).

Zaletel, M.P., R.S.K. Mong, F. Pollmann and E.H. Rezayi: Infinite density matrix renormalization group for multicomponent quantum Hall systems. Physical Review B **91**, 045115 (2015).

4.8 Semiclassics and Chaos in Quantum Systems

2013

Götte, J., M. Hentschel and W. Löffler: Beyond catoptrics. Journal of Optics **15**, 010301 (2013).

Götte, J.B., S. Shinohara and M. Hentschel: Are Fresnel filtering and the angular Goos-Hanchen shift the same? Journal of Optics **15**, 014009 (2013).

Goussev, A.: Diffraction in time: An exactly solvable model. Physical Review A **87**, 053621 (2013).

Goussev, A. and K. Richter: Scattering of quantum wave packets by shallow potential islands: A quantum lens. Physical Review E **87**, 052918 (2013).

Körber, M.J., M. Michler, A. Bäcker and R. Ketzmerick: Hierarchical Fractal Weyl Laws for Chaotic Resonance States in Open Mixed Systems. Physical Review Letters **111**, 114102 (2013).

Kotik, D. and M. Hentschel: How curvature affects the far-field emission from deformed optical microcavities. Journal of Optics **15**, 014010 (2013).

Kwon, T.-Y., S.-Y. Lee, J.-W. Ryu and M. Hentschel: Phase-space analysis of lasing modes in a chaotic microcavity. Physical Review A **88**, 023855 (2013).

Le Deunff, J., A. Mouchet and P. Schlagheck: Semiclassical description of resonance-assisted tunneling in one-dimensional integrable models. Physical Review E **88**, 042927 (2013).

Löbner, C., S. Löck, A. Bäcker and R. Ketzmerick: Integrable approximation of regular islands: The iterative canonical transformation method. Physical Review E **88**, 062901 (2013).

Mertig, N., S. Löck, A. Bäcker, R. Ketzmerick and A. Shudo: Complex paths for regular-to-chaotic tunnelling rates. EPL **102**, 10005 (2013).

Popkov, V. and R. Livi: Manipulating energy and spin currents in non-equilibrium systems of interacting qubits. New Journal of Physics **15**, 023030 (2013).

Rüegg, A., E. Gull, G.A. Fiete and A.J. Millis: Sum rule violation in self-consistent hybridization expansions. Physical Review B **87**, 075124 (2013).

2014

Ahnert K., D. Demidov and M. Mulansky: Solving Ordinary Differential Equations on GPUs. In: Numerical Computations with GPUs. Cham: Springer, 2014. 125-157.

Bittrich, L., A. Bäcker and R. Ketzmerick: Temporal flooding of regular islands by chaotic wave packets. Physical Review E **89**, 032922 (2014).

Dubertrand, R. and A.Goussev: Origin of the exponential decay of the Loschmidt echo in integrable systems. Physical Review E **89**, 022915 (2014).

Lee, S.Y., J.Le Deunff, M. Choi and R.Ketzmerick: Quantum Goos-Hanchen shift and tunneling transmission at a curved step potential. Physical Review A **89** 022120 (2014).

Ribeiro, P. and A.M. García-García: Interplay of classical and quantum capacitance in a one-dimensional array of Josephson junctions. Physical Review B **89**, 064513 (2014).

Singh, R., R. Kunjwal and R. Simon: Relative volume of separable bipartite states. Physical Review A **89**, 022308 (2014).

2015

Beugeling, W., A. Andreanov and M. Haque: Global characteristics of all eigenstates of local many-body Hamiltonians: participation ratio and entanglement entropy. Journal of Statistical Mechanics - Theory and Experiment **2015**, P02002 (2015).

Beugeling, W., R. Moessner and M. Haque: Off-diagonal matrix elements of local operators in many-body quantum systems. Physical Review E **91**, 012144 (2015).

Fyodorov, Y.V. and D.V. Savin: Resonance width distribution in RMT: Weak-coupling regime beyond Porter-Thomas. EPL **110**, 40006 (2015).

Schönwetter, M. and E.G. Altmann: Quantum signatures of classical multifractal measures. Physical Review E **91**, 012919 (2015).

Srivastava, S.C.L. and A. Lakshminarayanb: Records in the classical and quantum standard map. Chaos, Solitons & Fractals **74**, 67–78 (2015).

Zambrano, E., W.P. Karel Zapfe and A.M. Ozorio de Almeida: Local quantum ergodic conjecture. Physical Review E **91**, 042911 (2015).

4.9 Stochastic Processes

2013

Altmann, E.G., Z.L. Whichard and A.E. Motter: Identifying Trends in Word Frequency Dynamics. Journal of Statistical Physics **151**, 277-288 (2013).

Amancio, D.R., E.G. Altmann, D. Rybski, O.N. Oliveira Jr. and L. da F. Costa: Probing the Statistical Properties of Unknown Texts: Application to the Voynich Manuscript. PLoS One **8**, e67310 (2013).

Bauermeister, C., T. Schwalger, D.F. Russell, A.B. Neiman and B. Lindner: Characteristic Effects of Stochastic Oscillatory Forcing on Neural Firing: Analytical Theory and Comparison to Paddlefish Electroreceptor Data. PLoS Computational Biology **9**, e1003170 (2013).

Ben-Naim, E., N.W. Hengartner, S. Redner and F. Vazquez: Randomness in Competitions. Journal of Statistical Physics **151**, 458-474 (2013).

Chechkin, A.V., I.M. Zaid, M.A. Lomholt, I.M. Sokolov and R. Metzler: Bulk-mediated Surface Diffusion on a Cylinder in the Fast Exchange Limit. Mathematical Modelling of Natural Phenomena **8**, 114-126 (2013).

Chepizhko, O., E.G. Altmann and F. Peruani: Optimal Noise Maximizes Collective Motion in Heterogeneous Media. Physical Review Letters **110**, 238101 (2013).

Denisov, S.I., Yu.S. Bystrik and H. Kantz: Limiting distributions of continuous-time random walks with superheavy-tailed waiting times. Physical Review E **87**, 022117 (2013).

Gerlach, M. and E.G. Altmann: Stochastic Model for the Vocabulary Growth in Natural Languages. Physical Review X **3**, 021006 (2013).

Lenz, F., A.V. Chechkin and R. Klages: Constructing a Stochastic Model of Bumblebee Flights from Experimental Data. PLoS One **8**, e59036 (2013).

Niemann, M., H. Kantz and E. Barkai: Fluctuations of 1/f Noise and the Low-Frequency Cutoff Paradox. Physical Review Letters **110**, 140603 (2013).

Schulz, J.H.P., A.V. Chechkin and R. Metzler: Correlated continuous time random walks: combining scale-invariance with long-range memory for spatial and temporal dynamics. Journal of Physics A **46**, 475001 (2013).

Taloni, A., A. Chechkin and J. Klafter: Generalized Elastic Model: Fractional Langevin Description, Fluctuation Relation and Linear Response. Mathematical Modelling of Natural Phenomena **8**, 127-143 (2013).

Vincent, U.E., B.R. Nana-Nbendjo and P.V.E. McClintock: Collective dynamics of a network of ratchets coupled via a stochastic dynamical environment. Physical Review E **87**, 022913 (2013).

Vlaming, S.M., V.A. Malyshev, A. Eisfeld and J.Knoester: Subdiffusive exciton motion in systems with heavy-tailed disorder. Journal of Chemical Physics **138**, 214316 (2013).

Zaburdaev, V., S. Denisov and P. Hänggi: Space-Time Velocity Correlation Function for Random Walks. Physical Review Letters **110**, 170604 (2013).

2014

Bagchi, D. and P.K. Mohanty: A microscopic model of ballistic-diffusive crossover. Journal of Statistical Mechanics, P11025 (2014).

Batac, R.C. and H. Kantz: Observing spatio-temporal clustering and separation using interevent distributions of regional earthquakes. Nonlinear Processes in Geophysics **21**, 735-744 (2014).

Chapman, S.C., R.O. Dendy, T.N. Todd, N.W. Watkins, A.J. Webster, F. Calderon, J. Morris and JET EFDA Contributors: Relationship of edge localized mode burst times with divertor flux loop signal phase in JET. Physics of Plasmas **21**, 062302 (2014).

Chapman, S.C., R.O. Dendy, A.J. Webster, N.W. Watkins, T.N. Todd, J. Morris and JET EFDA Contributors: An apparent relation between ELM occurrence times and the prior phase evolution of divertor flux loop measurements in JET. EPS-41st EPS Conference on Plasma Physics **38**, P1.00 (2014).

Chechkin, A.V. and I. Pavlyukevich: Marcus versus Stratonovich for systems with jump noise. Journal of Physics A **47**, 342001 (2014).

Cherstvy, A.G., A.V. Chechkin and R. Metzler: Ageing and confinement in non-ergodic heterogeneous diffusion processes. Journal of Physics A **47**, 485002 (2014).

