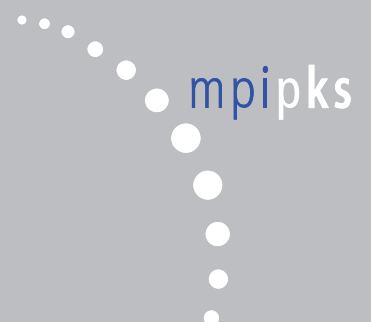


MAX-PLANCK-GESELLSCHAFT

Max Planck Institute
for the Physics of
Complex Systems

Scientific Report

7/2015–12/2018



Front cover

Dr. Steffen Rulands:

Microscopy image of a developing mouse heart where a subset of the earliest precursor cells has been labelled with fluorescent genetic markers. Physicists at the MPI-PKS have shown that the sizes of marked patches follow universal forms (S. Rulands et al., Nature Physics 2018, image by S. Chabab).

IMPRESSUM

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MAX PLANCK INSTITUTE FOR THE PHYSICS
OF COMPLEX SYSTEMS

Scientific Report 7/2015 – 12/2018

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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 (**mpipks**) was founded by the Senate of the Max Planck Society in November 1992. The concept for the institute envisaged 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 accommodation for the institute. The institute was officially inaugurated by *Prof. H. Zacher*, President of the Max Planck Society, on May 2nd, 1994. An administration was installed headed by *Mrs. I. Auguszt*. The Visitors Program began to operate, first guests were invited, and the first workshop took place in March 1994.

1995-1998 • In 1995, *Dr. H. Kantz* joined the institute as head of an independent Junior Research Group on *Nonlinear Time Series Analysis*. Moreover, the **mpipks** decided to broaden its research spectrum considerably by installing temporary Junior Research Groups: The group *Pattern Formation in Reaction-Diffusion-Systems* headed by *Dr. M. Bär* started its activities in 1995, the group *Quantum Chaos and Mesoscopic Systems* headed by *Dr. K. Richter* in January 1996, and the group *Quantum 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 Workshop and Visitors Program gained momentum with hundreds of scientists visiting the institute.

1999-2001 • In 1999, the *Finite Systems* division was installed under the direction 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*. *Dr. U. Birkenheuer* succeeded *Dr. Dolg* as head of the *Quantum Chemistry* group in March 2000. To strengthen 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 of 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.

2005-2006 • In 2005, 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.

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. 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 Helmholtz Center Dresden-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 *Quantum Chaos and Quantum Dynamics* 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 • Further new groups were established: Dr. F. Pollmann set up the activities of the Junior Research Group *Topology and Correlations in Condensed Matter*, and Dr. E. Gull launched the Junior Research Group *Computational Quantum Many-Body Physics*. The group *Physics of the Cytoskeleton* headed by Dr. G. Salbreux, the group *Computational Biology and Evolutionary Genomics* headed by Dr. M. Hiller, and the group *Collective Dynamics of Cells* headed by Dr. V. Zaburdaev 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 operated at the Center of Free-Electron Laser Science, Hamburg. To accommodate the increasing number of visiting scientists, a fourth guest house was built and inaugurated in November 2012. The joint research program of the **mpipks** 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 this period, the research at the **mpipks** has once more acquired new foci due to the installation of new temporary working 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 *Quantum Chaos and Quantum Dynamics* were extended to a second five-year period by the Max Planck Society.

06.2015-2018 • Over the past thirty months, several new research groups began their scientific work at **mpipks**. The Condensed Matter division is strengthened by the arrival of Dr. M. Heyl, heading the group *Dynamics in Correlated Quantum Matter*, and Dr. D. Luitz, heading the group *Computational Quantum Many-body Physics*. The Biological Physics division welcomes the groups of Dr. S. Rulands working on *Statistical Physics of Living Systems* and Dr. C. Weber who heads the group *Mesoscopic Physics of Life*. Moreover, the research profile of **mpipks** is complemented by the establishment of three Max

Planck Research groups, headed by *Dr. A. E. B. Nielsen* who focuses on *Quantum Many-body Systems*, *Dr. F. Piazza* studying *Strongly Correlated Light-Matter Systems* and *Dr. I. A. N. Sodemann Villadiego* investigating *Fractionalization and Topology in Quantum Matter*. The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* successfully passed the 12-years evaluation in September 2015 and was renewed for another six-year period with a new focus on *Many Particle Systems in Structured Environments*. The new building of the *Center for Systems Biology Dresden* was inaugurated in 2017. *Mrs. I. Auguszt*, who headed the administration of **mpipks** since its foundation, retired in 2017, with *Mrs. K. Huppertz* taking over the responsibility as head of administration.

Role of honor: Present status of former group leaders

group	active	leader	current affiliation
Pattern Formation in Reaction-Diffusion-Systems	1995 - 2004	M. Bär	Head of Department PTB Berlin
Quantum Chaos and Mesoscopic Systems	1996 - 2001	K. Richter	Professor University of Regensburg
Quantum Chemistry (first period)	1996 - 2000	M. Dolg	Professor University of Cologne
Quantum Chemistry (second period)	2000 - 2005	U. Birkenheuer	Staff Scientist HZ Dresden-Rossendorf
Nonlinear Dynamics in Quantum Systems	1999 - 2007	A. Buchleitner	Professor University of Freiburg
Complex Media and Mesoscopic Phenomena	2000 - 2005	H. Schomerus	Professor Lancaster University
Physics of Biological and Soft Matter	2002 - 2006	R. Everaers	Professor ENS de Lyon
Biological Physics of Olfaction: From Genes to Networks	2002 - 2008	M. Zapotocky	Senior Scientist Czech Academy of Sciences
Nonlinear Processes in Strong Fields	2002 - 2008	A. Becker	Associate Professor Univ. of Colorado Boulder
Electronic Structure of Finite Systems	2003 - 2005	S. Kümmel	Professor University of Bayreuth
Physics of Cell Division	2004 - 2006	K. Kruse	Prof. at Univ. of Geneva
Many Body Effects in Mesoscopic Systems	2006 - 2012	M. Hentschel	Professor TU Ilmenau
Motor Systems	2006 - 2013	S. Grill	Director at the MPI-CBG
Dynamics of Biological Networks	2007 - 2011	T. Gross	Reader University of Bristol
Stochastic Processes in Biophysics	2007 - 2011	B. Lindner	Professor HU Berlin
Computational Nonlinear and Relativistic Optics	2007 - 2014	S. Skupin	CNRS Researcher Université de Bordeaux
New States of Quantum Matter	2008 - 2011	A. Läuchli	Professor University of Innsbruck
Complex Dynamics in Cold Gases	2008 - 2017	T. Pohl	Professor Aarhus University
Molecular Quantum Optics	2009 - 2011	K. Hornberger	Professor University of Duisburg-Essen
Collective Phenomena in Solid State and Materials Physics	2009 - 2014	S. Kirchner	Professor Zhejiang University
Physics of the Cytoskeleton	2010 - 2015	G. Salbreux	Group Leader Francis Crick Institute
Dynamical Systems and Social Dynamics	2010 - 2016	E. Altmann	Associate Professor University of Sydney
X-Ray Quantum Optics	2011 - 2015	N. Rohringer	Professor University of Hamburg
Topology and Correlations in Condensed Matter	2011 - 2016	F. Pollmann	Professor TU Munich
Computational Quantum Many-Body Physics	2012	E. Gull	Associate Professor University of Michigan
Collective Dynamics of Cells	2012 - 2018	V. Zaburdaev	Professor FAU Erlangen-Nuremberg
Quantum Matter - Transport and Dynamics	2013 - 2017	J. H. Bardarson	Assistant Professor KTH Stockholm

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 activities 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 groups, which thematically expand, fortify and bridge the research activities:

- 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 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 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 *Statistical Physics of Living Systems* headed by *Dr. S. Rulands* studies mechanisms of cell fate regulation in tissue development, maintenance and disease with methods from statistical physics.
- The research group *Mesoscopic Physics of Life* headed by *Dr. C. Weber* applies concepts from the field of phase transitions, non-equilibrium thermodynamics, and non-linear dynamics to investigate the basic principles which underly the patterns and the morphology in biological systems.
- 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 *Ultrafast Laser-Matter Interaction* headed by *Dr. A. Landsman* focuses on the interaction of matter with ultrashort flashes of light, with the ultimate goal to image and control electron dynamics on the attosecond time-scale.
- The research group *Dynamics in Correlated Quantum Matter* headed by *Dr. M. Heyl* studies dynamics in quantum many-body systems at the interface between quantum many-body theory, non-equilibrium physics, quantum information science, and machine learning.
- The research group *Computational Quantum Many-body Physics* headed by *Dr. D. Luitz* uses computational techniques to explore the rich physics of strongly interacting quantum matter both in thermodynamic equilibrium as well as far from equilibrium.
- The research group *Nonequilibrium Quantum Matter* headed by *Prof. T. Oka* theoretically searches for new ways to control the quantum states in solid state materials via nonequilibrium external fields.
- The Max Planck research group *Strongly Correlated Light-Matter Systems* headed by *Dr. F. Piazza* investigates many-body phenomena at the boundary between condensed matter physics and quantum optics using non-equilibrium quantum-field-theoretical methods.
- The Max Planck research group *Quantum Many-Body Systems* headed by *Dr. A. E. B. Nielsen* focuses on phenomena in strongly-correlated quantum many-body systems with emphasis on fractional quantum Hall physics in lattice systems and related one-dimensional models.
- The Max Planck research group *Fractionalization and Topology in Quantum Matter* headed by *Dr. I. A. N. Sodemann Villadiego* explores the interplay of strong interactions, fractionalization and topology in quantum matter and studies unconventional forms of spin and charge transport.

- 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 as well as the non-equilibrium properties of isolated and driven-dissipative many-body systems.

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. 133), but also international workshops and seminars (p. 140). For these we offer both logistical and technical support as well as access to facilities (seminar rooms, offices, guest houses).

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. 50). 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. 134), 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. 138).

1.4 Teaching and Training

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

Training • The **mpipks** runs the IMPRS *Many Particle Systems in Structured Environments*, which offers a well-structured PhD training (p. 14). It also participates in the IMPRS for *Cell, Developmental and Systems Biology* run by the MPI-CBG, which provides a similarly broad spectrum of lectures and courses. In addition, it is part of various third party funded structured graduate programs (p. 184).

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. 147). In addition, the institute organizes soft skill training events such as German courses or a presentation series on professional skills and career coaching (p. 188). 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. 187). 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 **mpipks** 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 July 2015 and December 2018, junior scientists (including young group leaders) of the institute were involved in the coordination of 9 out of 56 events (p. 147).

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. In this way, we can tailor our support to individual needs, profiles, and backgrounds. On average the institute hosts scientists from about 40 countries at any given time.

The **mpipks** is committed 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 scientists to apply for positions. The percentage of female researchers has increased to 18% among postdocs and to 21% among predocs holding a contract of more than three months.

To accommodate the requirements of researchers with small children the institute provides a *parent & child apartment* in one of the guest houses. This facility also gives scientists who travel with children the opportunity to participate in workshops and seminars while their children are cared for on the premises. Contact to qualified staff is facilitated by the institute upon request. When not booked for workshop participants, the *parent & child apartment* can be used by members of the **mpipks** who need to bring their 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 activities at the *Long Night of the Sciences* (p. 192), and the lecture series *Science in the Theatre* (p. 193).

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. 194): 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, whom we hope to inspire through direct contact with young researchers.

On 14th September 2018, the Max Planck Society celebrated the Max-Planck-Day, on the occasion of the 70th anniversary of the Society, the 160th birthday of Max Planck and the 100th anniversary of the award of the Nobel Prize to Max Planck. All Max-Planck-Institutes throughout Germany organized full-day programs directed at a broad public audience in 32 cities. The **mpipks** joined forces with the two other Max Planck Institutes in Dresden with an event in the City Hall, offering a broad selection of formats for the public to get an insight into the research performed at the institutes – including hands-on experiments, talks, a podium discussion and a science café (p. 192).

1.7 Research Networking

Local • The **mpipks** 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 *Quantum Chaos and Quantum Dynamics* headed by *Prof. R. Ketzmerick*, as well as in the **mpipks** participation in three clusters of excellence: *Center for Advancing Electronics Dresden*, *Physics of Life*, and *Complexity and Topology in Quantum Materials*. Other joint initiatives include the collaborative research center *Correlated Magnetism: From Frustration To Topology*, the International Max Planck Research Schools for *Cell, Developmental and Systems Biology* and for *Many-Particle Systems in Structured Environments* (p. 14), and the research training group *Itinerant Magnetism and Superconductivity in Intermetallic Compounds*. The **mpipks** 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. 184). 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. 12). The division *Condensed Matter* cooperates with the Leibniz Institute for Solid State and Materials Research Dresden and runs a joint research group with the neighbouring Max Planck Institute for the Chemical Physics of Solids (p. 14). Further collaborations connect the **mpipks** 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).

1.7.1 Center for Systems Biology Dresden



The Center for Systems Biology Dresden (CSBD, www.csbdresden.de) was established by the Max Planck Society as an intersectional collaboration. It was founded in 2013 with the signing of an operational agreement between the **mpipks** and the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG). The center is built to extend the productive and long-standing partnership between the **mpipks** and the MPI-CBG. It aims to foster cross-disciplinary research between physics, computer science and biology in collaboration with the TU Dresden.

The **mpipks** and the MPI-CBG administer the center together. The Max Planck Society provides funds for three research groups that are affiliated with the two institutes and for the division headed by Prof. Eugene Myers at MPI-CBG. It also provides funds for the ELBE postdoc program administered by **mpipks** and the ELBE PhD program administered by MPI-CBG. The Free State of Saxony financed the new building of the center and the The Federal Ministry of Education and Research (BMBF) has supported the research at the CSBD via the award of large institutional grants in 2010, 2012 and 2016. The Dresden University of Technology (TUD) partly finances one professorship, to which Ivo Sbalzarini, who is also a group leader at MPI-CBG, was appointed in 2014.

From 2013 to 2017, the center has operated as a virtual entity achieving the development of an organizational structure. This includes the hiring of new group leaders and the development and execution of the ELBE Postdoc and PhD programs. The ELBE postdoc program 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 **mpipks** and administered by **mpipks**. The ELBE postdoc program has the important role to also foster collaborations between experimentalists and theorists. Therefore, ELBE postdocs are usually 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.

The planning and construction of a new building for the center began in 2013. The current evaluation period 2015 - 2018 saw the completion of the construction, the inauguration and the occupancy of the CSBD building in 2017. The ground breaking for the building was in Fall 2014 and the first groups moved in during March of 2017. The official inauguration was celebrated on June 1, 2017, with the Minister President of the Free State of Saxony, at that time Stanislaw Tillich, and the President of the Max Planck Society, Martin Stratmann, being amongst the speakers of the ceremony.