Cherstvy, A.G., A.V. Chechkin and R. Metzler: Particle invasion, survival, and non-ergodicity in 2D diffusion processes with space-dependent diffusivity. Soft Matter **10**, 1591-1601 (2014).

Demirel, G., F. Vazquez, G.A. Böhme and T. Gross: Moment-closure approximations for discrete adaptive networks. Physica D **267**, 68-80 (2014).

Gaveau, B., L. Granger, M. Moreau and L.S. Schulman: Dissipation, interaction, and relative entropy. Physical Review E **89**, 032107 (2014).

Gaveau, B., L. Granger, M. Moreau and L.S. Schulman: Relative Entropy, Interaction Energy and the Nature of Dissipation. Entropy **16**, 3173-3206 (2014).

Gerlach, M. and E.G. Altmann: Scaling laws and fluctuations in the statistics of word frequencies. New Journal of Physics **16**, 113010 (2014).

Ghanbarnejad, F., M. Gerlach, J.M. Miotto and E.G. Altmann: Extracting information from S-curves of language change. Journal of the Royal Society Interface **11**, 20141044 (2014).

Godec, A., A.V. Chechkin, E. Barkai, H. Kantz and R. Metzler: Localisation and universal fluctuations in ultraslow diffusion processes. Journal of Physics A **47**, 492002 (2014).

Gundermann, J., S. Siegert and H. Kantz: Improved predictions of rare events using the Crooks fluctuation theorem. Physical Review E **89**, 032112 (2014).

Hossein, S., M.D. Reichl and K.E. Bassler: Symmetry in critical random Boolean network dynamics. Physical Review E **89**, 042804 (2014).

Jeon, J.H., A.V. Chechkin and R. Metzler: First Passage Behavior of Multi-Dimensional Fractional Brownian Motion and Application to Reaction Phenomena. In: First Passage Phenomena and Their Applications. R. Metzler, G. Oshanin, S. Redner (Eds:). Singapore: World Scientific, 2014. S. 175-202.

Jeon, J.H., A.V. Chechkin and R. Metzler: Scaled Brownian motion: a paradoxical process with a time dependent diffusivity for the description of anomalous diffusion. Physical Chemistry Chemical Physics **16**, 15811-15817 (2014).

Kaiser, V. and T. Novotný: Loop exponent in DNA bubble dynamics. Journal of Physics A **47**, 315003 (2014).

Leitao, J.C., J.M.V.P. Lopes and E.G. Altmann: Efficiency of Monte Carlo sampling in chaotic systems. Physical Review E **90**, 052916 (2014).

Miotto, J.M. and E.G. Altmann: Predictability of Extreme Events in Social Media. PLoS One **9**, e111506 (2014).

Ndemanou, B.P., J. Metsebo, B.R. Nana Nbendjo and P. Woafo: Dynamics and magneto-rheological control of vibration of cantilever Timoshenko beam under earthquake loads. Nonlinear Dynamics **78**, 163-171 (2014).

Nezhadhaghighi, M.G., A. Chechkin and R. Metzler: Numerical approach to unbiased and driven generalized elastic model. Journal of Chemical Physics **140**, 024106 (2014).

Palyulin, V.V., A.V. Chechkin and R. Metzler: Lévy flights do not always optimize random blind search for sparse targets. PNAS **111**, 2931-2936 (2014).

Palyulin, V.V., A.V. Chechkin and R. Metzler: Space-fractional Fokker-Planck equation and optimization of random search processes in the presence of an external bias. Journal of Statistical Mechanics, P11031 (2014).

Suess, D., A. Eisfeld and W.T. Strunz: Hierarchy of Stochastic Pure States for Open Quantum System Dynamics. Physical Review Letters **113**, 150403 (2014).

Vitanov, N.K., N.P. Hoffmann and B. Wernitz: Nonlinear time series analysis of vibration data from a friction brake: SSA, PCA, and MFDFA. Chaos Solitons & Fractals **69**, 90-99 (2014).

2015

Chatterjee, S., P. Pradhan and P.K. Mohanty: Zeroth law and nonequilibrium thermodynamics for steady states in contact. Physical Review E **91**, 062136 (2015).

Deluca, A., N.R. Moloney and A. Corral: Data-driven prediction of thresholded time series of rainfall and self-organized criticality models. Physical Review E **91**, 052808 (2015).

Erdös, P.L., I Miklós and Z. Toroczkai: A Decomposition Based Proof for Fast Mixing of a Markov Chain over Balanced Realizations of a Joint Degree Matrix. SIAM Journal on Discrete Mathematics **29**, 481–499 (2015).

Font-Clos, F., G. Pruessner, N.R. Moloney and A. Deluca: The perils of thresholding. New Journal of Physics **17**, 043066 (2015).

Franzke, C.L.E., S.M. Osprey, P. Davini and N.W. Watkins: A Dynamical Systems Explanation of the Hurst Effect and Atmospheric Low-Frequency Variability. Scientific Reports **5**, 9068 (2015).

Froemberg, D., M. Schmiedeberg, E. Barkai and V. Zaburdaev: Asymptotic densities of ballistic Lévy walks. Physical Review E **91**, 022131 (2015).

Höll, M. and H. Kantz: The fluctuation function of the detrended fluctuation analysis - investigation on the AR(1) process. European Physical Journal B **88**, 126 (2015).

Kollmer, J.E., T. Pöschel and J.A.C. Gallas: Are physicists afraid of mathematics? New Journal of Physics **17**, 013036 (2015).

Maksymenko, M., R. Moessner and K. Shtengel: Reversible first-order transition in Pauli percolation. Physical Review E **91**, 062103 (2015).

Martinez, I.A., E. Roldan, L. Dinis, D. Petrov and R.A. Rica: Adiabatic Processes Realized with a Trapped Brownian Particle. Physical Review Letters **114**, 120601 (2015).

Romanczuk, P. and G. Salbreux: Optimal chemotaxis in intermittent migration of animal cells. Physical Review E **91**, 042720 (2015).

Sandev, T., A. Iomin and H. Kantz: Fractional diffusion on a fractal grid comb. Physical Review E **91**, 032108 (2015).

Saxena, R.K., Z. Tomovski and T. Sandev: Analytical solution of generalized space-time fractional cable equation. Mathematics **3**, 153-170 (2015).

Shin, J., A.G. Cherstvy and R. Metzler: Polymer Looping Is Controlled by Macromolecular Crowding, Spatial Confinement, and Chain Stiffness. ACS Macro Letters **4**, 202-206 (2015).

Sliusarenko, O.Y., A.V. Chechkin and Y.V. Slyusarenko: The Bogolyubov-Born-Green-Kirkwood-Yvon hierarchy and Fokker-Planck equation for many-body dissipative randomly driven systems. Journal of Mathematical Physics **56**, 043302 (2015).

Suess, D., W.T. Strunz and A. Eisfeld: Hierarchical Equations for Open System Dynamics in Fermionic and Bosonic Environments. Journal of Statistical Physics **159**, 1408-1423 (2015).

Watkins, N.W., G. Pruessner, S.C. Chapman, N.B. Crosby and H.J. Jensen: 25 Years of Self-organized Criticality: Concepts and Controversies. Space Science Reviews **5**, doi: 10.1007/s11214-015-0155-x (2015).

Wylomanska, A., A. Chechkin, J. Gajda and I.M. Sokolov: Codifference as a practical tool to measure interdependence. Physica A **42**, 412-429 (2015).

Yano, J.I., J.F. Geleyn, M. Köhler, D. Mironov, J. Quaas, P.M.M. Soares, V.T.J. Phillips, R.S. Plant, A. Deluca, P. Marquet, L. Stulic and Z. Fuchs: Basic Concepts for Convection Parameterization in Weather Forecast and Climate Models: COST Action E50905 Final Report. Atmosphere **6**, 88-147 (2015).

Zaburdaev, V., S. Denisov and J. Klafter: Levy walks. Reviews of Modern Physics **87**, 483-530 (2015).

4.10 Strongly Correlated Electrons

2013

Babichenko, V.S. and I.Y. Polishchuk: Coulomb correlations and electron-hole liquid in double quantum wells. JETP Letters **97**, 628-633 (2013).

Cayssol, J., B. Dóra, F. Simon and R. Moessner: Floquet topological insulators. Physica Status Solidi RRL **7**, 101-108 (2013).

Depenbrock, S. and F. Pollmann: Phase diagram of the isotropic spin-3/2 model on the z=3 Bethe lattice. Physical Review B **88**, 035138 (2013).

Dóra, B., I.F. Herbut and R. Moessner: Coupling, merging, and splitting Dirac points by electron-electron interaction. Physical Review B **88**, 075126 (2013).

Dora, B., F. Pollmann, J. Fortágh and G. Zaránd: Loschmidt Echo and the Many-Body Orthogonality Catastrophe in a Qubit-Coupled Luttinger Liquid. Physical Review Letters **111**, 046402 (2013).

Dyugaev, A.M., P.D. Grigoriev and E.V. Lebedeva: Ground-state energy of quantum liquids. JETP Letters **98**, 33-37 (2013).