A steering committee is responsible for the scientific management of the Center. It has representatives of both institutes and is responsible for deciding upon the scientific vision, profile of research activities, programs and technologies, as well as overseeing the allocation of shared resources (space, equipment, personnel, systems biology center funds). Only CSBD members serve on the Steering Committee. The CSBD Coordinator is responsible for external and internal communications of the CSBD, particularly ensuring the communication flow between the participating institutions. In addition, the coordinator supports the Steering Committee by enacting many of the decisions made.

The CSBD investigates integrated biological systems with a focus on spatio-temporal processes in cells and tissues. Interdisciplinary teams of physicists, computer scientists, mathematicians and biologists, work together closely, embracing the motto "Where computer science and physics meet biology". The center's vision is to develop theoretical and computational approaches to biological systems across different scales, from molecules to cells and from cells to tissues. Starting from primarily observations of spatio-temporal phenomena, we develop theoretical approaches that help to identify principles and

mechanisms underlying the self-organization of biological systems and processes. To answer such questions, we combine a unique blend of state-of-the-art genomic technologies and quantitative microscopy, with computer vision, computational science, and theoretical physics. The center engineers and develops microscopy techniques that are optimized for automated analysis by computer vision and machine learning algorithms. Such microscopy techniques provide high quality data in three space dimensions and in time that provide valuable insights that stimulate biophysical approaches. 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.

The current groups that use office space in the new CSBD building are

- Michael Hiller, (**mpipks**): Computational biology and evolutionary genomics
- Florian Jug, (MPI-CBG): Computer vision and machine learning for quantitative bioimage computation
- Frank Jülicher, (**mpipks**): Theory of biological systems
- Carl Modes, (MPI-CBG): Network complexity and systems biophysics
- Eugene Myers (MPI-CBG): Exploring cells & systems via image analysis, customized microscopy, and genomics
- Ivo Sbalzarini, (MPI-CBG and TU Dresden): Scientific computing for image-based systems biology
- Agnes Toth-Petroczy, (MPI-CBG): Protein plasticity and evolution
- Christoph Weber, (**mpipks**): Biophysics of mesoscale cellular dynamics
- Christoph Zechner, (MPI-CBG): Stochastic models of molecular networks

Furthermore, there is an additional depth in physics, computer science and biology brought by the following nine research groups that are involved in the governance and research of the CSBD as members: Jan Brugués (**mpipks**), Stephan Grill (TU Dresden), Suzanne Eaton (MPI-CBG), Tony Hyman (MPI-CBG), Moritz Kreysing (MPI-CBG), Steffen Rulands (**mpipks**), Pavel Tomancak (MPI-CBG), Vasily Zaburdaev (**mpipks**), and Marino Zerial (MPI-CBG). The program is further strengthened by its close involvement with all the researchers of the MPI-CBG and **mpipks** and the following additional CSBD affiliates: Carlo Vittorio Cannistraci (TU Dresden), Stefan Diez (TU Dresden), Benjamin Friedrich (TU Dresden), Carsten Rother (formerly TU Dresden, now University of Heidelberg), Guillaume Salbreux (formerly **mpipks**, now Francis Crick Institute London), and Axel Voigt (TU Dresden). Moreover, the CSBD has established a good relationship with the faculties of Physics, of Mathematics and of Computer Science at the TU Dresden and with the biotechnology center.



CSBD building. The Center for Systems Biology Dresden (CSBD) is jointly operated by **mpipks** and MPI-CBG in cooperation with the Technical University Dresden. Several computational and theory groups of the CSBD are accommodated in a new building that was inaugurated in 2017. The building is located next to the MPI-CBG and provides a stimulating environment for physicists and computer scientists that facilitates interactions between theory and nearby experiments. Pictures by Jussi Tiainen.

1.7.2 Joint research group with MPI-CPfS

One of the main research themes of **mpipks** is the study of collective phenomena in quantum matter. This started with Peter Fulde's activities in the field of strongly correlated electron systems, and continued after the creation of the condensed matter division headed by Roderich Moessner.

A focal point of present work is the collaboration with experimental activities at the neighbouring Max Planck Institute for the Chemical Physics of Solids (MPI-CPfS), one of whose main objectives is to study materials physics with an interdisciplinary approach from physics and chemistry. Recent years have seen the appointments of Hao Tjeng, Claudia Felser and Andy Mackenzie as directors.

This provides opportunities for a multi-faceted set of collaborations between the institutes. A joint research group between the institutes was established, which provides an organisational framework for seeding collaborations between the institutes, in particular enabling young scientists to benefit from both access to experimental work at MPI-CPfS and the theory environment at **mpipks**. It thus provides a conduit between the various groups involved in the study of strongly correlated electron physics, superconductivity and magnetism. Its current head is Takashi Oka, who established the joint group "Nonequilibrium quantum matter" in the second half of 2015.

In addition, there are many informal collaborations, for instance on the new field of electronic hydrodynamics, which has also attracted the attention of members of **mpipks** hailing from a high-energy theory background. Further, members of MPI-CPfS engaging primarily in theoretical studies can participate and contribute to activities at **mpipks**. The combined research activities of the institutes is also an important attractive aspect for recruiting young scientific talent to Dresden.

Finally, the two institutes collaborate in the framework of large-scale collaborative grant initiatives, such as in the Collaborative Research Centre "Correlated Magnetism: from Frustration to Topology" and the Cluster of Excellence "Complexity and Topology in Quantum Matter".

1.7.3 International Max Planck Research School

International Max Planck Research Schools (IMPRS) offer English language based structured doctoral programs based at Max Planck institutes in close collaboration with universities. There are about 60 such research schools across a wide range of interdisciplinary topics.

The IMPRS headquartered at **mpipks** was established in 2005 with a focus on Dynamical Processes in Atoms, Molecules and Solids. With two successful evaluations - in 2008 and 2015 - and a prolongation of the originally envisioned six year funding period through to the end of 2016, the IMPRS was renewed at the beginning of 2017 for a further six year period. With the renewal the IMPRS defined a new trajectory in response to changes in the research landscape in Dresden and further afield.

The current IMPRS for Many-Particle Systems in Structured Environments is a collaboration between groups at the following institutions in three countries

1. Technical University, Dresden - TUD
2. Max Planck Institute for the Physics of Complex Systems - **mpipks**
3. Leibniz Institute for Solid State and Materials Research - IFW
4. Institute of Low Temperature and Structure Research - ILTSR (Polish Academy of Sciences, Wrocław, Poland)
5. University of Wrocław - UW
6. Institute of Organic Chemistry and Biochemistry - IOCB (Prague, Czech Republic)
7. University of Chemistry and Technology - UCT (Prague, Czech Republic)

The IMPRS capitalizes on the strengths of the participating research groups in studying many-body interacting systems in various settings. The structured environments from which the IMPRS takes its name include optical lattice traps for cold atomic gases, solid state materials driven out of equilibrium,

organic molecules in solution undergoing light-induced chemical reactions and nuclear matter at high temperatures and densities. Understanding these systems requires exploring new directions in many-body physics and chemistry, including time-dependent ab initio calculations, quantum chaos in a many-particle context, thermalization and ergodicity breaking, and the possibility of new phases appearing in driven systems.



Participants at the joint IMPRS workshop 2017.

The school has 24 partners including 23 who act as PhD advisors for students of the graduate school and one coordinator. All matters concerning the large scale operation of the graduate school including the admission of new students, the allocation of IMPRS funds, the program of IMPRS event including the summer school and retreat are decided by the board that is composed of nine partner members. The following is a list of all IMPRS partners with board members highlighted with asterisks:

- Prof. A. Bäcker (TUD)
- * Prof. B. Büchner (IFW)
- Prof. D. Blaschke (UW)
- * Prof. G. Cuniberti (TUD)
- * Dr. A. Eckardt (mpipks)
- Dr. A. Eisfeld (mpipks)
- Dr. F. Grossmann (TUD)
- Dr. M. Heyl (MPI PKS)
- * Prof. P. Jungwirth (IOCB)
- Prof. R. Ketzmerick (TUD)
- Dr. A. Landsman (mpipks)
- * Dr. P. McClarty (coordinator, mpipks)
- * Prof. R. Moessner (spokesperson, mpipks)
- Dr. A. Nielsen (mpipks)
- Prof. T. Oka (mpipks)
- Dr. F. Piazza (mpipks)
- * Prof. J.-M. Rost (mpipks)
- Prof. U. Saalman
- Prof. P. Slavicek (UCT)
- Prof. R. Schmidt (TUD)
- Dr. I. Sodemann (mpipks)
- * Prof. W. Strunz (TUD)
- * Prof. J. Sznajd (ILTSR)
- Dr. hab. T. Zaleski (ILTSR)

The board meets approximately once per year.

There is an executive board composed of the spokesperson, coordinator and Prof. Strunz that meets biannually to carry out an initial evaluation of new applications.

1.8 Divisions and 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.

The focus of the division on many-body quantum dynamics in and out of equilibrium has intensified considerably over the last few years. We are now studying a range of selected topics in the realm of classical and quantum chaos, transport, equilibration and thermalisation, and the role of disorder and nontrivial (free) energy landscapes.

Besides this, our long-standing interest in exotic phases and topological materials is continuing, at a time when experimental studies are producing an unprecedented richness of interesting experimental findings.

Research Topics

Kitaev materials. Following the excitement surrounding the identification of a material – α - RuCl_3 – potentially realising Kitaev’s spin liquid, we have invested much effort into pinning down experimental signatures of this exotic phase, e.g. in signatures of Majorana fermions in neutron or Raman scattering. Many conceptual advances have resulted from this, e.g. the formulation of the concept of a proximate spin liquid. This has built on our exact solution of the dynamical structure factor of the pure Kitaev model, as well as our development of a matrix product operator based algorithm for simulating the real-time dynamics of quantum spin systems in two dimensions.

Inverted hysteresis. In collaboration with an experimental group at Dresden’s high magnetic field laboratory, we developed a theory for the inverted hysteresis loop found in a pyrochlore compound – in particular, exhibiting a remanent magnetisation in a direction opposite to its saturation field. This was based on the existence of a nonequilibrium population of magnetic domain walls separating nonmagnetic domains in zero field.

Discrete time crystals. In part motivated by experimental work, which detected signatures of the spatiotemporal order predicted by us, we have extended our study of such systems, now known under the name ‘discrete time crystals’ to include period tripling in parafermionic systems, as well as the fate of this phenomenon in open systems: coupling to a bath generally endows the effect with a finite lifetime.

Disordered flat bands. We have identified a family of disordered hopping models in which a flat band is present. This has built on our work on jamming in spin systems, which in turn has uncovered a rich phenomenology for static and dynamical properties of the relevant constraint-balanced disordered spin model.

Disorder-free localisation. We have identified routes for obtaining localisation in systems without quenched disorder. One of these, Stark many-body localisation, uses the presence of Bragg localisation for cold atoms in a trap, in order to mimic the phenomenology of many-body localisation; while another route involves integrability hidden by a duality transformation in a quantum quench with both translationally invariant Hamiltonian and initial state.

Topological electrons. Our extensive work on topological condensed matter physics has continued. This e.g. includes identification and analysis of a topological band structure reminiscent of a smoke ring, with a topologically protected nodal line; or the study of topological magnon band structures and their experimental signatures.

Hydrodynamic transport. We have studied signatures of the hydrodynamic transport regimes proposed for graphene and certain delafossite materials, e.g. the prediction of the emergence of a boundary layer

in the response of a laterally confined liquid ('duct flow') to an alternating external field.

Perspectives

The condensed matter division at the **mpipks** is now more than 10 years old. The period since the last scientific advisory board meeting has been a particularly dynamic period. Two group leaders, Jens Bardarson and Frank Pollmann, as well as a number of senior postdocs, have accepted offers of faculty positions. Newly arrived group leaders are Takashi Oka, whose joint group with MPI-CPfS, see below, is now firmly established; and more recently David Luitz, who specialises in computational quantum many-body physics; and Markus Heyl, who works on dynamics in correlated quantum matter. In addition, the institute has been fortunate to be able to host three independent Max Planck Research Groups leaders, two of which, Anne Nielsen, Inti Sodemann are affiliated with the condensed matter division. The third, Francesco Piazza, provides a valuable bridge to the finite systems division, to which he is affiliated.

This has provided a new focus, as well as broadened, the research profile of the division. In this context, of further note is the recruitment of Piotr Surowka, a high-energy physicist by training, who contributes a new perspective to our quantum dynamics research effort.

One research focus extending our long-standing research effort in the search for unconventional – topological nonequilibrium and other – new phases will be the investigation of regimes which are non-universal in the usual sense, but nonetheless generic. The abovementioned proximate spin liquid, as well as prethermal time crystalline regimes, provide instances of such behaviour, the importance of which lies in their robust observability compared to the concomitant 'pristine' but often masked or preempted universal regimes.

Another direction of investigation is the role of quasiparticles – and their absence – for various aspects of many-body dynamics, in particular in regimes exhibiting features of chaotic behaviour. This has received much impetus through recent studies of quantum chaos emanating from the high-energy physics community, whose relevance for realistic low-energy lattice models is in the process of being clarified. A thread combining these above two paths concerns the question of the role of (de)coherence for the observation of entangled phases in experiment.

Cooperations

- *Joint group with Max Planck Institute for the Chemical Physics of Solids:* This cooperative activity has received a redoubled impetus with the arrival of Andrew Mackenzie as a new director at MPI-CPfS, whose experimental activities have proven a popular subject for theoretical studies at MPI-PKS.

The group headed by Takashi Oka works under the heading of nonequilibrium quantum matter. Not only has it led to a number of interesting joint projects between the institutes, it has also functioned as a conduit for facilitating contact between members of MPI-PKS and experimental activities at MPI-CPfS.

The condensed matter division is actively involved in two large-scale cooperative grants. Firstly, the collaborative research center SFB 1143 at TU Dresden, entitled "Correlated magnetism: from frustration to topology"; and secondly, the cluster of excellence ct.qmat — "complexity and topology in quantum matter" where the TU Dresden has joined forces with the JMU Würzburg.