Jaubert, L.D.C., M.J. Harris, T. Fennell, R.G. Melko, S.T. Bramwell and P.C.W. Holdsworth: Topological-Sector Fluctuations and Curie-Law Crossover in Spin Ice. Physical Review X **3**, 011014 (2013).

Kjäll, J.A., M.P. Zaletel, R.S.K. Mong, J.H. Bardarson and F. Pollmann: Phase diagram of the anisotropic spin-2 XXZ model: Infinite-system density matrix renormalization group study. Physical Review B **87**, UNSP 235106 (2013).

Kovrizhin, D.L., B. Doucot and R. Moessner: Multicomponent Skyrmion Lattices and Their Excitations. Physical Review Letters **110**, 186802 (2013).

Langari, A., F. Pollmann and M. Siahatgar: Ground-state fidelity of the spin-1 Heisenberg chain with single ion anisotropy: quantum renormalization group and exact diagonalization approaches. Journal of Physics - Condensed Matter **25**, 406002 (2013).

Läuchli, A.M., Z. Liu, E.J. Bergholtz and R. Moessner: Hierarchy of Fractional Chern Insulators and Competing Compressible States. Physical Review Letters **111**, 126802 (2013).

LeBlanc, J.P.F. and E. Gull: Equation of state of the fermionic two-dimensional Hubbard model. Physical Review B **88**, 155108 (2013).

Miloshevich, G., T. Dauxois, R. Khomeriki and S. Ruffo: Dipolar needles in the microcanonical ensemble: Evidence of spontaneous magnetization and ergodicity breaking. EPL **104**, 17011 (2013).

Morawetz, K.: Quasiparticle parametrization of mean fields, Galilei invariance, and universal conserving response functions. Physical Review E **88**, 022148 (2013).

Motruk, J., E. Berg, A.M. Turner and F. Pollmann: Topological phases in gapped edges of fractionalized systems. Physical Review B **88**, 085115 (2013).

Munoz, E., C.J. Bolech and S. Kirchner: Comment on "Universal Out-of-Equilibrium Transport in Kondo-Correlated Quantum Dots: Renormalized Dual Fermions on the Keldysh Contour" Reply. Physical Review Letters **111**, 089702 (2013).

Petrova, O., P. Mellado and O. Tchernyshyov: Unpaired Majorana modes in the gapped phase of Kitaev's honeycomb model. Physical Review B **88**, 140405 (2013).

Pollmann, F., M. Haque and B. Dora: Linear quantum quench in the Heisenberg XXZ chain: Time-dependent Luttinger-model description of a lattice system. Physical Review B **87**, 041109 (2013).

Roy, B. and I.F. Herbut: Topological insulators in strained graphene at weak interaction. Physical Review B **88**, 045425 (2013).

Seabra, L. and F. Pollmann: Exotic Ising dynamics in a Bose-Hubbard model. Physical Review B **88**, 125103 (2013).

Toldin, F.P., J. Figgins, S. Kirchner and D.K. Morr: Disorder and quasiparticle interference in heavy-fermion materials. Physical Review B **88**, 081101 (2013).

Udagawa, M. and R. Moessner: Anomalous Hall Effect from Frustration-Tuned Scalar Chirality Distribution in $Pr_2Ir_2O_7$. Physical Review Letters **111**, 036602 (2013).

Zaletel, M.P., R.S.K. Mong and F. Pollmann: Topological Characterization of Fractional Quantum Hall Ground States from Microscopic Hamiltonians. Physical Review Letters **110**, 236801 (2013).

Zvyagin, A.A.: Possibility of Direct Observation of Edge Majorana Modes in Quantum Chains. Physical Review Letters **110**, 217207 (2013).

2014

Antipov, A.E., E. Gull and S. Kirchner: Critical Exponents of Strongly Correlated Fermion Systems from Diagrammatic Multiscale Methods. Physical Review Letters **112**, 226401 (2014).

Beugeling, W., R. Moessner and M. Haque: Finite-size scaling of eigenstate thermalization. Physical Review E **89**, 042112 (2014).

Braak, D., J.M. Zhang and M. Kollar: Integrability and weak diffraction in a two-particle Bose-Hubbard model. Journal of Physics A **47**, 465303 (2014).

Daoud, M., R.A. Laarriara and W. Kaydi: Unified scheme for correlations using linear relative entropy. Physics Letters A **378**, 3501-3508 (2014).

Dóra, B., I.F. Herbut and R. Moessner: Occurrence of nematic, topological, and Berry phases when a flat and a parabolic band touch. Physical Review B **90**, 045310 (2014).

Ghosh, S., P. Ribeiro and M. Haque: Real-space structure of the impurity screening cloud in the resonant level model. Journal of Statistical Mechanics, P04011 (2014).

Grimmer, D., A. Safavi-Naini, B. Capogrosso-Sansone and Ş.G. Söyler: Quantum phases of dipolar soft-core bosons. Physical Review A **90**, 043635 (2014).

Haghshenas, R., A. Langari and A.T. Rezakhani: Symmetry fractionalization: symmetry-protected topological phases of the bond-alternating spin-1/2 Heisenberg chain. Journal of Physics-Condensed Matter **26**, 456001 (2014).

Halász, G.B., J.T. Chalker and R. Moessner: Doping a topological quantum spin liquid: Slow holes in the Kitaev honeycomb model. Physical Review B **90**, 035145 (2014).

Hermanns, M., Y. Salimi, M. Haque and L. Fritz: Entanglement spectrum and entanglement Hamiltonian of a Chern insulator with open boundaries. Journal of Statistical Mechnics-Theory and Experiment, P10030 (2014).

Hozoi, L., H. Gretarsson, J.P. Clancy, B.G. Jeon, B. Lee, K.H. Kim, V. Yushankhai, P. Fulde, D. Casa, T. Gog, J. Kim, A.H. Said, M.H. Upton,Y.J. Kim and J. van den Brink: Longer-range lattice anisotropy strongly competing with spin-orbit interactions in pyrochlore iridates. Physical Review B **89**, 115111 (2014).

Kanungo, S., B.H. Yan, M. Jansen and C.Felser: Ab initio study of low-temperature magnetic properties of double perovskite Sr_2FeOsO_6. Physical Review B **89**, 214414 (2014).

Katukuri, V.M., K. Roszeitis, V. Yushankhai, A. Mitrushchenkov, H. Stoll, M. van Veenendaal, P. Fulde, J. van den Brink and I. Hozoi: Electronic Structure of Low-Dimensional $4d_5$ Oxides: Interplay of Ligand Distortions, Overall Lattice Anisotropy, and Spin-Orbit Interactions. Inorganic Chemistry **53**, 4833-4839 (2014).

Khuntia, P., P. Peratheepan, A.M. Strydom, Y. Utsumi, K.T. Ko, K.D. Tsuei, L.H. Tjeng, F. Steglich and M. Baenitz: Contiguous *3d* and *4f* Magnetism: Strongly Correlated *3d* Electrons in $YbFe_2Al_{10}$. Physical Review Letters **113**, 216403 (2014).

Kjall, J.A., J.H. Bardarson and F. Pollmann: Many-Body Localization in a Disordered Quantum Ising Chain. Physical Review Letters **113**, 107204 (2014).

Knolle, J., D.L. Kovrizhin, J.T. Chalker and R. Moessner: Dynamics of a Two-Dimensional Quantum Spin Liquid: Signatures of Emergent Majorana Fermions and Fluxes. Physical Review Letters **112**, 207203 (2014).

Merker, L., S. Kirchner, E. Muñoz and T.A. Costi: Reply to "Comment on 'Conductance scaling in Kondo-correlated quantum dots: Role of level asymmetry and charging energy' ". Physical Review B **90**, 077103 (2014).

Petrova, O., P. Mellado and O. Tchernyshyov: Unpaired Majorana modes on dislocations and string defects in Kitaev's honeycomb model. Physical Review B **90**, 134404 (2014).

Pollmann, F., K. Roychowdhury, C. Hotta and K. Penc: Interplay of charge and spin fluctuations of strongly interacting electrons on the kagome lattice. Physical Review B **90**, 035118 (2014).

Rodriguez-Lopez, P. and A.G. Grushin: Repulsive Casimir Effect with Chern Insulators. Physical Review Letters **112**, 056804 (2014).

Rüegg, A., H.H. Hung, E. Gull and G.A. Fiete: Comparative DMFT study of the e_g-orbital Hubbard model in thin films. Physical Review B **89**, 085122 (2014).

Sharma, A. and M. Haque: Fine structures in the spectrum of the open-boundary Heisenberg chain at large anisotropies. Physical Review A **89**, 043608 (2014).

Shchadilova, Y.E., P. Ribeiro and M. Haque: Quantum Quenches and Work Distributions in Ultralow-Density Systems. Physical Review Letters **112**, 070601 (2014).

Shchadilova, Y.E., M. Vojta and M. Haque: Single-impurity Kondo physics at extreme particle-hole asymmetry. Physical Review B **89**, 104102 (2014).