- *Manifold cooperations with theory groups internationally, e.g.:*
 - Canada: Simon Fraser University (Igor Herbut); University of Toronto (Yong-baek Kim; Sung-Sik Lee)
 - China: Chinese Academy of Sciences (Yuan Wan); Tsinghua University (Lih-king Lim)
 - France: University of Bordeaux (Ludovic Jaubert); CEA Grenoble (Mike Zhitomirsky); École Normale Supérieure Lyon (Peter Holdsworth); Université Paris VI-Jussieu (Benoît Douçot)
 - Great Britain: University of Cambridge (Claudio Castelnovo); Loughborough University (Ioannis Ruchosatzakis); Oxford University (John Chalker, Dima Kovrizhin); St. Andrew's (Chris Hooley)
 - Hungary: Budapest University of Technology and Economics (Balazs Dora)

- India: IACS Kolkata (Arnab Das, Arnab Sen); Raman Research Institute (Dibyendu Roy); Tata Institute for Fundamental Research (Kedar Damle, Subhro Bhattacharjee)
 - Italy: ICTP Trieste (Antonello Scardicchio)
 - Japan: Gakushuin University (Masafumi Udagawa); University of Tokyo (Yukitoshi Motome)
 - United States: Google (Sergei Isakov); Johns Hopkins (Oleg Tchernyshyov); University of Minnesota (Natalia Perkins); Princeton University (Shivaji Sondhi); UC Riverside (Kirill Shtengel)
- *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 – Jochen Wosnitza (ultrasound studies on frustrated magnets)
 - * MPI-CPfS - Andy Mackenzie (electron transport)
 - United States: Oak Ridge National Laboratory – Steve Nagler, Alan Tennant (Kitaev materials); Brown University - Kemp Plumb (spin liquids)

Research Group: Quantum Matter - Transport and Dynamics

(until August 2017, Head: Dr. Jens H. Bardarson)

The research group "Quantum Matter – Transport and Dynamics" was established at the **mpipks** in September 2013. Its members during the period of this report included three postdocs (Soumya Bera, Jacopo Viti and Jun-Won Rhim) and four PhD students (Jan Behrends, Younes Javanmard, Talia Lezama, and Emmanouil Xypakis). In September 2017 the group leader, Jens H Bardarson, moved to KTH Royal Institute of Technology in Stockholm, Sweden, where he took a faculty position.

The group's main interests are in the physics of quantum matter, whereby we refer to a class of materials where quantum phenomena are essential even at relatively large and experimentally relevant scales. In the last couple of years our research has focussed on three different classes of materials, topological insulator nanowires, Weyl semimetals, and many-body localized insulators. Our approach is mainly computational, and is motivated by explaining and/or suggesting possible experiments that would reveal the underlying physics, with the main probes being transport or quantum dynamics. We have collaborated with our experimental colleagues at the Max Planck Institute for Chemical Physics of Solids and The Leibniz Institute for Solid State and Materials Research both in Dresden on the topics of Weyl semimetals and topological insulator nanowires, respectively.

Topological insulators are materials that have an insulating bulk but a robust metallic surface. The metallic surface states result from an unavoidable unknottedness of the wave function of the material at the interface with vacuum (or air). On the inside the wave function is tied into a knot but not on the outside—the surface state is therefore topologically protected, as the untying of the knot needs to take place somewhere, and this results in the metallic state. An even more exotic state is obtained when such material is made into a nanowire and coupled to a superconductor. This results in the formation of Majorana modes at the ends of the wires. Majorana fermions are their own antiparticles, and in the current context the Majorana modes are best understood as resulting from the splitting of a single regular fermion into two parts, each part residing on their respective end of the wire. On the topic of topological insulator nanowires we have (i) introduced a simplified transport model that allows for an easier direct comparison with experimental results, (ii) studied the emergence of a $\nu = 0$ quantum Hall plateau induced by disorder and shown how it is reflected in conductance fluctuations, (iii) demonstrated how in the presence of magnetic field thermoelectric current through such wires can under certain circumstance flow from the cold to the hot electrode, and (iv) studied the effect of ripples in the surface of the wire on transport properties.

Weyl semimetals constitute another topological phase of matter, but one that is metallic. The topology still arises from the properties of the wave function; this time the band structure of the electrons has isolated points where the conduction and valence points touch. These points act as monopoles of Berry phase, which is a measure of the winding of the wave function. The low energy degrees of freedom, which dominate transport properties, are given in terms of Weyl fermions that come in pairs with opposite

chirality or handedness: Weyl fermions are left or right handed. We have studied several different aspect of the physics of Weyl semimetals, here we mention a few: (i) we introduced one way in which one can realize a fractional version of the Weyl semimetal through the combination of interactions and a magnetic field, (ii) we uncovered a strong dependence of the magnetoresistance in Weyl semimetals on the angle between the Weyl node separation and the magnetic field, (iii) showed that in tilted Weyl semimetals one can obtain anomalous Nernst and thermal Hall effects, and discussed how they can be experimentally observed, and (iv) showed how coupling of the different Weyl nodes can in some cases lead to a different phase of matter called nodal-line semimetal, in which the conduction and valence bands touch in a line instead of in a set of points.

Many-body localization is the interacting version of Anderson localization, in which all quasiparticles are localized and immobile. As a result, thermalization does not take place and processes and order otherwise forbidden by statistical mechanics are allowed. In particular, zero modes can be stabilized at high energies or temperatures. Many-body localization is characterized by area law entanglement in eigenstates and slow logarithmic growth after global quantum quenches. We have shown how one can (i) think of each eigenstate as being equivalent to a ground state in the sense of having a step function in the occupations (eigenvalues) of the one particle density matrix, equivalent to what happens in Fermi liquid ground states, and how (ii) the step is smeared in quantum quenches, phenomenologically similar to the effects of temperature in Fermi liquids. We have furthermore studied signatures of many-body localization in (iii) the bipartite fluctuations after a quantum quench, and (iv) the quantum mutual information.

External collaborations

- Jerome Cayssol, Universite Bordeaux et CNRS, France.
- Sigurdur I. Erlingsson and Andrei Manolescu, Reykjavik University.
- Romain Giraud and Joseph Dufouleur, Leibniz Institute for Solid State and Materials Research, IFW Dresden, Germany.
- Adolfo G. Grushin, Institut Neel, CNRS and Universite Grenoble.
- Fabian Heidrich-Meisner, Ludwig-Maximilians-Universität München, Germany
- Roni Ilan, Tel Aviv University.
- Tobias Meng, TU Dresden.
- Henning Schomerus, Lancaster University, United Kingdom.
- Kirill Shtengel, University of California at Riverside.

Research Group: Dynamics in Correlated Quantum Matter

(since September 2016, Head: Dr. Markus Heyl)

The research group Dynamics in correlated quantum matter started at the **mpipks** in September 2016. It currently consists of three postdocs (Yi-Ping Huang, Petr Karpov, and Adrien Bolens) and three PhD students (Daniele Trapin, Heiko Bura, and Roberto Verdel Aranda). During the first two years also two summer internship students were hosted (Vikram Ravindranath and Abijith Krishnan).

The central research objective of this group is the study of the dynamics in quantum many-body systems. The interplay of quantum correlations imposed by interactions and dynamics can lead to complex phenomena ranging from new kinds of phase structures to universal behavior in real-time evolution. It is the main goal to identify general principles underlying such complex dynamical quantum processes and to develop a systematic understanding not only for specific problems but rather whole classes of phenomena. This research is not only driven by fundamental theoretical questions. It is also guided by the recent experimental progress in so-called quantum simulators, where nowadays access to the dynamics in correlated quantum matter has been achieved with unprecedented control. In this context we also work closely with experimental groups to identify and propose feasible experiments. Within the last two years, the group has focused particularly onto the following main lines of research:

Dynamics in nonergodic and constrained quantum many-body systems

It is the central property of ergodic systems to exhibit relaxation towards equilibrium independent of initial conditions when they are evolved for a long time. Thus, in order to generate long-lived quantum states with inherent nonequilibrium properties it is essential to induce nonergodic behavior. We have explored various questions in this direction. First, we have studied many-body localized systems, where nonergodicity originates from imposing strong disorder. In this context we have (i) studied implications

of nonergodicity onto time-irreversibility, (ii) formulated a theory of dynamical potentials in order to explore whether a macroscopic description of many-body localized systems is possible, (iii) constructed an experimentally feasible observable to measure many-body localized spin-glass order, and (iv) developed an efficient solution of many-body localized systems at very strong disorder, which we further utilized to study the influence of an environment onto the many-body localized phase. Second, we have investigated nonergodic and metastable states imposed by other constraints: (i) we have shown that lattice gauge theories can generically exhibit nonergodic behavior without imposing disorder but rather caused by gauge invariance and (ii) we have contributed to an experiment which has observed a metastable prethermalized state in a periodically driven quantum many-body system, where the dynamical constraint is imposed by a large driving frequency.

Dynamical quantum phase transitions

Another general route towards creating nonequilibrium states of quantum matter is to perturb a system strongly at some instant of time and to study the subsequent dynamics on intermediate time scales before final relaxation takes place in the long run. It is one main purpose of the research in this group to identify general principles of such dynamics through the lens of the theory of dynamical quantum phase transitions. As opposed to conventional equilibrium phase transitions which are driven by a control parameter such as temperature, these dynamical transitions occur during nonequilibrium real-time dynamics with physical quantities becoming nonanalytic as a function of time. In this context we have (i) been working on ideas to formulate analogs to Landau theories for these dynamical quantum phase transitions, (ii) collaborated with several experimental groups to observe signatures in systems of ultra-cold atoms in optical lattices, trapped ions, and quantum walks, (iii) contributed reviews summarizing the recent progress in this field, and (iv) have studied dynamical quantum phase transitions for particular model systems such as lattice gauge theories or collapse and revival oscillations in a superfluid.

Quantum dynamics and quantum information

Many concepts from quantum information theory have become central for the characterization of quantum many-body systems and their dynamics. This includes quantum entanglement, which we (i) have analyzed in the nonequilibrium dynamics of a quantum spin model experiencing dynamical quantum phase transitions in a recent experiment and (ii) have studied its spatial structure both in ground and finite-temperature states of the paradigmatic transverse-field Ising chain. Further, we have shown that so-called out-of-time ordered correlators, originally proposed to quantify the spreading and scrambling of quantum information, can also be utilized to detect phase transitions in quantum Ising models in a dynamical fashion. Today, the rapid development in quantum computing devices opens up a further interface between quantum many-body theory and quantum information science. Specifically, these devices are now beginning to touch a regime, where many-body effects play an important role. In this context, we have studied an inherent error source originating from time discretization in so-called digital quantum simulation, where quantum computers are utilized to simulate the dynamics of quantum many-body models. In particular, we have shown that the formal question of time discretization errors is intimately linked to a quantum localization phenomenon and therefore endowed it with a physical meaning. This further explains the weak discretization error observed experimentally in the digital quantum simulation of quantum electrodynamics in one dimension, which was supported by our theoretical contributions.

Collaborations with theory groups

- Prof. Peter Zoller (IQOQI Innsbruck, Austria): quantum information
- Prof. Marcello Dalmonte (ICTP Trieste, Italy): lattice gauge theories and constrained systems
- Prof. Balazs Dora (Budapest University of Technology and Economics, Hungary): universal behavior in quantum dynamics
- Prof. Soumya Bera (Indian Institute of Technology Bombay, India): Many-body localization
- Prof. Frank Pollmann (TU Munich, Germany): Quantum dynamics and many-body localization
- Dr. Philipp Hauke (University of Heidelberg, Germany): quantum dynamics and quantum information
- Prof. Michael Knap (TU Munich, Germany): Quantum quenches
- Prof. Alessandro Silva (SISSA Trieste, Italy): Dynamical quantum phase transitions
- Prof. Jan Carl Budich (TU Dresden, Germany): Dynamical quantum phase transitions

Collaborations with experimental groups

- Prof. Rainer Blatt (IQOQI Innsbruck, Austria): Quantum dynamics in spin chains

- Prof. David Weld (University of California, Santa Barbara, USA): Floquet prethermalization
- Prof. Guang-Can Guo (University of Science and Technology of China, Hefei, China): Quantum walks
- Prof. Klaus Sengstock and Christoph Weitenberg (Institut für Laserphysik, Universität Hamburg, Hamburg, Germany): Nonequilibrium dynamics in topological systems

Research Group: Topology and Correlations in Condensed Matter

(until December 2016, Head: Dr. Frank Pollmann)

The research group “Topology and Correlations in Condensed Matter” was established at the **mpipks** in January 2011. In 2017 Frank Pollmann took up an associate professorship appointment at the Technical University of Munich and the group successively moved to Munich.

Our group is interested in a variety of problems in Condensed Matter Theory. The main focus lies on the study of phenomena which arise due to quantum mechanical effects in systems of correlated electrons. Areas of research include the study of topological phases of matter, dynamical properties of quantum many-body systems 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 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 a number of strongly correlated electron and spin-systems: (i) We showed that the kagome chiral spin liquid can be understood as a gauged $U(1)$ symmetry protected topological phase. (ii) We found a bosonic integer quantum Hall effect in an interacting lattice model— a prominent example of a symmetry protected topological phase. (iii) We studied one-dimensional symmetry protected topological phases and their transitions. For specific critical points, we identified exponentially localized symmetry protected edge modes despite the presence of algebraic correlations in the bulk.

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 found, using large scale density matrix renormalization group simulations, that the paradigmatic kagome Heisenberg antiferromagnet shows signatures of Dirac cones. (ii) We investigated the stability of the spin-1/2 kagome ground state with breathing anisotropy. (iii) We identified a continuous easy-plane deconfined phase transition on the kagome lattice.

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 developed new algorithms that allow to efficiently obtain highly excited eigenstates of MBL systems using the matrix-product state representation. (ii) We explored quantum mutual information as a probe for MBL. (iii) We characterized the time-irreversibility in disordered fermionic systems by the effect of local perturbations.

Dynamics of two-dimensional quantum spin systems—Determining the dynamical properties of quantum spin systems is a very challenging task. We introduced a combination of the density-matrix renormalization (DMRG) ground state method and a matrix-product states based dynamical algorithm to obtain response functions for generic two-dimensional spin systems. With this we are able to access the dynamics of different phases that can occur in frustrated systems. Moreover it is also very useful for regular ordered phases where one would conventionally use large- S approximations, which in some cases cannot qualitatively explain certain high energy features: (i) We investigated the dynamics of the Kitaev-Heisenberg model with and without an applied magnetic field (ii) We studied the quantum dynamics of the square-lattice Heisenberg model. (iii) We demonstrated that strong quantum interactions can prevent quasiparticle decay—we found this mechanism at work in the spin-1/2 triangular lattice Heisenberg antiferromagnet.

Collaborations

- *University of California, Berkeley*: Collaborations with Joel Moore, Mike Zaletel, and Ehud Altman and several members of their groups on numerically simulating the dynamics of quantum-many body systems out of equilibrium
- *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
- *Princeton University*: Collaboration with Shivaji Sondhi on efficient simulations of many-body localized systems

Research Group: Computational Quantum Many-body Physics

(since April 2018, Head: Dr. David Luitz)

The research group “*Computational Quantum Many-Body Physics*” was established at **mpipks** in April 2018. It currently consists of two PhD students (Luis Andres Colmenarez Gomez and Robin Schäfer) and has hosted one summer intern (Owen Howell) from June to September 2018.