Sirker, J., M. Maiti, N. P. Konstantinidis and N. Sedlmayr: Boundary fidelity and entanglement in the symmetry protected topological phase of the SSH model. Journal of Statistical Mechanics, P10032 (2014).

Zhang, J.M., M. Haque: Nonsmooth and level-resolved dynamics illustrated with a periodically driven tight-binding model. ScienceOpen Research, DOI: 10.14293/S2199-1006.1.SOR-PHYS.A2CEM4.v1 (2014).

Ziesche, P.: Erratum: Momentum distribution and structure factors of a high-density homogeneous electron gas from its cumulant two-body reduced density matrix [Phys. Rev. A 86, 012508 (2012)]. Physical Review A **89**, 059902 (2014).

Ziesche, P. and J. Cioslowski: Cumulant Structure Factors of Jellium. Journal of Modern Physics **5**, 725-742 (2014).

Zvyagin, A.A.: Spin-orbit interaction in the supersymmetric antiferromagnetic t-J chain with a magnetic impurity. Low Temperature Physics **40**, 65-72 (2014).

Zvyagin, A.A. and H. Johannesson: Spin-orbit and impurity scattering in an integrable electron model: Exact results for dynamic correlations. Physical Review B **89**, 205135 (2014).

2015

Bergholtz, E.J., Z. Liu, M. Trescher, R. Moessner, M. Udagawa: Topology and Interactions in a Frustrated Slab: Tuning from Weyl Semimetals to $C > 1$ Fractional Chern Insulators. Physical Review Letters **114**, 016806 (2015).

Derzhko, O., J. Richter and M. Maksymenko: Strongly correlated flat-band systems: The route from Heisenberg spins to Hubbard electrons. International Journal of Modern Physics B **29**, 1530007 (2015).

Fuji, Y., F. Pollmann and M. Oshikawa: Distinct Trivial Phases Protected by a Point-Group Symmetry in Quantum Spin Chains. Physcial Review Letters **114**, 177204 (2015).

Gulacsi, M.: Ordering of correlated electrons in rare-earth compounds. Physica Status Solidi B **252**, (2015).

Isakov, S.V., R. Moessner, S.L. Sondhi and D.A. Tennant: Analytical theory for proton correlations in common-water ice I-h. Physical Review B **91**, 245152 (2015).

Konstantinidis, N.P.: Antiferromagnetic Heisenberg Model on the Icosahedron: Influence of Connectivity and the Transition from the Classical to the Quantum Limit. Journal of Physics-Condensed Matter **27**, 076001 (2015).

Konstantinidis, N.P.: Thermalization away from integrability and the role of operator off-diagonal elements. Physical Review E **91**, 052111 (2015).

Lin, S.Y., M. Chen, X.B. Yang, Y.J. Zhao, S.C. Wu, C. Felser and B.H. Yan: Theoretical search for half-Heusler topological insulators. Physical Review B **91**, 094107 (2015).

Ma, Y.D., X. Li, L.Z. Kou, B.H. Yan, C.W. Niu, Y. Dai and T. Heine: Two-dimensional inversion-asymmetric topological insulators in functionalized III-Bi bilayers. Physical Review B **91**, 235306 (2015).

Mellado, P., O. Petrova and O. Tchernyshyov: Projective symmetry of partons in the Kitaev honeycomb model. Physical Review B **91**, 04113 (2015).

Moudgalya, S. and F. Pollmann: Fragility of symmetry-protected topological order on a Hubbard ladder. Physcial Review B **91**, 155128 (2015).

Quinn, E., S. Bhattacharjee and R. Moessner: Phases and phase transitions of a perturbed Kekule-Kitaev model. Physical Review B **91**, 134419 (2015).

Roy, S., K. Saha and S. Das: Probing surface states exposed by crystal terminations at arbitrary orientations of three-dimensional topological insulators. Physical Review B **91**, 195415 (2015).

4.11 Structure Formation and Active Systems

2013

Bai, L., M. Eyiyurekli, P.I. Lelkes and D.E. Breen: Self-organized sorting of heterotypic agents via a chemotaxis paradigm. Science of Computer Programming **78**, 594-611 (2013).

Bertin, E., H. Chaté, F. Ginelli, S. Mishra, A. Peshkov and S. Ramaswamy: Mesoscopic theory for fluctuating active nematics. New Journal of Physics **15**, 085032 (2013).

Bialonski, S. and K. Lehnertz: Assortative mixing in functional brain networks during epileptic seizures. Chaos **23**, 033139 (2013).

Cioslowski, J. and J. Albin: Oscillatory and fluctuating terms in energies of assemblies of equicharged particles subject to spherically symmetric power-law confining potentials. Journal of Chemical Physics **139**, 104306 (2013).

Droste, F., A.-L. Do and T. Gross: Analytical investigation of self-organized criticality in neural networks. Journal of the Royal Society Interface **10**, 20120558 (2013).

Ferrante, E., A.E. Turgut, M. Dorigo and C. Huepe: Collective motion dynamics of active solids and active crystals. New Journal of Physics **15**, 095011 (2013).

Ferrante, E., A.E. Turgut, M. Dorigo, and C. Huepe: Elasticity-Based Mechanism for the Collective Motion of Self-Propelled Particles with Springlike Interactions: A Model System for Natural and Artificial Swarms. Physical Review Letters **111**, 268302 (2013).

Grassberger, P.: On the continuum time limit of reaction-diffusion systems. EPL **103**, 50009 (2013).

Grassberger, P.: Polymer collapse and crystallization in bond fluctuation models. EPL **103**, 26003 (2013).

Grassberger, P.: Two-Dimensional SIR Epidemics with Long Range Infection. Journal of Statistical Physics **153**, 289-311 (2013).

Großmann, R., L. Schimansky-Geier and P. Romanczuk: Self-propelled particles with selective attraction-repulsion interaction: from microscopic dynamics to coarse-grained theories. New Journal of Physics **15**, 085014 (2013).

Kuehn, C. and T. Gross: Nonlocal Generalized Models of Predator-Prey Systems. Discrete and Continuous Dynamical Systems - Series B **18**, 693-720 (2013).

Kuhnert, M.T., S. Bialonski, N. Noennig, H. Mai, H. Hinrichs, C. Helmstaedter and K. Lehnertz: Incidental and Intentional Learning of Verbal Episodic Material Differentially Modifies Functional Brain Networks. PLoS One **11**, e80273 (2013).

Vitanov, N.K. and Z.I. Dimitrova: Traveling waves and statistical distributions connected to systems of interacting populations. Computers and Mathematics with Applications **66**, 1666-1684 (2013).

Weber, C.A., T. Hanke, J. Deseigne, S. Léonard, O. Dauchot, E. Frey and H. Chaté: Long-Range Ordering of Vibrated Polar Disks. Physical Review Letters **110**, 208001 (2013).

2014

Berthoumieux, H., J.L. Maitre, C.P. Heisenberg, E.K. Paluch, F. Jülicher and G. Salbreux: Active elastic thin shell theory for cellular deformations. New Journal of Physics **16** 065005 (2014).

Bhattacharjee, S., I. Dey, K.R. Chowdhury, D. Sahu, S. Pandey and S. Chatterjee, S: Trapping of electrons in troughs of self generated electromagnetic standing waves in a bounded plasma column. Physics of Plasma **21**, 012111 (2014).

Caussin, J.B., A. Solon, A. Peshkov, H. Chaté, T. Dauxois, J. Tailleur, V. Vitelli and D. Bartolo: Emergent Spatial Structures in Flocking Models: A Dynamical System Insight. Physical Review Letters **112**, 148102 (2014).

Dierkes, K., A. Sumi, J. Solon and G. Salbreux: Spontaneous Oscillations of Elastic Contractile Materials with Turnover. Physical Review Letters **113**, 148102 (2014).

Gingell, P.W., S.C. Chapman and R.O. Dendy: Plasma blob formation by ion kinetic Kelvin-Helmholtz and interchange instabilities. Plasma Physics and Controlled Fusion **56**, 035012 (2014).

Hyman, A.A., C.A. Weber and F. Jülicher: Liquid-Liquid Phase Separation in Biology. Annual Review of Cell and Developmental Biology **30**, 39-58 (2014).

Ihle, T.: Towards a quantitative kinetic theory of polar active matter. European Physical Journal-Special Topics **223**, 1293-1314 (2014).

Ihle, T. and Y.L. Chou: Discussion on Ohta et al., "Traveling bands in self-propelled soft particles". European Physical Journal-Special Topics **223**, 1409-1415 (2014).

Jülicher, F.: Theme Issue in memory of Tom Duke. Interface Focus **, 4**, 20140072 (2014).

Kumar, K.V., J.S. Bois, F. Jülicher and S.W. Grill: Pulsatory Patterns in Active Fluids. Physical Review Letters **111**, 208101 (2014).

Romensky, M., V. Lobaskin and T. Ihle: Tricritical points in a Vicsek model of self-propelled particles with bounded confidence. Physical Review E **90**, 063315 (2014).

Scharrel, L., R. Ma, F. Jülicher and S. Diez: Bimodality in a System of Active and Passive Kinesin-1 Motors. Biophysical Journal **106**, 443A (2014).

Scharrel, L., R. Ma, R. Schneider, F. Jülicher and S. Diez: Multimotor Transport in a System of Active and Inactive Kinesin-1 Motors. Biophysical Journal **107**, 365-372 (2014).

Servidio, S., K.T. Osman, F. Valentini, D. Perrone, F. Califano, S. Chapman, W.H. Matthaeus, and P. Veltri: Proton Kinetic Effects in Vlasov and Solar Wind Turbulence. Astrophysical Journal Letters **781**, L27 (2014).

Sharma, A.K., B. Shtylla and D. Chowdhury Distribution of lifetimes of kinetochore–microtubule attachments: interplay of energy landscape, molecular motors and microtubule (de-)polymerization. Physical Biology **11**, 036004 (2014).

2015

Lade, S.J., M. Coelhob, I.M. Tolić and T. Gross: Fusion leads to effective segregation of damage during cell division: An analytical treatment. Journal of Theoretical Biology **378**, 47-55 (2015).

Lin, Y.T., H. Kim and C.R. Doering: Demographic stochasticity and evolution of dispersion I. Spatially homogeneous environments. Journal of Mathematical Biology **70**, 647-678 (2015).

Lin, Y.T., H. Kim and C.R. Doering: Demographic stochasticity and evolution of dispersion II: Spatially inhomogeneous environments. Journal of Mathematical Biology **70**, 679-707 (2015).

Ramaswamy, R., G. Bourantas, F. Jülicher and I.F. Sbalzarini: A hybrid particle-mesh method for incompressible active polar viscous gels. Journal of Computational Physics **291**, 334-361 (2015).

Romanova-Michaelides, M., D. Aguilar-Hidalgo, F. Jülicher and M. Gonzalez-Gaitan: The Wing and the Eye: a Parsimonious Theory for Scaling and Growth Control? WIREs Developmental Biology **2015**, doi: 10.1002/wdev.195 (2015).

Werner, S., T. Stückemann, A. Beiran Amigo, J.C. Rink, F. Jülicher and B.M. Friedrich: Scaling and Regeneration of Self-Organized Patterns. Physical Review Letters **114**, 138101 (2015).

4.12 Superconductivity and Magnetism

2013

Abbagari, S., T.B. Bouetou and T.C. Kofane: Generating a New Higher-Dimensional Coupled Integrable Dispersionless System: Algebraic Structures, Backlund Transformation and Hidden Structural Symmetries. Communications in Theoretical Physics **60**, 145-149 (2013).

Andreev, A.V., S. Yasin, Y. Skourski, A.A. Zvyagin, S. Zherlitsyn and J. Wosnitza: Magnetic and magnetoelastic properties of UCo_2Si_2 as studied by high-field magnetization and ultrasound measurements. Physical Review B **87**, 214409 (2013).

Bouhou, S., I. Essaoudi, A. Ainane, F. Dujardin, R. Ahuja and M. Saber: Magnetic Properties of Diluted Magnetic Nanowire. Journal of Superconductivity and Novel Magnetism **26**, 201-211 (2013).

Chern, G.-W. and R. Moessner: Dipolar Order by Disorder in the Classical Heisenberg Antiferromagnet on the Kagome Lattice. Physical Review Letters **110**, 077201 (2013).

Cohen, G., E. Gull, D.R. Reichman, A.J. Millis and E. Rabani: Numerically exact long-time magnetization dynamics at the nonequilibrium Kondo crossover of the Anderson impurity model. Physical Review B **87**, 195108 (2013).

Crespo, Y, A. Andreanov and N. Seriani: Competing antiferromagnetic and spin-glass phases in a hollandite structure. Physical Review B **88**, 014202 (2013).

Dufouleur, J., L. Veyrat, A.Teichgräber, S. Neuhaus, C. Nowka, S. Hampel, J. Cayssol, J. Schumann, B. Eichler, O.G. Schmidt, B. Büchner and R. Giraud: Quasiballistic Transport of Dirac Fermions in a Bi_2Se_3 Nanowire. Physical Review Letters **110**, 186806 (2013).

Gaafar, M. and Y. Shukrinov: Effect of microwave irradiation on parametric resonance in intrinsic Josephson junctions. Physica C **491**, 56-58 (2013).

Goussev, A., R.G. Lund, J.M. Robbins, V. Slastikov and C. Sonnenberg: Fast domain-wall propagation in uniaxial nanowires with transverse fields. Physical Review B **88**, 024425 (2013).

Gull, E., O. Parcollet and A.J. Millis: Superconductivity and the Pseudogap in the Two-Dimensional Hubbard Model. Physical Review Letters **110**, 216405 (2013).

Herbut, I.F. and V. Mastropietro: Universal conductivity of graphene in the ultrarelativistic regime. Physical Review B **87**, 205445 (2013).

Karevski, D., V. Popkov and G.M. Schuetz: Exact Matrix Product Solution for the Boundary-Driven Lindblad XXZ Chain. Physical Review Letters **110**, 47201 (2013).

Knolle J. and I. Eremin: The Antiferromagnetic Phase of Iron-Based Superconductors: An Itinerant Approach. In: Iron-Based Superconductors. Singapore : Pan Stanford Publishing Pte. Ltd., 2013. S. 431-472.

Knolle J. and C. Joas: Supraleitung und Interkontinentalraketen, "On-line computing" zwischen Militär, Industrie und Wissenschaft. In: Physik im Kalten Krieg. Berlin, Heidelberg : Springer Spektrum, 2013. S. 225-239.

Lee, S.-Y., A. Goussev, O. Georgiou, G. Gligorić and A. Lazarides: Sticky Goos-Hänchen effect at normal/superconductor interface. EPL **103**, 20004 (2013).

Lee, T.-H., K.Y.-J. Zhang, C.-H. Chung and S. Kirchner: Universal scaling of nonlinear conductance in the two-channel pseudogap Anderson model: Application for gate-tuned Kondo effect in magnetically doped graphene. Physical Review B **88**, 085431 (2013).

Plakida, N.M. and V.S. Oudovenko: On the theory of superconductivity in the extended Hubbard model. European Physical Journal B **86**, 115 (2013).

Powalski, M., K. Coester, R. Moessner and K.P. Schmidt: Disorder by disorder and flat bands in the kagome transverse field Ising model. Physical Review B **87**, 54404 (2013).

Rousochatzakis, I., R. Moessner and J. van den Brink: Frustrated magnetism and resonating valence bond physics in two-dimensional kagome-like magnets. Physical Review B **88**, 195109 (2013).

Roy, B., V. Juricic and I.F. Herbut: Quantum superconducting criticality in graphene and topological insulators. Physical Review B **87**, 041401 (2013).

Wang, J. and G.-Z. Liu: Competition between the superconductivity and nematic order in the high-T-c superconductor. New Journal of Physics **15**, 073039 (2013).

Wang, J.-R. and G.-Z. Liu: Additional electron pairing in a d-wave superconductor driven by nematic order. New Journal of Physics **15**, 063007 (2013).

Zvyagin, A.A.: New physics in frustrated magnets: Spin ices, monopoles, etc. Low Temperature Physics **39**, 901-922 (2013).

2014

Ahn, F., I. Eremin, J. Knolle, V.B. Zabolotnyy, S.V. Borisenko, B. Büchner and A.V. Chubukov: Superconductivity from repulsion in LiFeAs: Novel s-wave symmetry and potential time-reversal symmetry breaking. Physical Review B **89**, 144513 (2014).

Andreanov, A. and A.A. Fedorenko: Localization of spin waves in disordered quantum rotors. Physical Review **B**, 014205 (2014).

Berashevich, J. and A. Reznik: Possible route to d_0 magnetism in α-PbO compound. Journal of Physics and Chemistry of Solids **75**, 1132-1136 (2014).

Chernodub, M.N., A. Cortijo, A.G. Grushin, K. Landsteiner and M.A.H. Vozmediano: Condensed matter realization of the axial magnetic effect. Physical Review B **89**, 081407 (2014).

Coldea, A.I., L. Seabra, A. McCollam, A. Carrington, L. Malone, A.F. Bangura, D. Vignolles, P.G. van Rhee, R.D. McDonald, T. Sorgel, M. Jansen, N. Shannon and R. Coldea: Cascade of field-induced magnetic transitions in a frustrated antiferromagnetic metal. Physical Review B **90**, 020401 (2014).

de Juan, F., R. Ilan and J.H. Bardarson: Robust Transport Signatures of Topological Superconductivity in Topological Insulator Nanowires. Physical Review Letters **113**, 107003 (2014).

Derzhko, O. and J. Richter: Dispersion-driven ferromagnetism in a flat-band Hubbard system. Physical Review B **90**, 045152 (2014).