Our group studies quantum many-body systems relevant in condensed matter and ultracold atoms experiments. We focus in particular on phenomena which are due to strong interactions between particles and consider both equilibrium and out of equilibrium situations. Recent research foci include frustrated quantum magnets, thermalization of quantum systems with unitary dynamics, periodically driven and open quantum systems and many-body localization. We develop state of the art numerically exact techniques to simulate quantum many-body systems such as exact diagonalization, Krylov space exact time evolution, matrix product state techniques as well as tensor networks and Quantum Monte Carlo.

Thermalization. Isolated quantum systems undergo unitary dynamics governed by the Schrödinger equation and can therefore not reach a mixed state of the full system if prepared initially as a pure state. Consequently, this appears to be an obstacle for thermalization. It is now understood that thermalization can nevertheless occur for a subsystem, since the rest of the isolated system can serve as a heat bath. We have shown numerically that the entire reduced density matrix of eigenstates of the Hamiltonian of generic spin chain becomes indeed identical to the grand canonical density matrix. This implies that the eigenstate thermalization hypothesis (ETH) holds for any operator in the subsystem. Interestingly, if disorder is added to interacting spin chains, the dynamics in the system slows down, leading to subdiffusive transport. We have found that this is accompanied by a slow power law growth of the entanglement entropy, while diffusive systems exhibit a linear growth. A detailed study of the statistics of eigenstate expectation values of local operators not only represented the so far largest quantitative test of ETH but also revealed that subdiffusive transport leads to a modified scaling of these expectation values with system size, leading to a generalized formulation of ETH.

Many-body localization. Strong disorder leads to exponential localization of noninteracting particles, a phenomenon which is known as Anderson localization. Surprisingly, strong enough disorder leads to a localized phase even in the presence of interactions, and there is a dynamical many-body localization transition in one dimensional quantum many-body systems at a critical disorder strength. We have found in one of the largest exact diagonalization studies in the field that the critical disorder strength depends on the energy density of the considered eigenstates of the Hamiltonian. This was an important confirmation of the theoretical prediction of the existence of a many-body mobility edge. Current work focuses on a deeper understanding of the nature of the MBL transition, since theoretical works suggest that it is driven by an instability towards thermal inclusions, which can thermalize the entire system under certain conditions. We have provided numerical confirmation of this picture in a simple toy model.

Periodically driven quantum many-body systems. Time dependent Hamiltonians generally do not conserve energy and are therefore of fundamental interest for the understanding of the role of conservation laws, but are also important to describe experiments e.g. with periodic modulations of electromagnetic fields by microwaves. The stroboscopic dynamics of periodically driven quantum systems can be understood by introducing an effective Hamiltonian, however it is not immediately clear if this Hamiltonian is local. We have studied transport properties of the stroboscopic dynamics and provided the first clear evidence that stroboscopic transport in generic periodically driven systems is diffusive. Furthermore, we have constructed an interacting driving protocol which can lead to a perfect subharmonic revival of the initial wave function at arbitrary multiples of the underlying driving period.

Frustrated quantum magnets. As part of a collaboration in the SFB1143, our group studies model systems for frustrated quantum magnets, relevant for example for the understanding of α RuCl₃ or pyrochlore. We develop several techniques for a numerically exact simulation of such systems at finite and zero temperature, to extract thermodynamic and dynamical properties. One particular goal of this project is the calculation of the frequency and momentum resolved dynamical spin structure factor. We use powerful exact Krylov space time evolution techniques based on quantum typicality as a computational baseline and are currently developing tensor network approaches to tackle larger system sizes.

Collaborations.

- Ben Gurion University, Beer Sheva, Israel: Collaboration with Yevgeny Bar Lev on quantum information spreading, slow dynamics and many-body localization.
- Technical University of Munich, Germany: Collaboration with Frank Pollmann on tensor network techniques for one and two dimensional quantum many-body systems.
- KU Leuven, Belgium: Collaboration with Wojciech de Roeck on the stability of many-body localization.
- University of Loughborough, UK: Collaboration with Achilleas Lazarides on open quantum many-body systems.
- Harvard University, USA: Collaboration with Vedika Khemani on prethermal time crystals.
- CNRS and Université Paul Sabatier, Toulouse, France: Collaboration with Fabien Alet on dynamical simulations of quantum many-body systems.

Division: Finite Systems

(Head: Prof. Jan Michael Rost)

The department *Finite Systems* studies the behavior of finite microscopic systems and their interaction with an environment in the extreme regimes of ultracold and ultrafast dynamics. Finiteness can refer to a finite number of particles, e.g., atoms or molecules, to geometric restrictions in real space or in abstract mathematical spaces, such as the Hilbert space for quantum problems. The environment can consist of similar entities as the atom or molecule under consideration (e.g., clusters, quantum aggregates, ultracold gases). Light from intense pulses or in microcavities provides another, quite universal kind of environment. Thirdly, noise creates an important class of environments, also studied at **mpipks** outside the *Finite Systems* department in various contexts, from breathers over chaotic dynamics to biological systems.

The research group *Finite Systems* within the department concentrates on fundamental time-dependent mechanisms in light-matter coupling inspired by rapid technological development towards ultrashort pulses (attosecond science) and short X-ray pulses (project leader *Ulf Saalmann*), strong field dynamics in matter with periodic structures (project leader *Lukas Medisauskas*) and on Rydberg excitations in random as well as regular environments. 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*. Through the research group *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. Furthermore, the affiliated Research Group *Strongly Correlated Light-Matter Systems*, headed by *Francesco Piazza* provides a fruitful bridge to the condensed matter department.

Research topics

Non-adiabatic light driven electrons in ultrafast and ultracold dynamics. Loosely bound electrons cannot follow the change of the envelope of ultrashort pulses. Ensuing non-adiabaticity leads to new ionization phenomena such as photoionization by pulse envelope derivatives. Since the condition for non-adiabatic driving is the slow electron time scale relative to the driving period, such phenomena can occur also in experiments of ultracold molecular photo-association to bound states with energies of less than a MHz by pulsed magnetic fields of milliseconds duration.

Deconvolution of dynamics induced by noisy XFEL pulses with machine learning. SASE generated XFEL pulses without seeding are naturally noisy. In other situations the measured signal is noisy due to unavoidable experimental circumstances. We use machine learning concepts to “purify” a noisy measurement in order to predict what the de-noised pulse looks like and how, e.g., the purified electron spectrum would look like under the de-noised pulse.

Low-energy electrons. 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. Measuring slow electrons poses a challenge to experiment and we have collaborated with experimental groups to understand the influence of laser pulse length and very small electric fields on low energy photoionization dynamics in generic situations. Low energy electron escape (also in non-adiabatic light driven dynamics) builds an obvious bridge to ultra cold Rydberg dynamics, a major activity in the department.

Ultracold Rydberg aggregates. Embedded Rydberg systems with their inherently small energy scales require an ultracold environment to be sustainable. In most applications the focus is on electron dynamics (“frozen gas”) with the atomic motion as an annoying but unavoidable fact. With Rydberg aggregates we incorporate atomic motion explicitly and focus on its interplay with electronic dynamics akin to chemical dynamics which preserves coherence by motion of the atoms moving according to the forces exerted by the electronic (Rydberg) excitations.

Nano-mechanical Rydberg hybrid systems. Apart from their very small energy scale Rydberg systems are also quite large and provoke the question if this property can be beneficially used to interface them with nanomechanical systems. In this context we have explored the possibility to achieve cavity-free cooling by coupling a nanomechanical mirror with an ultracold gas exploiting EIT with laser light. In a second scenario we have investigated the feasibility of quantum non-demolition experiments using the coherent interaction of a nanomechanical oscillator with a Rydberg-atomic waveguide, both hosted on a microfabricated chip.

Rydberg excitations in structured environments. Triggered by our counter-intuitive discovery that long-range Rydberg molecules formed from a Rydberg atom and a ground state atom, so called “trilobites”, thrive in their natural environment of an ultracold gas (of ground state atoms) with thousands of atoms in the volume of the Rydberg orbital, we have started to investigate Rydberg excitations in structured environments. Particularly promising is the symmetry-breaking combination of a highly excited Rydberg atom (high density of states) with an atomic monolayer which leads to an intriguing electron spectrum with energy bands as a function of lattice spacing.

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 the general trend to simulate experimental results in particular in FEL-matter interactions, we will 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, in particular by extracting (timescale-)separations often hidden.

Along the same lines our interest in machine learning concepts is geared not to simulating specific situations but rather towards the question if ML is of value to aid theory and to identify (may be hidden) physical mechanisms in the interaction of light with matter.

Regarding ultracold Rydberg dynamics we will exploit the high density of Rydberg states to address questions of localization of Rydberg systems in structured environments and the relation to semiclassical dynamics and scarring phenomena.

Cooperations

- Prof. M. Beims (Curitiba, Brazil) on semiclassical theory,
- Prof. Dörner (Uni Frankfurt) regarding slow electrons in strong field ionization,
- Prof. Greene (Purdue University, USA) on ultracold non-adiabatic effects,
- Prof. L. di Mauro, (Ohio State Univ., USA) on long-wavelength light illuminating clusters,
- Prof. Pfeifer (MPI for Nuclear Physics, Heidelberg) regarding ionization in XUV pulses,
- Prof. Singh (ITER, Mohali, India) on attosecond ionization.
- Through participation in two Priority Networks of the DFG, PP 1840 *Quantum Dynamics in Tailored Intense Fields* and PP 1929 *Giant Interactions in Rydberg Systems*, we are closely connected to groups active in those fields of ultrafast and ultracold dynamics, respectively.

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 one PhD student (Ghassan Abumwis) and one postdoc (Fulu Zheng). During the evaluation period three students finished their PhD (David Schönleber, Alan Celestino, Panpan Zhang) and the group hosted several postdoctoral guest scientists (Zengzhao Li, Himangshu Goswami, Chris Bentley, Xing Gao).

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

Self-assembled organic-dye aggregates. In recent years we focussed on organic dyes on surfaces. For example, together with the experimental group of Prof. Sokolowski (U. Bonn) we investigated organic molecules which form two-dimensional domains on dielectric materials like KCl or NaCl. The dielectric is used as a template to induce specific arrangements of adsorbed molecules. We found that electronic excitation of these molecules is delocalized across hundreds of molecules at low temperature. This results in superradiance. By investigating the temperature dependence of the superradiance we predicted the existence of optically dark states at the bottom of the exciton band. This finding motivated us to suggest the use of metallic-tip-based near-field spectroscopy to gain access to the many optically dark states. We found that with this technique one can indeed obtain detailed information about the interactions and decoherence properties of the aggregate. Another system we investigated was acene molecules deposited on neon clusters. The experimentally observed lifetime reduction was traced back to a combination of superradiance and singlet fission. These studies were carried out together with the experimental group of Prof. Stienkemeier (U. Freiburg).

In addition to these studies that are directly related to experiment, we have also considered general questions about the non-radiative decay of dipole-dipole interacting molecules. Here we have, for example, found that via aggregation one can strongly tune the non-radiative loss dynamics. This has important consequences for the design of optical systems where a strong fluorescence intensity is desired. As a possible new application of molecular aggregates we suggested tubular aggregates of organic dyes to be used in luminescent solar concentrators.

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 in deriving 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. In the last years we have made important improvements regarding the truncation of the hierarchy, which allows us now to treat systems with up to 100 molecules. 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. We were also able to extend the formalism to time-dependent Hamiltonians, which allowed us to treat multidimensional femtosecond spectroscopy in a non-perturbative way.

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 the group of Prof. Aspuru-Guzik (Harvard) we investigated the possibility to use superconducting circuits for this task. 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 also promising candidates. In particular, in both cases we could show that it is possible to achieve thermalization of the system eigenstates. The parameters entering the simulator are obtained using machine learning approaches.

Phase-modulated femtosecond spectroscopy. Recently, the experimental group of Prof. Stienkemeier (Uni Freiburg) developed a new variant of phase-modulated femtosecond spectroscopy, that allowed them to detect many-body coherences in dilute atomic gases. We provided the basic theoretical framework to describe their technique. At the moment we are trying to discover the origin of strong many-body signals that have experimentally been observed in extremely dilute gases.

Cooperations

- Prof. Aspuru-Guzik (Harvard University, Cambridge, USA): Quantum simulators.
- Dr. Croy (TU Dresden): Nano-electro mechanical devices; quantum rotors.
- Prof. Engel (University of Würzburg, Germany): Molecular dimers, 2D spectroscopy.
- Prof. El-Ganainy (Michigan Tech, USA): Non-linear photonics.
- Prof. Hauer (Wien, Austria): Spectroscopy of organic dye aggregates.
- Prof. Knoester (University of Groningen, Netherlands): Unconventional disorder and localization.
- Prof. Rost (**mpipks**): Rydberg trilobites.
- Prof. Sokolowski (Uni Bonn, Germany): PTCDA monolayers on dielectric surfaces, superradiance.
- Prof. Stienkemeier (Uni Freiburg, Germany): Phase-modulated femtosecond spectroscopy
- Prof. Strunz (TU Dresden, Germany): Stochastic Schrödinger equations.
- Prof. Whitlock (Strassburg, France): Dynamics of driven Rydberg assemblies
- Prof. Wüster (IISER Bhopal): Rydberg aggregates.
- Prof. Yacomotti (CNRS UPR 20): Photonic molecules

Research Group: Complex Dynamics in Cold Gases

(until February 2017, Head: Dr. Thomas Pohl)

The group was established in September 2008, and hosted an average number of 8 to 10 group members. During the reporting period we have been active in several national and European wide initiatives, such as the SPP 1929 GiRyd, H2020 FET-Open (Xtrack) project "HAIRS", H2020 FET-PROACTIVE network "RySQ" and most recently the H2020 FET-Open (Xtrack) project "ErBeStA". In early 2017, the group moved to Aarhus University, Denmark, where it is currently funded through a Niels Bohr Professorship by the Danish National Research Foundation. Two PhD students, Callum Murray and Valentin Walther, have moved with the group from the **mpipks** to Aarhus at an early stage of their studies and will graduate in Dresden this year.

During its final year at the **mpipks**, the group's primary research interest was focussed on the physics of highly excited atomic gases in the context of quantum optical phenomena, atomic and molecular processes and many-body dynamics. Understanding the interplay of interactions, coherence and dissipation that drives the quantum dynamics of light and matter excitations in such systems lies at the core of our research. Specific research directions include:

Quantum simulations The pursuit of synthetic systems for quantum simulations of many-body systems has remained an active frontier in AMO research. Our research aims at advancing the scope and capabilities of this approach by exploring new ways of manipulating ultracold atoms with laser light and other external fields. In particular, we are interested in the properties and many-body dynamics of such synthetic quantum systems in and out of equilibrium and closely collaborate with experimental groups on actual implementation. One such experiment, performed at the MPQ, succeeded to generate a strongly interacting quantum magnet with record-setting coherence times using weak optical coupling to high-lying states of atoms in an optical lattice.

Quantum many-body optics Rooted in our elementary understanding of light lies the notion that photons in vacuum do not interact with one another. This defining property is crucial to optical communication technologies, as it enables low-loss and light-speed transmission of information over long distances. Yet, the ability to engineer such interactions synthetically holds profound implications for both fundamental and applied science, and has since ushered in a new era of research into nonlinear optics at the ultimate quantum level. In our group, we investigate such interactions and search for new mechanisms for their emergence and control in various systems from cold atoms and thermal vapour to solid-state settings, such as semiconductor cavities or excitons in two-dimensional monolayer materials.

Quantum gases Related to the activities outlined above, the physics of ultracold quantum gases has generally been a continual focus of our research interest. Here, we have explored new collective phenomena that emerge from long-range interactions, as induced by dipolar exchange reactions or mediated by photons in constrained geometries. Most recently, we have studied quantum impurity problems in atomic Bose Einstein condensates, whereby the immersion of an impurity atom, in the form of another atomic species or electronic state, triggers the formation of a polaron quasiparticle state. Here we are investigating the quantum dynamics of this formation process, aiming to understand and identify the general mechanisms and characteristic timescales of the associated dynamics. Ultimately, such a dynamical theory will provide an enabling framework for studying quantum optical settings in which photons couple to internal states of atoms, leading to the emergence of quasiparticles with polaronic and polaritonic character, suggesting a promising route to quantum nonlinear optics in ultracold quantum gases. The coherence properties and emerging interactions of such systems have remained largely unexplored and are currently being studied using various approaches in our group.

Cooperations

- Collaborations with theory groups
 - Prof. Georg Bruun (Aarhus University) [Bose polarons]
 - Prof. Alexey Gorshkov (Joint Quantum Institute) [photon interactions]
 - Prof. Stefan Scheel (Rostock University) [Rydberg excitons]
 - Prof. Tommaso Calarco (Forschungszentrum Jülich) [optimal control of lattice gases]
 - Prof. Stefan Skupin (University of Lyon), [nonlocal nonlinear optics]
 - Prof. Wieslaw Krolikowski (Australian National University) [nonlocal nonlinear optics]
- Collaborations with experimental groups
 - Prof. Jan Arlt (Aarhus University), [Bose polarons]
 - Prof. Immanuel Bloch (MPQ), [synthetic quantum magnets]
 - Prof. Mikhail Lukin (Harvard University), [interacting photons]
 - Prof. Vladan Vuletic (MIT), [interacting photons]
 - Prof. Sebastian Hofferberth (University of Southern Denmark), [interacting photons]
 - Prof. Manfred Bayer (University of Dortmund), [Rydberg excitons]
 - Prof. Vinod Menon (CUNY), [quantum optics in 2D materials]

Division: Biological Physics

(Head: Prof. Frank Jülicher)

The division *Biological Physics* focuses on the study of spatiotemporal phenomena in biological systems ranging from molecules to cells and tissues. Living matter is fundamentally active and driven far from thermodynamic equilibrium by constant supply of free energy. It can exhibit a number of fascinating behaviors that are associated with its active nature. Examples are active force generation, spontaneous movements and flows, nonlinear oscillations, the formation of complex spatial patterns and morphologies and unconventional active material properties. A key insight of research of the last decade is that biological morphologies and dynamic structures typically emerge from mechanochemical processes which tightly integrate mechanically active processes with chemical patterns. We develop the theory of nonequilibrium systems and of living matter with the aim to identify fundamental principles and key concepts that underlie the spatiotemporal organization of biological systems.

Recent research activities include:

Theory of active surfaces. The dynamics of cells is driven by active processes on the molecular scale such as the force generation of molecular motors that move along filaments of the cytoskeleton. Such active processes on small scales lead on large scales to emergent out-of-equilibrium phenomena. Key examples are spontaneous flows and oscillations, active stresses and unconventional material properties. We have extended hydrodynamic theories of active fluids and gels to address the physics of effectively two-dimensional thin sheets of active matter that are embedded in three-dimensional space. Such active surfaces can exhibit flows and pattern formation on curved manifolds and can undergo spontaneous shape changes driven by internally generated forces and torques. A key example is the self-organized dynamics of surface shape driven by mechano-chemical processes. This theory has applications for cell and tissue shape changes as well as the organization of the cytoskeleton during cell division.

Generic properties of stochastic entropy production. Stochastic thermodynamics captures fluctuations of thermodynamic quantities in mesoscopic systems. We have addressed fluctuations of entropy production in nonequilibrium steady states. Entropy production quantifies the degree of irreversibility of a process. Application of decision theory reveals that the optimal time to decide on the arrow of time for a given stochastic process is when the entropy production for the first time passes a threshold value. Furthermore, it can be shown that the negative exponential of entropy production in units of k_B is a so-called martingale, i.e. a stochastic process without drift. From this martingale property a number of universal properties of stochastic entropy production can be derived that provide for example bounds on the distribution of extrema and infima of entropy production. These theoretical insights in irreversibility and fluctuations of nonequilibrium systems have implications for the behaviors of molecular motors and other active molecular processes.

Physics of chemically active droplets. Droplets formed by liquid-liquid phase separation concentrate specific chemical components and can therefore act to spatially organize chemical processes. We are developing general theoretical approaches that combine the physics of multicomponent phase separation with the thermodynamics of chemical reactions. We have identified shape instabilities that can lead to the spontaneous division of active droplets, providing a minimal model for division that stimulates our thinking about physical mechanisms underlying early division of protocells at the origin of life.

Phase separation as organizer of cellular biochemistry. Living cells use phase separation of protein components and nucleic acid polymers to assemble organelles that localize specific biochemical processes. In collaboration with biologists in Dresden we investigate the physics and the material properties of such intracellular protein condensates. Important questions concern mechanisms of positioning of protein condensates in a cell, the effects of temperature changes as well as the role of pH changes on phase separation.

Symmetry breaking of cells. During morphogenesis when complex structures form from initially symmetric cells, spatial symmetries have to be broken. One important situation is that cells themselves break symmetries. We have investigated physical mechanisms underlying the establishment of cell polarity, axial asymmetries and cell chirality. In many cases, symmetry breaking cues guide cell symmetry breaking. In the case of cell polarity, the position of the centrosome can provide such cues. In the case of cell chirality, it is the chirality of biomolecules that guides symmetry breaking.

Emergence of tissue shape and size. Developing tissues form complex shapes and morphologies and have to grow to a specific size. Shape and size arise from the collective interplay of cell populations in a

tissue. We have recently identified a critical point in the dynamics of tissue growth regulated by growth factors. This critical point introduces scale invariance and ensures scalable morphologies during growth. Tissue shape is governed by anisotropic active processes in a tissue. Furthermore, mechanical boundary conditions at the tissue margins can guide the emergence of the tissue shape.

Collective dynamics of oscillators in biology and engineering. Interacting dynamical oscillators play important roles in many biological systems. Such oscillations can be mechanical, genetic or biochemical in nature. We are also applying concepts initially developed for biological systems to engineering and study the self-organization of phase-locked loops to provide common time references in distributed electronic networks. Because of the high clock rate of such systems (GHz), centimeter distances at the speed of light imply significant communication delays that can help synchronisation.

Integration in the Dresden scientific environment

This research program is conducted in close collaboration with several experimental groups. Most important is a tight and longstanding collaboration with the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG) in Dresden. This collaboration is fostered by the Center for Systems Biology Dresden (CSBD) which is jointly operated by the two Max Planck Institutes in collaboration with the technical university Dresden. The new building of the center was inaugurated in 2017. It now provides ideal opportunities for close collaborations between physics, computer science and biology. Our group is integrated in the International Max-Planck Research School for Cell, Developmental and Systems Biology, managed by the MPI-CBG. This provides many opportunities for recruitment and training of interdisciplinary PhD students. Within the Dresden campus, we also interact closely with the Biotec Center of the TU Dresden. In the context of the excellence initiative of German universities, our group participated in the cluster for excellence "Center for advancing electronics Dresden" that was funded from 2012-2018. We contributed strongly to the design of a proposal for a new cluster of excellence on the "Physics of Life". This project was recently approved for funding and will start operations in 2019. The new cluster will substantially strengthen the biophysics research environment in Dresden with the establishment of several new professorships at TU Dresden, and it will also raise the attractiveness of Dresden for biophysics students.

Cooperations

- Max Planck Institute of Molecular Cell Biology and Genetics, Dresden
 - Collaborations with Anthony Hyman and Moritz Kreysing on protein condensates and cellular biophysics.
 - Collaborations with Suzanne Eaton, Gene Myers, Jochen Rink and Marino Zerial on the dynamic organization of tissues
- TU Dresden
 - Collaboration with Christian Dahmann on fold formation in two-dimensional tissues.
 - Collaboration with Gerhard Fettweis on the use of distributed clocks in electronic networks.
 - Collaboration with Stephan Grill on the establishment of cell polarity.
 - Collaboration with Jens-Uwe Sommer on the positioning of droplets.
- Institut Curie, Paris
 - Collaboration with Jean-Francois Joanny and Jacques Prost on cell and tissue physics.
 - Collaboration with Pascal Martin on the physics of collective motor systems.
- Francis Crick Institute, London
 - Collaboration with Guillaume Salbreux on the physics of active surfaces.
- École Polytechnique Fédérale de Lausanne
 - Collaboration with Andy Oates on oscillating gene expression.
- University of Geneva
 - Collaboration with Marcos González-Gaitán on the dynamics of tissue growth factors and mechanisms of growth control.

Research Group: Collective Dynamics of Cells (until December 2018, Head: Dr. Vasily Zaburdaev)

The group *Collective Dynamics of Cells* was active at **mpipks** from 2012 to 2018. Our focus is on developing and applying methods of statistical physics to biological problems. We greatly benefited from the very active biophysical community and participated in a number of joint projects with experimental groups in Dresden. In this period, 7 postdocs passed through the group, while one of them moved on to a Junior Professorship position (W1, Tenure-track) and another later joined **mpipks** as a group leader. Furthermore, 2 PhD students graduated in 2018 and 3 Master students wrote their thesis in our group. Most of our research projects are performed in close collaboration with experimental groups. Here we briefly describe some of them while below two further projects are presented in greater detail.

Exactly solvable dynamics of polymer loops. In our previous work, we introduced a model of forced polymer loops to describe chromosomes during meiosis in fission yeast. In meiosis, the chromosomes are forming loops and are actively pulled together with the whole nucleus through the elongated cell in an oscillatory manner. It is believed that the oscillations are necessary to help aligning the chromosomes for recombination. We have shown that the viscous drag force indeed can suppress the fluctuations in chromosome conformation and thus reduces the distance between the homologous regions of the DNA. Our approach based on theory of random walks with a loop constraint could only address the statistics of the steady-state configurations of the chromosomes while leaving the dynamics out of reach. In a recent effort, we could also analytically solve for the dynamics of loops. We could show that a problem of forced polymer loops could be mapped to an asymmetric simple exclusion process with reflecting boundary conditions. The dynamics of the particle system can be solved exactly using the Bethe ansatz. We thus can fully describe the relaxation dynamics of forced polymer loops. In the steady state, the conformation of the loop can be approximated by a combination of Fermi–Dirac and Brownian bridge statistics, while the exact solution is found by using the fermion integer partition theory. With the theoretical framework presented here we establish a link between the physics of polymers and statistics of many-particle systems opening new paths of exploration in both research fields. Our results could be applied to the dynamics of the biopolymers which form closed loops. In application to fission yeast chromosomes dynamics in meiosis, we could estimate the characteristic relaxation times of the loops and show that it was below the typical period of nuclear oscillations. This observation thus justifies that the steady-state statistics we obtained previously indeed can be used to estimate the effect of chromosome alignment by pulling in the viscous nucleoplasm.

Stochastic model for polymerase transcription through nucleosomal barriers. In eukaryotes, gene expression depends on chromatin organization. However, how chromatin affects the transcription dynamics of individual RNA polymerases has remained elusive. The basic unit of DNA compaction into chromatin are nucleosomes – protein complexes around which the DNA molecule is wrapped and thus forms a structure which is often referred to as beads on a string. In a project together with the Grill lab in Dresden, we investigated the process of RNA polymerase II (Pol II) transcription on a DNA template containing just two nucleosomes. In experiments, we used dual trap optical tweezers to study a single yeast Pol II molecule transcribing along the DNA template. The observed slowdown and changes in pausing behavior of Pol II within the nucleosomal region allowed us to determine the so called drift coefficient, χ which characterizes the ability of the enzyme to recover from a nucleosomal backtrack (a switch from the directed elongation to a random-walk-like motion of the polymerase before it returns to the elongation mode). Notably, χ can be used to predict the probability to pass the first nucleosome. Importantly, the presence of a second nucleosome changes χ in a manner that depends on the spacing between the two nucleosomes, as well as on their rotational arrangement on the helical DNA molecule. We could develop an advanced stochastic model of Pol II transcription on the nucleosomal DNA. This model includes most major processes of Pol II transcription such as directed elongation, backtracking, recovery and cleavage, effects of the assisting force, and the slowing down of the polymerase in the nucleosomal region. Remarkably, this model has no free parameters: all necessary rates can be directly obtained from the experimental data. The model predicts the Pol II passage probabilities in full agreement with the experiments. Our results indicate that the ability of Pol II to pass the first nucleosome is increased when the next nucleosome is turned away from the first one to face the opposite side of the DNA template. These findings help to rationalize how chromatin arrangement affects Pol II transcription dynamics.

Multi-dimensional Lévy walks. The model of Lévy walks was suggested in 1982 by Shlesinger and Klafter and since then was used in numerous applications. The length of steps in the Lévy random walk model is power-law distributed while the steps themselves are performed with a constant velocity. These two peculiarities of the model are responsible for its noticeable success in describing the anomalous diffusion processes in physics, biology and ecology. Power-law distributed steps are responsible for anomalous diffusion, while the finite velocity of steps mirrors the generic feature of most real transport processes where particles or living organisms always move with a well defined velocity. However, the majority of analytical results for the model were obtained in the one-dimensional case, while most of real transport phenomena take place in two or three dimensions. To bridge this important gap in the theory of Lévy walks we decided to study the model on the plane (and later also in higher dimensions). We showed that the model admits three different formulations that differ by geometry of performing the random walks steps and correspond to the three specific classes of physical transport processes. Asymptotic analysis of the exact analytical solution and numerical simulations uncovered a very interesting peculiarity of Lévy walks in two dimensions. Geometry of random walks is imprinted in the profiles of the density of particles even at asymptotically large times, an effect which is absent in the case of normal diffusion. We also proposed a method of trajectory analysis based on the generalized Pearson coefficient that helps to determine the type of the underlying model from the data. A natural continuation of this work was the generalization of our results to higher dimensions.