Eremin, I., J. Knolle, R.M. Fernandes, J. Schmalian and A.V. Chubukov: Antiferromagnetism in Iron-Based Superconductors: Selection of Magnetic Order and Quasiparticle Interference. Journal of the Physical Society of Japan **83**, 061015 (2014).

Erfanifam, S., S. Zherlitsyn, S. Yasin, Y. Skourski, J. Wosnitza, A.A. Zvyagin, P. McClarty, R. Moessner, G. Balakrishnan and O.A. Petrenko: Ultrasonic investigations of the spin ices $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ in and out of equilibrium. Physical Review B **90**, 064409 (2014).

Gingras, M.J.P. and P.A. McClarty: Quantum spin ice: a search for gapless quantum spin liquids in pyrochlore magnets. Reports on Progress in Physics **77**, 056501 (2014).

Goussev, A., J.M. Robbins and V. Slastikov: Domain wall motion in thin ferromagnetic nanotubes: Analytic results. EPL **105**, 67006 (2014).

Gulacsi, M.: Magnetism in rare-earth alloys. International Journal of Modern Physics B **28**, 1430016 (2014).

Gulacsi, M.: Erratum: Magnetism in rare-earth alloys. International Journal of Modern Physics B **28**, 1492006 (E) (2014).

Gulacsi, M.: One-dimensional periodic Anderson model. Modern Physics Letters B **28**, 1450041 (2014).

Gulacsi, M.: Pseudospin Exchange in Rare Earth Alloys. Journal of Superconductivity and Novel Magnetism **27**, 2585-2594 (2014).

Hamad, B.: Magnetic structure calculations of $Ir_{0.5}Mn_{0.5}$ over- and sub-layer at Co(001) surface. Journal of Magnetism and Magnetic Materials **369**, 1-4 (2014).

Hegde, S.S., H. Katiyar, T.S. Mahesh and A. Das: Freezing a quantum magnet by repeated quantum interference: An experimental realization. Physical Review B **90**, 174407 (2014).

Katukuri, V.M., S. Nishimoto, V. Yushankhai, A. Stoyanova, H. Kandpal, S. Choi, R. Coldea, I. Rousochatzakis, L. Hozoi and J. van den Brink: Kitaev interactions between j=$_1/_{2y}$ moments in honeycomb Na_2IrO_3 are large and ferromagnetic: insights from ab initio quantum chemistry calculations. New Journals of Physics **16**, 013056 (2014).

Katukuri, V.M., V. Yushankhai, L. Siurakshina, J. van den Brink, L. Hozoi and I. Rousochatzakis: Mechanism of Basal-Plane Antiferromagnetism in the Spin-Orbit Driven Iridate Ba_2IrO_4. Physical Review X **4**, 02105 (2014).

Knolle, J., G.W. Chern, D.L. Kovrizhin, R. Moessner and N.B. Perkins: Raman Scattering Signatures of Kitaev Spin Liquids in A_2IrO_3 Iridates with A = Na or Li. Physical Review Letters **113**, 187201 (2014).

Langridge, S., G.M. Watson, D. Gibbs, J.J. Betouras, N.I. Gidopoulos, F. Pollmann, M.W. Long, C. Vettier and G.H. Lander: Distinct Magnetic Phase Transition at the Surface of an Antiferromagnet. Physical Review Letters **112**, 167201 (2014).

LeBlanc, J.P.F.: Signatures of a momentum independent pseudogap in the electronic density of states and Raman spectroscopy of the underdoped cuprates. New Journal of Physics **16**, 113034 (2014).

Lee, E.K.H., S. Bhattacharjee, K. Hwang, H.S. Kim, H. Jin and Y.B. Kim: Topological and magnetic phases with strong spin-orbit coupling on the hyperhoneycomb lattice. Physical Review B **89**, 205132 (2014).

Lipavsky, P., K. Morawetz, B. Šopík and M. Männel: Stability of supercurrents and condensates in type I superconductors. European Physical Journal B **87**, 8 (2014).

Mandal, S., A. Andreanov, Y. Crespo and N. Seriani: Incommensurate helical spin ground states on the hollandite lattice. Physical Review B **90**, 104420 (2014).

Matthews, P., P. Ribeiro and A.M. García-García: Dissipation in a Simple Model of a Topological Josephson Junction. Physical Review Letters **112**, 247001 (2014).

McClarty, P.A., P. Stasiak and M.J.P. Gingras: Order-by-disorder in the XY pyrochlore antiferromagnet. Physical Review B **89**, 024425 (2014).

Moessner, R.: Magnetische Monopole in Spineis. Physik Journal **13**, 41-48 (2014).

Mostame, S., C. Castelnovo, R. Moessner, and S.L. Sondhi: Tunable nonequilibrium dynamics of field quenches in spin ice. Proceedings of the National Academy of Sciences of the United States of America **111**, 640-645 (2014).

Oliveira, T.P., P. Ribeiro and P.D. Sacramento: Entanglement entropy and entanglement spectrum of triplet topological superconductors. Journal of Physics-Condensed Matter **26**, UNSP 425702 (2014).

Rousochatzakis, I., Y. Wan, O. Tchernyshyov and F. Mila: Quantum dimer model for the spin-$_1/_2$ kagome Z_2 spin liquid. Physical Review B **90**, 100406 (2014).

Roy, B., F.F. Assaad and I.F. Herbut: Zero Modes and Global Antiferromagnetism in Strained Graphene. Physical Review X **4**, 021042 (2014).

Sharma, A., A. Andreanov and M. Müller: Avalanches and hysteresis in frustrated superconductors and XY spin glasses. Physical Review E **90**, 042103 (2014).

Xu, G., J. Wang, B.H. Yan and X.L. Qi: Topological superconductivity at the edge of transition-metal dichalcogenides. Physical Review B **90**, 100505 (2014).

Zhao, J.Z., S.J. Hu, J. Chang, P. Zhang and X.Q. Wang: Ferromagnetism in a two-component Bose-Hubbard model with synthetic spin-orbit coupling. Physical Review A **89**, 043611 (2014).

Zhao, J.Z., S.J. Hu, J. Chang, F.W. Zheng, P. Zhang and X.Q. Wang: Evolution of magnetic structure driven by synthetic spin-orbit coupling in a two-component Bose-Hubbard model. Physical Review B **90**, 085117 (2014).

Zvyagin, A.A.: Dynamics of the Kitaev chain model under parametric pumping. Physical Review B **90**, 014507 (2014).

Zvyagin, A.A.: Longitudinal spin pumping and topological superconductivity: Search for Majorana edge states. Physical Review B **89**, 214420 (2014).

Zvyagina, G.A., K.R. Zhekov, I.V. Bilych, A.A. Zvyagin, A.N. Bludov, V.A. Pashchenko and I.A. Gudim: Magnetic field-induced phase transitions in the antiferromagnet $Nd_{0.6}Dy_{0.4}Fe_3(BO_3)_4$. Low Temperature Physics **40**, 146-150 (2014).

2015

Andreanov, A. and P.A. McClarty: Order induced by dilution in pyrochlore XY antiferromagnets. Physical Review B **91**, 064401 (2015).

Beugeling, W., E. Kalesaki, C. Delerue, Y.M. Niquet, D. Vanmaekelbergh and C. Morais Smith: Topological states in multi-orbital HgTe honeycomb lattices. Nature Comunications **6**, 6316 (2015).

Bouhou, S., M. El Hamri, I. Essaoudi, A. Ainane and R. Ahuja: Magnetic properties of a single transverse Ising ferrimagnetic nanoparticle. Physica B **456**, 142-150 (2015).

Chudnovskiy, A.L. and V. Kagalovsky: Thermal and electrical quantum Hall effects in ferromagnet/topological insulator/ferromagnet junction. Physical Review B **91**, 195105 (2015).

El Hamri, M., S. Bouhou, I. Essaoudi, A. Ainane and R. Ahuja: Investigation of the surface shell effects on the magnetic properties of a transverse antiferromagnetic Ising nanocube. Superlattices and Microstructures **80**, 151-168 (2015).

Gulacsi, M.: Ferromagnetic order in the one-dimensional Anderson lattice. Journal of Magnetism and Magnetic Materials **374**, 690-695 (2015).

He, Y.C. and Y. Chen: Distinct Spin Liquids and Their Transitions in Spin-*1/2 XXZ* Kagome Antiferromagnets. Physical Review Letters **114**, 037201 (2015).

Jaubert, L.D.C. and R. Moessner: Multiferroicity in spin ice: Towards magnetic crystallography of $Tb_2Ti_2O_7$ in a field. Physical Review B **91**, 214422 (2015).

LeBlanc, J.P.F. and A.G. Grushin: Unparticle mediated superconductivity. New journal of Physics **17**, 033039 (2015).

Li, G., B.H. Yan, R. Thomale, W. Hanke: Topological nature and the multiple Dirac cones hidden in Bismuth high-Tc superconductors. Scientific Reports **5**, 10435 (2015).

Maghrebi, M.F., N.Y. Yao, M. Hafezi, T. Pohl, O. Firstenberg and A.V. Gorshkov: Fractional quantum Hall states of Rydberg polaritons. Physical Review A **91**, 033838 (2015).

Maksymenko, M., V.R. Chandra and R. Moessner: Classical dipoles on the kagome lattice. Physical Review B **91**, 184407 (2015).

Ovchinnikov, Y.N. and A.A. Varlamov: Phase slips in a current-biased narrow superconducting strip. Physical Review B **91**, 014514 (2015).

Rousochatzakis, I., J. Richter, R. Zinke and A.A. Tsirlin: Frustration and Dzyaloshinsky-Moriya anisotropy in the kagome francisites $Cu_3Bi(SeO_3)_2O_2X$ (X = Br, Cl). Physical Review B **91**, 024416 (2015).

Sen, A. and R. Moessner: Topological Spin Glass in Diluted Spin Ice. Physical Review Letters **114**, 247207 (2015).

Sticlet, D., L. Seabra, F. Pollmann and J. Cayssol: Topological superconductivity in the one-dimensional interacting Creutz model. Journal of Physics: Conference Series **592**, 012133 (2015).

Van Bijnen, R.M.W. and T. Pohl: Quantum Magnetism and Topological Ordering via Rydberg Dressing near Forster Resonances. Physical Review Letters **114**, 243002 (2015).

Wang, Q.Z., S.C. Wu, C. Felser, B.H. Yan and C.X. Liu: Spin texture and mirror Chern number in Hg-based chalcogenides. Physical Review B **91**, 165435 (2015).

Zherlitsyn, S., V. Tsurkan, A.A. Zvyagin, S. Yasin, S. Erfanifam, R. Beyer, M. Naumann, E. Green, J. Wosnitza and A. Loidl: A Novel phase transition and metastable regions in the frustrated magnet $CdCr_2O_4$. Physical Review B **91**, 060406 (2015).

4.13 Time Dependent Processes

2013

Gligoric, G., K. Rayanov and S. Flach: Make slow fast -How to speed up interacting disordered matter. EPL **101**, 10011 (2013).

Granger, L. and H. Kantz: Differential Landauer's principle. EPL **101**, 50004 (2013).

Gundermann, J., H. Kantz and J. Broecker: Crooks Fluctuation Theorem for a Process on a Two-Dimensional Fluid Field. Physical Review Letters **110**, 234502 (2013).

Kaiser, V., S.T. Bramwell, P.C.W. Holdsworth and R. Moessner: Onsager's Wien effect on a lattice. Nature Materials **12**, 1032-1036 (2013).

Laptyeva, T.V., J.D. Bodyfelt and S. Flach: Do nonlinear waves in random media follow nonlinear diffusion equations? Physica D **256**, 1-6 (2013).

Lucas, F. and K. Hornberger: Adaptive Resummation of Markovian Quantum Dynamics. Physical Review Letters **110**, 240401 (2013).

Mulhern, C.: Persistence of uphill anomalous transport in inhomogeneous media. Physical Review E **88**, 022906 (2013).

Osman, K.T., W.H. Matthaeus, K.H. Kiyani, B. Hnat and S.C. Chapman: Proton Kinetic Effects and Turbulent Energy Cascade Rate in the Solar Wind. Physical Review Letters **111**, 201101 (2013).

Roy, A., R. Dasgupta, S. Modak, A. Das and K. Sengupta: Periodic dynamics of fermionic superfluids in the BCS regime. Journal of Physics - Condensed Matter **25**, 205703 (2013).

Sharafi, N., J. Benda and B. Lindner: Information filtering by synchronous spikes in a neural population. Journal of Computational Neuroscience **34**, 285-301 (2013).

Vorberg, D., W. Wustmann, R. Ketzmerick and A. Eckardt: Generalized Bose-Einstein Condensation into Multiple States in Driven-Dissipative Systems. Physical Review Letters **111**, 240405 (2013).

2014

Caso, A., B. Horovitz and L. Arrachea: Model for electron spin resonance in STM noise. Physical Review B **89**, 075412 (2014).

Gorin, T., L. Alonso and P.C.L. Vázquez: Scattering approach to fidelity and fidelity recovery. In: AIP Conference Proceedings. Special Topics on Transport Theory: Electrons, Waves, and Diffusion in Confined Systems: V Leopoldo García-Colín Mexican Meeting on Mathematical and Experimental Physics **1579**, 11-20 (2014).

Jörg, D.J., L.G. Morelli, S. Ares and F. Jülicher: Synchronization Dynamics in the Presence of Coupling Delays and Phase Shifts. Physical Review Letters **112**, 174101 (2014).

Lucas, F. and K. Hornberger: Optimally convergent quantum jump expansion. Physical Review A **89**, 012112 (2014).

Ma, T., L. Fletcher, A. Pak, D.A. Chapman, R.W. Falcone, C. Fortmann, E. Galtier, D.O. Gericke, G. Gregori, J. Hastings, O.L. Landen, S. Le Pape, H.J. Lee, B. Nagler, P. Neumayer, D. Turnbull, J. Vorberger, T.G. White, K. Wünsch, U. Zastrau, S.H. Glenzer and T. Döppner: Observations of strong ion-ion correlations in dense plasmas. Physics of Plasma **21**, 056302 (2014).

Matthaeus, W.H., S. Oughton, K.T. Osman, S. Servidio, M. Wan, S.P. Gary, M.A. Shay, F. Valentini, V. Roytershteyn, H. Karimabadi and S.C. Chapman: Nonlinear and Linear Timescales Near Kinetic Scales in Solar Wind Turbulence. Astrophysical Journal **790**, 155 (2014).

Morawetz, K.: Universal short-time response and formation of correlations after quantum quenches. Physical Review B **90**, 075303 (2014).

Osman, K.T., K.H. Kiyani, S.C. Chapman and B. Hnat: Anisotropic Intermittency of Magnetohydrodynamic Turbulence. Astrophysical Journal Letters **783**, L27 (2014).

Osman, K.T., W.H. Matthaeus, J.T. Gosling, A. Greco, S. Servidio, B. Hnat, S.C. Chapman and T.D. Phan: Magnetic Reconnection and Intermittent Turbulence in the Solar Wind. Physical Review Letters **111**, 215002 (2014).

Pollakis, A., L. Wetzel, D.J. Jörg, W. Rave, G. Fettweis and F. Jülicher: Synchronization in networks of mutually delay-coupled phase-locked loops. New Journal of Physics **16**, 113009 (2014).

Saleh, M., B.B. Thomas and T.C. Kofane: Quasinormal modes of scalar perturbation around a quantum-corrected Schwarzschild black hole. Astrophysics and Space Science **350**, 721-726 (2014).

Sandev, T., I. Petreska and E.K. Lenzi: Time-dependent Schrodinger-like equation with nonlocal term. Journal of Mathematical Physics **55**, 092105 (2014).

Sartori, P., L. Granger, C.F. Lee and J.M. Horowitz: Thermodynamic Costs of Information Processing in Sensory Adaptation. PLoS Computational Biology **10**, e1003974 (2014).

Seabra, L., F.H.L. Essler, F. Pollmann, I. Schneider and T. Veness: Real-time dynamics in the one-dimensional Hubbard model. Physical Review B **90**, 245127 (2014).

Silk, H., G. Demirel, M. Homer and T. Gross: Exploring the adaptive voter model dynamics with a mathematical triple jump. New Journal of Physics **16**, 093051 (2014).

Teimourpour, M.H., R. El-Ganainy, A. Eisfeld, A. Szameit and D.N. Christodoulides: Light transport in PT-invariant photonic structures with hidden symmetries. Physical Review A **90**, 053817 (2014).

Yeakel, J.D., M.M. Pires, L. Rudolf, N.J. Dominy, P.L. Koch, P.R. Guimaraes and T. Gross: Collapse of an ecological network in Ancient Egypt. PNAS **111**, 14472-14477 (2014).

Zhu, H., S.C. Chapman, R.O. Dendy and K. Itoh: Transitions to improved confinement regimes induced by changes in heating in zero-dimensional models for tokamak plasmas. Physics of Plasmas **21**, 062307 (2014).

2015

Belobo, D.B., G.H. Ben-Bolie and T.C. Kofane: Dynamics of kink, antikink, bright, generalized Jacobi elliptic function solutions of matter-wave condensates with time-dependent two- and three-body interactions. Physical Review E **91**, 042902 (2015).

Grothe, T. and J. Baumgart: Assessment of Bassoon Tuning Quality from Measurements under Playing Conditions. Acta Acustica united with Acustica **101**, 238-245 (2015).

Laumann, C.R., R. Moessner, A. Scardicchio and S.L. Sondhi: Quantum annealing: The fastest route to quantum computation? European Physical Journal-Special Topics **224**, 75-88 (2015).

Pugliese, E., R. Meucci, S. Euzzor, J.G. Freire, J.A.C. Gallas: Complex dynamics of a dc glow discharge tube: Experimental modeling and stability diagrams. Scientific Reports **5**, 8447 (2015).