Cooperations

- Dr. Simon Alberti (MPI-CBG, Dresden) Understanding the physics of dormancy.
- Prof. Eli Barkai (Bar Ilan University, Israel) Theory of Lévy walks.
- Prof. Nicolas Biais (CUNY Brooklyn College, New York, USA) Experiments on *N. gonorrhoeae* bacteria biofilms.
- Prof. Sergey Denisov (Augsburg University, Germany) Theory of Lévy walks.
- Prof. Stephan Grill (BIOTEC, TU Dresden) Theory and experiments on RNA-polymerase transcription.
- Prof. Jochen Guck (BIOTEC, TU Dresden) Experiments on physics of dormancy.
- Prof. Teymuraz Kurzchalia (MPI-CBG, Dresden) Experiments on metabolic pathways of dauers.
- Prof. Iva Tolić (Ruder Bošković Institute, Zagreb, Croatia) Experiments on chromosome organisation during meiosis.
- Dr. Nadine Vastenhouw (MPI-CBG, Dresden) Experiments on genome activation and chromatin architecture during early embryo development.

Research Group: Statistical Physics of Living Systems

(since January 2017, Head: Dr. Steffen Rulands)

The self-organisation of cells during the development and regeneration of tissues is one of the most intriguing non-equilibrium processes in nature. How do cells coordinate their behaviour in order to build a complex structure like a living organism? The ability to self-renew places stem and progenitor cells, which have the remarkable capacity to generate multiple cell types in the developing and adult body, at the apex of theories of tissue maintenance and development. To ensure that the correct composition of differentiated cell types is generated at the right time and place, the fate of stem cells must be precisely regulated. Understanding mechanisms of cell fate regulation is pivotal for understanding diseases that arise due to dysregulation, such as cancer, and for the development of stem-cell-based therapies in regenerative medicine.

The fate of stem cells is regulated across many scales, from molecular interactions to tissue-level signalling or mechanical feedback. Despite the multi-scale nature of cell fate regulation experimental measurements are typically restricted to a single scale. On the population level, the recent advent of experimental methods, which are capable of genetically labelling and tracing cells *in vivo*, allows us to understand the functional behaviour of stem cells. On the molecular level, recent advances in single-cell profiling methods afford unprecedented access to detailed molecular information on single cells. For the first time, it is now possible to obtain information on the expression of thousands of genes, on epigenetic modifications of the DNA on single loci, and on the local organisation of chromatin on the level of

single cells from living organisms. These technological developments provide the exciting opportunity to gain mechanistic insight into the molecular processes underlying stem cell fate behaviour. But how can detailed quantitative information on the microscopic scale be translated into a mechanistic understanding of the collective degrees of freedom that determine biological function at the cellular and tissue scale?

In the realm of “low-energy” physics, the processes governing the smallest scales have long been described. Yet, almost a century after the formulation of quantum theory collective phenomena such as high-temperature superconductivity remain poorly understood. The reason for this is that the collective properties of interacting many-particle systems do not necessarily obey the symmetries that govern on the microscopic scale, a concept often referred to as emergence. In other words, the collective degrees of freedom cannot straightforwardly be inferred from the microscopic dynamics, and it requires the methodologies of statistical physics to understand macroscopic consequences of microscopic behaviour. Therefore, despite the excitement that novel developments in single-cell biology are causing, insights from these experiments will remain descriptive until matched with methodologies to identify collective degrees of freedom. Concepts from (non-equilibrium) statistical physics, such as scaling and renormalisation, provide a powerful framework to begin to understand the collective processes underlying cell fate decision making.

In the Statistical Physics of Living Systems group we combine novel experimental technologies developed by our collaborators with methods from non-equilibrium physics to understand the mechanisms controlling cellular behaviour. Our work not only contributes to the understanding of processes relevant to development, regeneration and ageing, but these biological questions also give rise to interesting and challenging problems at the frontier of non-equilibrium statistical physics. Our group is involved in multiple collaborations with experimental groups on the local and international level. We regularly contribute to public outreach events, such as the Long Night of Science, and teach in the framework of the International Max Planck Research School for Cell, Developmental, and Systems Biology.

The group follows four broad research directions:

Molecular processes underlying cell fate regulation. In several collaborations with experimental groups we combine methods from non-equilibrium statistical physics with novel tools from single-cell genomics to understand the molecular processes underlying cell fate decisions. A specific focus is on the interplay between different layers of epigenetic regulation. These are molecular processes not encoded in the DNA sequence that have in recent years been identified to be dynamically involved in cellular decision making. For example, in collaboration with the group of Wolf Reik we showed that the interplay between topological and chemical modifications of the DNA gives rise to long-range correlation in the modifications and to genome-wide oscillations in the concentration of methyl groups deposited on the DNA.

Collective dynamics of cells. While historically research on stem cells has focussed on the genetic mechanisms underlying their behavior with the advent of genetic mouse models and live imaging techniques recently more and more emphasis has been placed on the functional level. We are interested in collective properties of cellular systems and how mechanisms of fate regulation can be inferred from population-level measurements. For example, we recently showed that the size progeny of embryonic precursor cells follows universal scaling behavior, an important step in the interpretation of genetic tracing experiments.

Regulation of plasticity and specialisation. Biological systems are characterised by a high degree of specialisation and differentiation. In recent years it has become evident that despite this robust differentiation many biological systems exhibit a surprising amount of plasticity. For example, robustly differentiated cells in the lung have been found to rapidly reprogram into stem cells after injury although these transitions do not occur by chance fluctuations. Together with the group of Solenn Patalano we investigate how the interplay between population-level interactions and epigenetic dynamics can give rise to plasticity in robustly specialised populations.

Technology development. Using concepts from non-equilibrium physics together with our collaborators we develop computational and statistical methods that allow employing sequencing and imaging technologies in new contexts.

Cooperations

- Wolf Reik, The Babraham Institute, Cambridge (UK) on DNA methylation dynamics during development and ageing and on the development of live microscopy methods for epigenetic states

- Solenn Patalano, BSRC Institute "Alexander Fleming", Athens (Greece) on epigenetic plasticity and self-organisation in social insects
- Philipp Mergenthaler, Charite, Berlin (Germany) on metabolic regulation of neuronal cell death and the development of therapeutic strategies for MELAS disease patients
- Michael Brandt, Center for Regenerative Therapies, Dresden (Germany) on zebrafish neurogenesis and brain regeneration
- Laure Bally-Cuif, Institut Pasteur, Paris (France) on adult zebrafish neurogenesis
- Aydan Bulut-Karslioglu, Max Planck Institute for Molecular Genetics, Berlin (Germany) on the metabolic regulation of chromatin states
- Cedric Blanpain, Université Libre de Bruxelles, Brussels (Belgium) on heart morphogenesis and epidermal wound healing
- Alessandra Sacco, Sanford-Burnham Prebys Medical Discovery Institute, La Jolla (USA) on muscle regeneration and ageing
- Henrik Boije, Upsala University, Upsala (Sweden) on cell fate decisions in retina development
- Meri Huch, Wellcome Trust Gurdon Institute, Cambridge (UK) on early liver development
- Anna Philpott, University of Cambridge (UK) on Neurogenin3 phosphorylation in pancreas organoids
- Michaela Fre, Institut Curie, Paris (UK) on pancreas development
- Maria Pilar Alcolea, Wellcome Trust Gurdon Institute, Cambridge (UK) on regeneration and tumour initiation
- Benjamin D Simons, University of Cambridge, Cambridge (UK) on the theory of clonal dynamics
- Marianne Bauer, Princeton (USA) on evolutionary game theory and social dilemmas

Research Group: Mesoscopic Physics of Life

(since February 2018, Head: Dr. Christoph Weber)

We are interested in the physics involved in the spatial organization of the cell cytoplasm and the formation of proto-cells at the origin of life. In both cases we focus on the role of compartmentalization as a mechanism to achieve biological function. The resulting compartments can provide a stable and protective environment, a controlled chemical composition and the property to selectively host certain molecular species. Moreover, they offer a robust environment that can guide the folding of biofunctional molecules or facilitate their replication. Additionally, such compartments are capable to spatially regulate chemical reactions and can also promote nucleation and growth of aggregates.

In our group we aim to identify the physico-chemical mechanisms that underlie assembly, regulation and ageing of these compartments. We would like to understand the link between these mechanisms and how biological function emerges, either for the organization of the cellular cytoplasm or the development of life-like features arising from a set of inanimate molecular species. Our group uses concepts from the field of phase transitions, non-equilibrium thermodynamics, and non-linear dynamics, but also develops new approaches to describe these systems. All approaches are developed in close back and forth collaboration with experimental groups. Below we present some research questions that we currently investigate.

Droplet positioning inside cells. Living cells use phase separated protein droplets to achieve the spatial-temporal organisation of biomolecules. To this end, cells use concentration gradients that can spatially organize these protein droplets. To understand the positioning of droplets we consider how concentration gradients of a so-called regulator component affect phase separation of two components. We have worked out the cases in which the position of a condensed phase is influenced by an external field such as gravitation, electric or magnetic fields, or by a regulator gradient that is driven and maintained by boundary conditions. An extension of the classical Lifschitz and Slyozov theory by concentration gradients has been derived that approximately captures the kinetics of droplet position even inside living cells. However, open questions remain such as how concentration gradients affect the statistics of coalescence of protein droplets, how these droplets in turn affect the concentration gradients and a quantitative comparison of our theoretical predictions with studies in living cells.

Phase separation of membrane scaffolding proteins as a mechanism to control cell adhesion. Tight junctions regulate para-cellular flux of solutes across body compartments. Assembly of tight junctions into a continuous sub-apical belt requires a mechanism to accumulate junctional proteins and facilitate polymerization of claudin receptors and actin filaments. This assembly process is dependent on ZO proteins which are enriched in a dynamic protein dense plaque on the cytoplasmic side of the

tight junction. Our collaborators from the Honigmann Laboratory (Max Planck Institute of Molecular Cell Biology and Genetics, Dresden) have recently discovered that the main scaffolding proteins of the tight junction form domains at the membrane via liquid-liquid phase separation. Together we study the mechanism and the function of phase separation of these proteins in the context of the formation of the tight junction. Within our collaboration we address this problem via a combination of cell biology and in vitro biochemistry/biophysics (Honigmann) with non-equilibrium thermodynamic theory (Weber). In particular, we address the questions: How is phase separation of scaffolding ZO proteins induced at specific sites at the cell membrane, and how is phase separation involved in the assembly of claudin / actin polymerization and the supra-molecular structure of tight junctions? Answering these questions will allow us to elucidate the mechanisms that drive the assembly of a functional tight junction.

Ostwald ripening in active emulsions. Phase separating systems that are maintained away from thermodynamic equilibrium via molecular processes represent a class of active systems referred to as *active emulsions*. These systems are driven by external energy input for example provided by an external fuel reservoir. The external energy input gives rise to novel phenomena that are not present in passive systems. For instance, in active emulsions where droplets are subject to chemical reactions that are not at thermodynamic equilibrium, droplet nucleation and droplet size can be controlled, and droplets can spontaneously divide. The physics underlying the dynamics of active emulsions is relevant to the spatial organisation of the biochemistry in living cells, for the novel development of applications in chemical engineering and models for the origin of life.

In collaboration with the Boekhoven Laboratory (Technical University Munich) we study a class of chemical systems where the consumption of fuel leads to a state where the fraction of an unstable product is strongly enriched. At large enough concentrations of product oil droplets solely composed of product molecules form spontaneously. The degradation of products requires water which only exists outside of these droplets. We have found that Ostwald ripening is strongly accelerated due to the active assembly and degradation of product. We were able to derive analytic predictions for average volume and droplet number which quantitatively coincide with the experimental measurements. Currently, we work on the predictions for the droplet size distributions and a full treatment based on irreversible thermodynamics. The considered active, chemical system is relevant for drug delivery and may also serve as a synthetic model system for cellular emulsions and for proto-cells at the origin of life.

Control of phase transitions. Cells use phase transitions to achieve biological function. Since most phase transitions inside cells are discontinuous (e.g. phase separation, positioning, polymerisation, protein aggregation), i.e. the occurrence of a phase transition is accompanied by an abrupt change of the corresponding order parameter, cells aim to control such transitions. Such control may include the emergence as well as the ability to reverse phase transitions. We study this question by considering how phase separation in living cells is affected for example by temperature and pH, but also study the generic scenarios of how discontinuous phase transitions can be controlled by chemical cues in general. Understanding the cellular control of phase transitions is of particular importance for the heat shock response in living cells and how chaperones affect cellular assemblies.

Collaborations:

Theoretical Collaborations:

- Chris H. Rycroft (Harvard University, Cambridge, USA) on numerics of multi-phase flow.
- Vasily Zaburdaev (Friedrich Alexander Universität Erlangen-Nürnberg) on motility of bacterial colonies.
- Chiu Fan Lee (Imperial College, London) on Ostwald ripening in concentration gradients.
- Thomas C.T. Michaels (Harvard University, Cambridge, USA) on optimal control of phase transitions and optimal drug control.
- L. Mahadevan (Harvard University, Cambridge, USA) on the physics of active poroelastic materials and optimal drug control.
- Frank Jülicher (Max Planck Institute for the Physics of Complex Systems, Dresden) on theory of active emulsions.

Experimental Collaborations:

- Job Boekhoven (Technical University of Munich) on Ostwald ripening in active emulsions.
- Dieter Braun and Christof Mast (Ludwig Maximilian University Munich) on physical principles of replication at the onset of life.
- Simon Alberti (Max Planck Institute of Molecular Cell Biology and Genetics, Dresden) on ageing of phase separated compartment.
- Anthony Hyman (Max Planck Institute of Molecular Cell Biology and Genetics, Dresden) on P granule segregation in living cells.
- Alf Honigmann (Max Planck Institute of Molecular Cell Biology and Genetics, Dresden) on the formation of the tight junctions.

1.9 Groups

Research Group: Dynamical Systems and Social Dynamics

(until August 2016, Head: Dr. Eduardo G. Altmann)

The Otto Hahn group *Dynamical Systems and Social Dynamics* started in January 2011 and ended in August 2016. The research of the group concentrated on the interface between Complex Systems and Data Science, with focus on dynamics and on applications 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 digital 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), records of language usage over the last two centuries, textual and bibliometric data of millions of scientific papers, and data of socio-economical activities of cities. 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. This opens new opportunities to obtain a mechanistic understanding of problems of technological and societal interest, profiting from the computational and mathematical models and methods coming from dynamical systems theory, stochastic processes, and statistical physics.

During the one year period of this report, before the end of the group, the four Ph.D. students of the group successfully defended their Thesis and moved forward with their careers: three of them for postdoc positions (in the USA, Netherlands, and Denmark) and one to the private sector (in Germany). Research directions investigated in this period include:

Scaling laws in Urban Systems. Socio-economical indicators of different cities show universal scaling relationships with city sizes. Exploring new datasets we found that the statistical fluctuations of the data around the proposed scaling laws play a central role in the quantification and characterization of these scaling laws.