Trevino, S., A. Nyberg, C.I. Del Genio and K.E. Bassler: Fast and accurate determination of modularity and its effect size. Journal of Statistical Mechanics - Theory and Experiment **2015**, P02003 (2015).

Yeakel, J.D., M.M. Pires, L. Rudolf, N.J. Dominy, P.L. Koch, P.R. Guimarães and T. Gross: Reply to Evans and Bar-Oz et al.: Recovering ecological pattern and process in Ancient Egypt. Proceedings of the National Academy of Sciences of the United States of America **112**, E240 (2015).

Zaletel, M.P., R.S.K. Mong, C. Karrasch, J.E. Moore and F. Pollmann: Time-evolving a matrix product state with long-ranged interactions. Physical Review B **91**, 165112 (2015).

4.14 Ultracold Matter

2013

Alba, V., M. Haque and A.M. Läuchli: Entanglement Spectrum of the Two-Dimensional Bose-Hubbard Model, Physical Review Letters **110**, 260403 (2013).

Alba, V., K. Saha and M. Haque: Bethe ansatz description of edge-localization in the open-boundary XXZ spin chain. Journal of Statistical Mechanics, P10018 (2013).

Bannasch, G., T.C. Killian and T. Pohl: Strongly Coupled Plasmas via Rydberg Blockade of Cold Atoms. Physical Review Letters **110**, 253003 (2013).

Castro, J., G. Bannasch, P. McQuillen, T. Pohl and T.C. Killian: Creating Non-Maxwellian Velocity Distributions in Ultracold Plasmas. AIP Conference Proceedings **1421**, 31-43 (2012).

Daghofer, M. and M. Haque: Viewpoint: Toward Fractional Quantum Hall Physics with Cold Atoms. Physics **6**, 49 (2013).

Gammelmark, S. and A. Eckardt: Quantum crystal growing: adiabatic preparation of a bosonic antiferromagnet in the presence of a parabolic inhomogeneity. New Journal of Physics **15**, 033028 (2013).

Haque, M. and F.E. Zimmer: Slow interaction ramps in trapped many-particle systems: Universal deviations from adiabaticity. Physical Review A **87**, 033613 (2013).

Heinze, J., J.S. Krauser, N. Fläschner, K. Sengstock and C. Becker: Engineering Spin Waves in a High-Spin Ultracold Fermi Gas. Physical Review Letters **110**, 250402 (2013).

Lenz, M., S. Wuester, C.J. Vale, N.R. Heckenberg, H. Rubinsztein-Dunlop, C.A. Holmes, G.J. Milburn and M.J. Davis: Dynamical tunneling with ultracold atoms in magnetic microtraps. Physical Review A **88**, 013635 (2013).

Macri, T., F. Maucher, F. Cinti and T. Pohl: Elementary excitations of ultracold soft-core bosons across the superfluid-supersolid phase transition. Physical Review A **87**, 061602 (2013).

Möbius, S., M. Genkin, S. Wüster, A. Eisfeld, and J.M. Rost: Breakup of Rydberg-blockaded atom clouds via dipole-dipole interactions. Physical Review A. **88**, 012716 (2013).

Ribeiro, P., M. Haque and A. Lazarides: Strongly interacting bosons in multichromatic potentials supporting mobility edges: Localization, quasi-condensation, and expansion dynamics. Physical Review A **87**, 043635 (2013).

Simonet, J, J. Struck, M. Weinberg, C. Ölschläger, P. Hauke, A. Eckardt, M. Lewenstein, K. Sengstock and P. Windpassinger: Tunable gauge potential for spinless particles in driven lattices. EPJ Web of Conferences **57**, 01004 (2013).

Struck, J., M. Weinberg, C. Ölschläger, P. Windpassinger, J. Simonet, K. Sengstock, R. Höppner, P. Hauke, A. Eckardt, M. Lewenstein and L. Mathey: Engineering Ising-XY spin-models in a triangular lattice using tunable artificial gauge fields. Nature Physics **9**, 738-743 (2013).

Tieleman, O., O. Dutta, M. Lewenstein and A. Eckardt: Spontaneous Time-Reversal Symmetry Breaking for Spinless Fermions on a Triangular Lattice. Physical Review Letters **110**, 096405 (2013).

Tschischik, W., R. Moessner and M. Haque: Breathing mode in the Bose-Hubbard chain with a harmonic trapping potential. Physical Review A **88**, 063636 (2013).

Vidanovic, I., N.J. van Druten and M. Haque: Spin modulation instabilities and phase separation dynamics in trapped two-component Bose condensates. New Journal of Physics **15**, 035008 (2013).

Wüster, S., S. Möbius, M. Genkin, A. Eisfeld, and J.M. Rost: Source of entangled atom pairs on demand using the Rydberg blockade. Physical Review A **88**, 063644 (2013).

Zvyagin, A.A. and P. Schlottmann: Effects of spin-orbit interaction in the Hubbard chain with attractive interaction: Application to confined ultracold fermions. Physical Review B **88**, 205127 (2013).

2014

Belobo, D.B., G.H. Ben-Bolie and T.C. Kofane: Generation of Bright Matter-Wave Soliton Patterns in Mixtures of Bose-Einstein Condensates with Cubic and Quintic Nonlinearities. International Journal of Modern Physics B **28**, 1450003 (2014).

Bonnes, L., D. Charrier and A.M. Läuchli: Dynamical and steady-state properties of a Bose-Hubbard chain with bond dissipation: A study based on matrix product operators. Physical Review A **90**, 033612 (2014).

Ebling, U., J.S. Krauser, N. Flaschner, K. Sengstock, C. Becker, M. Lewenstein and A. Eckardt: Relaxation Dynamics of an Isolated Large-Spin Fermi Gas Far from Equilibrium. Physical Review X **4**, 021011 (2014).

Gaul, C. and C.A. Müller: A grand-canonical approach to the disordered Bose gas. Applied Physics B **117**, 775-784 (2014).

Gaul, C. and J. Schiefele: Bose-Einstein condensation in a minimal inhomogeneous system. Journal of Physics A **47**, 025002 (2014).

Genkin, M., S. Wüster, S. Möbius, A. Eisfeld and J.M. Rost: Dipole-dipole induced global motion of Rydberg-dressed atom clouds. Journal of Physics B **47**, 095003 (2014).

Gil, L.I.R., R. Mukherjee, E.M. Bridge, M.P.A. Jones and T. Pohl: Spin Squeezing in a Rydberg Lattice Clock. Physical Review Letters **112**, 103601 (2014).

Glaetzle, A.W., M. Dalmonte, R. Nath, I. Rousochatzakis, R. Moessner and P. Zoller: Quantum Spin-Ice and Dimer Models with Rydberg Atoms. Physical Review X **4**, 041037 (2014).

Golshani, M., S. Weimann, K. Jafari, M.K. Nezhad, A. Langari, A.R. Bahrampour, T. Eichelkraut, S.M. Mahdavi and A. Szameit: Impact of Loss on the Wave Dynamics in Photonic Waveguide Lattices. Physical Review Letters **113**, 123903 (2014).

Hauke, P., M. Lewenstein and A. Eckardt: Tomography of Band Insulators from Quench Dynamics. Physical Review Letters **113**, 045303 (2014).

Krauser, J.S., U. Ebling, N. Fläschner, J. Heinze, K. Sengstock, M. Lewenstein, A. Eckardt and C. Becker: Giant Spin Oscillations in an Ultracold Fermi Sea. Science **343**, 157-160 (2014).

Lebedeva, E.V., A.M. Dyugaev and P.D. Grigor'ev: On the thermodynamics of quantum liquids. Low Temperature Physics **40**, 475-481 (2014).

Leonhardt, K., S. Wüster and J.M. Rost: Switching Exciton Pulses Through Conical Intersections. Physical Review Letters **113**, 223001 (2014).

Macri, T. and T. Pohl: Rydberg dressing of atoms in optical lattices. Physical Review A **89**, 011402 (2014).

Quinn, E. and M. Haque: Modulated trapping of interacting bosons in one dimension. Physical Review A **90**, 053609 (2014).

Schlottmann, P. and A.A. Zvyagin: Superfluid instability in ultra-cold gas of fermionic atoms with attractive potential in a one-dimensional trap. Journal of Physics Conference Series **529**, 012013 (2014).

Sevinçli, S. and T. Pohl: Microwave control of Rydberg atom interactions. New Journal of Physics **16**, 123036 (2014).

Zoubi, H., A. Eisfeld and S. Wüster: van der Waals-stabilized Rydberg aggregates. Physical Review A **89**, 053426 (2014).

2015

Schlottmann, P. and A.A. Zvyagin: Threshold singularities in a Fermi gas with attractive potential in one dimension. Nuclear Physics B **892**, 269-287 (2015).

Tschischik, W. and M. Haque: Repulsive-to-attractive interaction quenches of a one-dimensional Bose gas in a harmonic trap. Physical Review A **91**, 053607 (2015).