Machine-learning methods based on networks of words. The unprecedented amount of written texts available on the Internet requires novel computational methods to extract information from them. The most popular machine-learning method is topic models, an unsupervised tool that allows for a summarization and classification of documents. We have been able to formally connect traditional topic-model approaches to the field of complex networks, obtaining improved methods based on existing community-detection methods developed in network science.

Predictions and fluctuations in fat-tailed distributions. The attention of a community typically concentrates on 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 developed computational methods to find rare trajectories in chaotic dynamical systems (e.g., in transient chaos) by adapting Importance Sampling Monte Carlo methods used in statistical physics (e.g., multicanonical simulations).

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. We investigated the organization of science by quantifying the similarity of scientific fields based on the similarity of their language and on citation patterns between them.

Research Group: Self-Organization of Biological Structures

(Head: Dr. Jan Bruges)

The group Self-organization of biological structures started in September 2013 and aims to understand how cells organize their contents in space and time. One way cells do this is by compartmentalizing their contents. These compartments or cellular structures assemble and disassemble according to specific needs and must have the right size and dynamics to function properly. In my lab we work at the interface between soft matter physics, cell biology, and systems biology to understand how the properties of cellular compartments emerge from the interaction of individual molecules. As model system we use two classic examples of cellular compartments, the metaphase spindle and the interphase nucleus. We combine in vitro and in vivo systems as well as theory and a range of biophysical methods. In vitro, we use the versatile *Xenopus laevis* egg extract system, which allows excellent imaging, mechanical accessibility, and ease of biochemical perturbations. In vivo, we use both zebrafish embryos, a model system traditionally used in developmental biology due to the ease of imaging of its large transparent cells, and tissue culture cells. Our long-term goals are to understand how cellular structures regulate their size and shape, and what are the principles of nuclear organization and compartmentalization.

Mechanisms of spindle scaling and size control during embryogenesis. Within an organism, cells change in size during early embryogenesis and later tissue differentiation. Mitotic spindles must adjust to this cell size changes in order to robustly segregate the chromosomes into the daughter cell. Recent in vitro evidence led to the proposal that scaling of spindles is dependent on limiting amounts of tubulin. However, a limiting component model cannot explain how spindles reach a finite size in very large cells or extract with virtually unlimited components. Alternatively, our recent findings (Decker et al., 2018) suggest that autocatalytic microtubule nucleation may regulate spindle size by scaling nucleation instead. How spindles scale in-vivo remains elusive due to the lack of direct measurements of the spindle architecture and microtubule nucleation. Do microtubules maintain the same organization in large and small spindles and scale down by decreasing individual microtubule lengths, or instead change their microtubule number and organization? Is the profile of microtubule nucleation independent of the cell size, or is it being regulated according the cell size? How do spindles orient properly during division in a system where astral microtubules are not in contact with the cell boundary? To answer these questions we are quantitatively characterizing the scaling of the spindle during the first rounds of cell division in the large and transparent cells of zebrafish embryos and in spindles assembled in encapsulated *X. laevis* egg extracts—which mimics the size scaling in tissues. To this end we will perform time-resolved measurements with a custom-built microscope of cell divisions in all cells simultaneously in 3D. Combining these measurements with laser ablation perturbations and theory we will systematically measure the spindle orientation, movement, architecture and microtubule nucleation profile as a function of cell size.

Theory and simulations of spindle morphology. The combination of theory and experiments allowed us to show that microtubule nucleation is autocatalytic and spatially regulated (Decker et al., 2018). These findings on microtubule nucleation show that previous models of spindle assembly are incomplete and suggest a mechanism of spindle formation that resembles classic Fisher-waves and Turing mechanisms. However, our mechanism has the fundamental difference that microtubule autocatalytic waves do not require diffusion or advection to propagate. Instead they are a consequence of the finite extension and dynamics of the reactant (the microtubule). The interplay between dynamic microtubules growing according to an autocatalytic process and fluxes driven by motors had not been considered and could lead

to unexpected properties of cytoskeletal organization. In this research line we are incorporating motor activities and autocatalytic microtubule growth into a continuum theory and a microscopic simulation that recapitulates spindle assembly and scaling but also explores the phase space of the interplay between motor activities and autocatalytic growth. We have already established a microscopic simulation that includes microtubule dynamics, nucleation and one type of molecular motor. We aim to add a second class of molecular motor to recapitulate the extensile and contractile forces that exist in spindles. We will combine this simulation with measurements of spatio-temporal correlation functions in spindles to validate the simulation. Together, our approach will allow us to understand how the activities of individual motors and filaments give rise to the emergence of the spindle material properties, active stress generation, and morphology.

Reconstitution of genome activation in synthetic nucleus. There is increasing evidence that the function of the genome should be understood in the context of its three-dimensional organization. In parallel, localized accumulations of RNA polymerase and transcription factors suggest that transcriptional activity is confined in local microenvironments. How the organization of genome and transcriptional machinery together impact transcriptional output is, however, not understood. To uncover basic principles of nuclear organization, we are developing an assay to reconstitute functional nuclei in encapsulated *Xenopus laevis* egg extracts using microfluidics (synthetic nuclei). These nuclei self-organize in extract upon the addition of pre-engineered synthetic chromosomes (such as long plasmids or BACs), properly assemble a nuclear membrane, lamina, chromatin, and are capable of nuclear import and export. The synthetic nuclei allows to study nuclear organization with total control of sequences, genetic to cytoplasmic ratio, labeling, and addition or depletion of components. We have successfully initiated transcription in extract nuclei, which is concentrated in several micron-sized foci. We aim to characterize the identity of these foci by labeling the known developmental genes that are turned on during maternal to zygotic transition. After that, we will characterize the biophysical properties of these foci and their dependence on histone levels and test models of genome activation. Our cell free approach will allow for unprecedented quantitative measurements and perturbations that are not amenable in vivo. Our ultimate goal is to recapitulate and model the processes that lead to genome activation in a synthetic nucleus. The orchestrated events that turn on an inactive nucleus are the hallmark of the beginning of life. By reconstituting the basic circuitry that leads to a genome activation event, we will uncover the basic principles of spatial and temporal regulation in the nucleus.

Dynamics of pattern formation in the nucleus. Genome activation is a gradual process that starts as localized transcription in foci followed by wide spread transcription in the nucleus. How transcription spreads from localized foci to the whole nucleus is not understood. We will combine our synthetic nucleus with in vivo imaging in the zebrafish embryo in collaboration with the Vastenhouw lab to investigate how the concentration of transcription factors, transcription activity and concentration of active transcription sites lead to the formation of transcription foci. One possible mechanism is that genes that share similar regulators (transcription factors, chromatin remodelers) physically move together to form a microenvironment, which would be predicted by phase separation. Alternatively, the activity of a gene may create a permissive environment for transcription that extends in space, influencing the activity of nearby genes. In this line of research, we are determining (i) if activating genes in the synthetic nucleus leads to recruiting and clustering of other genes, (ii) at what distance a microenvironment impacts the activation of genes, and (iii) whether its effect on transcription is general, or limited to genes that require the same regulators. Remarkably, we have already shown that addition of pioneering transcription factors in the synthetic nuclei is sufficient to both create micron-sized clustering and fluidization of the nucleus. The possibility that transcription activation is mediated by a change in the fluid properties of chromatin and subsequent clustering brings an exciting new perspective on how to think of nuclear organization and regulation. The use of the synthetic nucleus and the control over labeling, protein amounts, and genetic composition, will allow us to perform quantitative measurements to determine how the dynamics and level of transcription activation depends on the amount and identity of transcription factors and clustering. These type of measurements are currently not possible in the in vivo situation and will complement measurements in the zebrafish embryo. Together this will uncover how the spatial organization of transcriptionally active foci orchestrate the initiation of transcription nucleus-wide.

Cooperations

Nadine Vastenhouw (MPI-CBG Dresden)

Christoph Zechner (CSBD Dresden)

Tony Hyman (MPI-CBG Dresden)

Jochen Guck (MPI for the Science of Light Erlangen)
Frank Jülicher (**mpipks** Dresden)
Ivo Sbalzarini (CSBD Dresden)
Jan Huisken (Morgridge Institute for Research, US)

Research Group: Computational Biology and Evolutionary Genomics

(Head: Dr. Michael Hiller)

Since Oct 2011, our research group is jointly affiliated with the **mpipks** 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 long-term mission of the group is to combine comparative genomics and experimental approaches to address a key question in genetics and evolutionary biology: *What is the genomic basis of phenotypic differences between species?* Our research focus is explicitly on differences *between* species and not on differences *within* a species. Discovering the genomic changes that underlie particular phenotypic changes is a challenging task because numerous phenotypic and millions of genomic changes exist between each pair of species. However, numerous sequenced genomes provide an unprecedented opportunity to use statistical approaches, such as our Forward Genomics framework, to discover such associations by comparative analysis.

In order to discover the genomic changes that underlie phenotypic changes between species, my group has developed several computational methods that accurately detect evolutionary changes in functional genomic regions. This includes the development of a computational pipeline to discover gene loss events at very high accuracy (Research Report 1), the development of an unbiased genomic approach to detect signals of parallel protein evolution between any independent lineages, and novel methods to capture functional divergence in *cis*-regulatory elements by analyzing differences in transcription factor binding sites in a phylogenetic framework (Research Report 2). To improve our ability to discover statistical associations between genomic and phenotypic changes, we also developed new Forward Genomics methods that control for phylogenetic relatedness between species and differences in their evolutionary rates.

Given that accurate and sensitive genome alignments are required to detect genomic differences that could affect function, we have also developed methods to improve genome alignments. This includes a new approach that substantially increases alignment sensitivity. We showed that increased sensitivity enables the detection of thousands of novel alignments between orthologous exons, which is a significant advance when using genome alignments to project coding genes from a reference species (such as human) to other aligned species, as we have demonstrated for 143 non-human vertebrates. We also developed a new method that improves the specificity in genome alignments by accurately detecting and removing paralogous and random local alignments.

Applying these approaches to various genomes has led to many interesting discoveries. First, we discovered numerous gene losses that provide mechanistic explanations for well-known examples of mammalian adaptations, such as life in water, extreme diving abilities, or specializations to herbivorous, carnivorous or frugivorous diets (Research Report 1). Second, we discovered that echolocating bats and dolphins have an exceptionally high number of parallel substitutions in proteins that are specific to the contractile machinery of fast-twitch muscle fibers. This is exciting as both bats and dolphins rely on specialized superfast muscles to produce an extremely rapid call rate when homing in on their prey. By combining gene expression profiling of the superfast laryngeal muscle of bats with *in vitro* experiments that revealed functional convergence between a bat and dolphin calcium-storage protein, our results provide insights into the molecular underpinnings of this convergent vocalization aspect of echolocation. Third, by combining genome assembly with functional and comparative genomics, we could show that loss of limbs in snakes is associated with a widespread sequence and transcription factor binding site divergence in limb-regulatory elements. Furthermore, we could show that eye degeneration in subterranean mammals is associated with a large-scale divergence of eye-regulatory elements (Research Report 2). Overall, these and other discoveries demonstrate the potential of genome-wide screens, using the methods developed in my lab, to discover the genomic basis underlying phenotypic changes in mammals. This is not only fundamental for understanding molecular mechanisms underlying phenotypic adaptations, but also uncovered general principles of macroevolutionary processes and provided new insights into organismal biology.

In further projects, we collaborated with Elly Tanaka (IMP Vienna) and Gene Myers (MPI-CBG) to annotate and analyze the 32 Gb axolotl genome, the largest genome ever assembled. Our analysis, which

was published in Nature 2018, revealed key characteristics of genome size expansion in this regeneration model and showed that intron size in developmental genes, such as Hox genes and other key transcription factors, is under evolutionary constraint. Furthermore, we collaborated with Wieland Huttner (MPI-CBG) to discover genes involved in the expansion of the neocortex during primate, and notably human, evolution. By tracing the evolution of genes that are preferentially expressed in progenitor cells of the fetal human neocortex, our analysis revealed distinct evolutionary mechanisms that gave rise to primate- and human-specific genes, and uncovered promising candidates that may contribute to human-specific developmental differences in the neocortex.

Research Group: Nonlinear Time Series Analysis

(Head: Prof. Dr. Holger Kantz)

The world surrounding us is in permanent motion, most of which is irregular in detail despite regularities on coarser scales. An evident example is the weather, which is subject to clear and easy to understand seasonality, but which poses severe challenges when we want to predict the fluctuations around the annual cycle. The “fuel” for such fluctuations is transport through a system, usually energy or mass, which means that such systems are open or driven. The research of our group is devoted to temporal fluctuations. More precisely, we aim for the characterization, modeling, understanding, and prediction of fluctuations in various settings, and to use this methodology for the study of specific systems and phenomena.

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. A recurrent issue in the context of climate change is the potential change of the frequency and intensity of extreme weather conditions. The analysis of such extreme events poses particular challenges due to their rareness and hence the lack of a robust observational basis.

Long range temporal correlations Since the invention of the Detrended Fluctuation Analysis (DFA) by Peng et al [1994], about 10000 articles have been published where this tool revealed long range temporal correlations (LRC) in data. If these results were correct, then it would mean that the overwhelming majority of real world phenomena are affected by memory, i.e., they are neither Markovian (when seen as a stochastic process) nor exponentially mixing (when seen as dynamical system). Our long-lasting attempts to understand this issue better led to major break-throughs in the past 3 years. We were able to show that DFA relies exclusively on the auto-covariance function of a data set, i.e., that DFA results are neither influenced by multipoint-correlations nor by the marginal distribution of the data. We were able to derive analytic expressions for the signatures of DFA for simple memory-less processes such as AR(1) and AR(2). They show the existence of cross-over regimes, where the asymptotic scaling in the length of the time interval is not yet reached. Indeed, memory-less signals can, in these cross-overs, appear to be LRC, and if the data set is too short, the asymptotic regime cannot be reached by DFA. Hence, lack of data can make short range data appear to be LRC. In turn, we were able to extract, using DFA, short range properties such as relaxation times and noisy oscillation periods. In surface temperature data we could show that their LRC signatures in DFA can be generated by AR models, and this way we were able to confirm a previously detected 3-4 year period in El Niño data. Our current understanding is that DFA is a very useful tool when data sets are sufficiently long, that due to cross-over regimes short data sets can be erroneously interpreted as LRC even if they are not, and that the analytical study of DFA signatures of simple models can reveal this and even produce useful information about short range features. Also, we have understood how to model LRC data when they are non-Gaussian, which is a relevant class of signals for which before no data models existed.

Fluctuations in atmospheric physics. The atmosphere is one of the most complex physical systems, with dynamics on many spatial and temporal scales. Climate change as the consequence of rising greenhouse gas concentrations is nowadays an indisputable fact, however, details of which changes in particular on the regional scale are to be expected is 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. An automated analysis of more than 500 weather stations in Germany and of more than 10^6 grid points of the world-covering re-analysis data set *ERAinterim* showed clear limits of extreme value statistics: Calculated trends for return levels of hot temperatures are often negative and hence counter-intuitive, see p. 101. We conclude that this is not an effect of regionally diverse climate responses, but that this is within the error bars of the method. Although the details of climate change are regionally heterogeneous, the overall tendency towards hotter summer temperatures is very pronounced and negative trends in extremes must be artefacts of the analysis in most cases.

A direct consequence of fluctuations in all atmospheric variables are fluctuations in the production of renewable energy, in particular wind and solar power. Intermittency in the atmospheric dynamics leads to anomalous statistical behaviour of these fluctuations and hence poses challenges in their stochastic modeling, while at the same time the stability of the power grid might be affected by these. However, also fluctuations induced by consumers might play a relevant role, and we investigate various such aspects, also in collaboration with Prof. Timme at TU Dresden and Prof. Witthaut at University of Cologne.

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. Such systems can also be interpreted as models of extreme intermittency, 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. Together with Eli Barkai (Bar Ilan University), we generalized the Green-Kubo relation to such processes and elaborate some examples, including the deterministic Pomeau-Manneville map.

Root causes for anomalous statistics While strong intermittency in the Pomeau-Manneville map has been shown to generate anomalous statistics, the precise mechanisms of how and why were unclear. In particular, there is a transition from sub- to superdiffusion, which had been understood in terms of which dynamical phases of the map's iterates are relevant, but not in fundamental terms. In collaboration with Kevin Bassler (Houston) we were able to change this (see p. 103). Kevin Bassler was able to decompose anomalous scaling of a probability density function as violation of the central limit theorem into three root causes: dependence, non-stationarity, and infinite variance of the increments. In the Pomeau-Manneville map, all these three phenomena are present, depending on values of the control parameter. For this system, we succeeded to decompose the Hurst exponent characterizing the anomalous diffusion into exponents characterizing these three causes and hence have established a pseudo-physical model as a paradigm for such behaviour.

Coherent sets in two-dimensional flows Hydrodynamic transport in the atmosphere and ocean can be quite complicated due to turbulence and its intermittent nature. While one would naively expect hyperdiffusive mixing of fully turbulent flows, the existence of eddies leads to coherent sets. These are blobs of air or water with very slow mass exchange with the surrounding current. Therefore, the quality of the interior medium might differ strongly from the outside, e.g., in terms of temperature, salinity, pollutant or nutrient concentration. Such coherent sets are known to be relevant for many phenomena in climate (e.g., Agulhas rings), in aquatic population dynamics, and in pollutant transport. Due to their Lagrangian nature, it is a challenge to precisely delineate their boundaries. We extended the well established transfer operator approach, which implies a mapping of the Lagrangian hydrodynamic particle transport onto a stochastic process, and are thereby able to reliably detect the boundaries of coherent sets also for time dependent velocity fields. The method was applied to velocity fields taken from the Baltic sea.

Cooperations

- Center for Dynamics at the TU Dresden: Holger Kantz is member of the board of directors of this Centre which establishes scientific interchange on dynamics in the Dresden area. Through this centre, we collaborate with Katrin Padberg-Gehle (University of Lüneburg) 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-foundation 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), Freddy Bouchet, (ENS Lyon) collaboration on nonequilibrium fluctuations and large deviations in atmospheric dynamics.
- CAFE project: A European ITN on medium range weather prediction coordinated by Alvaro Corral in Barcelona with colleagues from Spain, France, UK, Uruguay, and Germany.
- Fluctuations in the electric power grid: Marc Timme (TU Dresden) and Dirk Witthaut (University Cologne).

Research Group: Ultrafast Laser-Matter Interaction

(Head: Dr. Alexandra Landsman)

Our group was founded in the beginning of 2015 as part of the Max Planck Center for Attosecond Science, aiming to increase collaboration and exchange of ideas between the Max Planck Institutes and the leading centers for Attosecond Science in Asia. Hence our group involves extensive collaborations with Max Planck Korea (MPK) and POSTECH (Pohang, South Korea), as well as collaborations with experimental groups at the Max Planck Institute for Quantum Optics (MPQ).

We study the interaction of matter with ultrashort flashes of light. Such fast flashes of light are on a time scale of attoseconds to femtoseconds, which is fast enough to capture the motion of bound electrons inside atoms, molecules and solids. Below is the overview of our research activities.

Strong field physics. A fundamental process in ultrafast science is tunnel ionization, whereby a strong laser field bends the binding potential of the atom or molecule so that the bound electron tunnels out and is subsequently accelerated in the strong laser field. This process also underlies the creation of high frequency (in the XUV range) attosecond pulses via the process known as High Harmonic Generation (HHG). We investigate how experimental observables, such as electron momentum distributions or HHG spectra, can be used to reconstruct the interaction between strong ultrafast laser pulses and atoms, molecules, and condensed matter systems.

Pump-probe spectroscopy. Many state-of-the-art experiments employ a pump-probe scheme, combining relatively weak attosecond pulses to excite the dynamics (pump), which are subsequently probed with an infrared (IR) pulse. This pump-probe scheme can be used to study electronic and vibrational properties of atoms and molecules or probe the delays in single photon ionisation. Much theoretical analysis relies on the solution of the time-dependent Schrödinger equation (TDSE), which, however, is possible only in simple atoms or highly symmetric molecules. Our group is developing classical and semi-classical methods to accurately describe ionisation of atoms and molecules using attosecond pulses. Such methods are less computationally expensive than TDSE and can be used to accurately treat multi-electron dynamics in more complex systems, such as organic molecules.

Attosecond physics at the nanoscale. Electron tunnelling emission from a nanostructure due to strong DC fields has been widely used in modern science and technology because it produces bright and coherent electron beams. AC fields of an ultrashort laser pulse can produce ultrashort coherent sources of electron beams, if the dominant ionization mechanism is via tunnel (as opposed to multi-photon) emission. We are developing analytical and numerical methods to understand interaction of nano-structures with ultrafast laser pulses. This is a relatively new field where common analytic tools of strong field physics (such as the dipole approximation) break down and new behaviour emerges.

Collaborations

With experimental groups

Prof. Matthias Kling (LMU and MPQ) on photoionization delays in molecules

Prof. Ferenc Krausz and Dr. Martin Schultze (MPQ) on photoionization delays in atoms, strong field phenomena in atoms and nanostructures

Prof. Ursula Keller (ETH Zurich) on tunneling delays in strong field ionization of atoms and photoionization delays in simple molecules

Prof. Seungchul Kim (Pusan, S. Korea) on high harmonic generation in solids

Prof. Dong Eon Kim (POSTECH) on strong field phenomena near nanostructures, streaking in noble gases, high harmonic generation in solids

With theoretical groups

Prof. Jan Michael Rost (MPI-PKS) on theoretical modeling of single photon ionization delays

Prof. Siddhartha Mishra (ETH Zurich) on strong field phenomena in atoms and nanostructures, ultrafast phenomena in plasmas

Prof. Maciej Lewenstein (ICFO) on high harmonic generation in solids and attosecond physics at the nanoscale

Max Planck Research Group: Quantum Many-Body Systems

(since January 2016, Head: Dr. Anne Nielsen)

The independent Max Planck Research Group "Quantum Many-Body Systems" was established in 2016. It currently hosts two PhD students (Sourav Manna and Srivatsa N.S) and four postdocs (Xikun Li, Aniket Patra, Wei Wang, and Julia Wildeboer). It has also hosted two summer interns (Saptarshi Majumdar and Shriya Pai).

We study the collective behavior of strongly correlated quantum many-body systems. We are particularly interested in topological properties. We also study the dynamics of quantum systems. In the following, we describe our main research directions.

Anyons: Anyons are a type of quasiparticles that are neither bosons nor fermions, and they can have fractional charge. Anyons can appear in topologically ordered systems, such as the fractional quantum Hall effect. We study how one can create and trap anyons in different model systems, and we investigate their size, shape, charge, and braiding properties. The size is, e.g., important experimentally in determining how far the anyons should be separated, when they are braided. We also search for the presence of anyons in new types of systems, where they have not been seen before. We have, e.g., shown that anyons can exist in dimensions between one and two. We have also shown that it is much simpler to construct analytical states containing fractional quantum Hall quasielectrons in lattices than one would expect from the corresponding problem in the continuum.

Infinite-dimensional matrix product states: Quantum many-body systems are highly complex, and therefore (partially) analytical models are important tools to gain insight into the possible behaviors of quantum matter. It is relatively difficult to find non-trivial examples of Hamiltonians that can be diagonalized analytically. Another possible approach is to find analytical wavefunctions with interesting properties and then derive parent Hamiltonians for the states. It is known that some fractional quantum Hall states can be expressed as correlation functions of conformal fields, and we use this to construct fractional quantum Hall models on lattices with analytical ground states. The analytical form of the ground states makes it much easier to analyze the properties of the models accurately. The states have a form that is similar to matrix product states, but the matrices are infinite-dimensional. Using a similar approach, we have also constructed interesting models in 1D and on ladders, e.g. a generalization of the Haldane-Shastry model, which has correlation functions that decay as a power law for short distances and exponentially for large distances.

Simplification of conformal field theory Hamiltonians: The Hamiltonians constructed from conformal field theory are typically few-body, but nonlocal. The nonlocal property makes it more difficult to implement the models experimentally. On the other hand, the fractional quantum Hall ground states have correlations that decay exponentially with distance. It hence seems that it should not be necessary to have nonlocal interactions in the Hamiltonians. We have previously shown for particular models that the Hamiltonians constructed from conformal field theory can be used as a starting point to find local, few-body Hamiltonians with almost the same ground state. We have now investigated a different strategy to construct local Hamiltonians from the conformal field theory Hamiltonians, which can be applied more generally than the previous method.

Unitary dynamics of quantum systems: The time evolution of quantum systems constitutes a rich field of research. We have, e.g., studied particle dynamics in fractional quantum Hall models derived from conformal field theory. The results suggest that the fractional quantum Hall properties of these systems appear through a different mechanism than they do in other fractional quantum Hall models. We have also proposed an effective description of the dynamics of few-fermion systems in a double well potential.

Quantum control: We investigate how one can achieve a desired time evolution or state preparation in quantum many-body or few-body systems by controlling the time variation of parameters. A typical problem, which is important for experiments, is that one starts from a system in the ground state with Hamiltonian H_1 and would like to prepare the system in the ground state of another Hamiltonian H_2 . This can be done by changing the Hamiltonian adiabatically, but if the transition needs to be completed within a given amount of time, it is nontrivial to find out how one should change the parameters as a function of time to get the desired state with the highest possible fidelity. We have, e.g., computed how to speed up the preparation of states of few-fermion systems, and how to speed up transitions in ultracold atoms in optical lattices.

Disordered systems: We study how disorder affects the properties of quantum many-body systems. The aim is to find systems with new types of behavior. So far, we have studied a critical model in one dimension and found that the ground state properties remain the same when disorder is added, but the states in the middle of the spectrum show Poisson statistics and low entanglement. In the future, we plan to investigate the interplay between topology and disorder.

Stochastic dynamics of quantum systems: Quantum measurements provide an interesting toolbox to manipulate the state of quantum systems. This is because the dynamics resulting from measurements is often quite different from the dynamics that can be achieved with unitary time evolution. We are investigating how measurements influence the dynamics of ultracold atom systems and how measurements can be used to detect particular properties of these systems.

Collaborations:

- Prof. Jacob Sherson (Aarhus University, Denmark)
- Prof. Ignacio Cirac (Max Planck Institute of Quantum Optics, Germany)
- Prof. German Sierra (UAM-CSIC, Spain)
- Prof. Masud Haque (Maynooth University, Ireland)
- Prof. Tomasz Sowiński (Polish Academy of Sciences, Poland)
- Prof. Maria Hermanns (Nordita, Sweden)
- Prof. Eddy Ardonne (Stockholm University, Sweden)

Research Group: Nonequilibrium Quantum Matter

(since August 2015, Head: Prof. Dr. Takashi Oka)

The Joint Research Group *Nonequilibrium Quantum Matter* is co-sponsored by the **mpipks** and the MPI-CPfS, and was established in August 2015. During the report period it hosted six postdocs (Leda Bucciantini from 2015 to 2017, Tanay Nag from 2016 to 2018, Robert-Jan Slager from 2017 to 2018, Sota Kitamura from 2017 to 2019, Shintaro Takayoshi from 2018 and Francesco Peronaci from 2019), while the first four have already moved out. As the group is a joint research group of two institutes, efforts are made to integrate the groups in both institutes. The goal of the group is to understand strongly correlated quantum systems based on analytical and numerical methods, and to uncover and characterize new quantum states emerging in these systems. We study problems ranging from topological band theory, quantum magnetism and Mott insulators. During the report period we worked particularly on the following three topics:

Topology and correlation in 2D delafossite materials The two-dimensional (2D) delafossite are renowned for the lowest room temperature resistivity among all oxides. In the department of Andy Mackenzie at MPI-CPfS, the transport and spectral properties in this family is being studied extensively. As a theory group half affiliated in MPI-CPfS, we are making effort to support the understanding of their experimental findings and to propose new theoretical concepts. This is done through an international collaboration that includes the group of Philip D. C. King (St. Andrews) performing angle resolved photo emission spectroscopy as well as Kazuhiro Kuroki (Osaka) working on the first principle band structure calculation of these materials.

Current induced "Mott semimetal" A collaboration with an experimental group in Kyoto university led by Yoshiteru Maeno is going on with the aim to study the nonequilibrium steady state of the Mott insulator Ca_2RuO_4 . From nonlinear transport measurements, it is suggested that the steady state can be characterized as a "Mott semimetal" since the temperature dependence of the resistivity is strongly suppressed. In addition, strong diamagnetic response was discovered, which turned out to be the strongest among all non-superconducting materials. We are making effort to establish the theoretical framework for the current induced "Mott semimetal" state starting from simple tight binding models derived by first principle band structure calculation.

Floquet engineering of quantum matter One particular research interest of the group centers around the control of quantum materials by external means such as lasers and application of strong electric fields in non-linear devices. Topology is one of the key concepts in modern condensed matter physics. It is often said that "topology is robust against perturbation" and is considered to be a property that is fixed when a material is synthesized. There is a way to cheat this. We found the first example of the so-called Floquet topological insulator in 2009; We showed that the Berry curvature, Chern number, and the chiral edge state in almost ANY two-dimensional multi-band system can be controlled or induced by external time-periodic fields such as lasers. During the last decade, Floquet engineering, i. e. the control of quantum systems using time-periodic perturbations, has become an important technique to realize topological bands in solid state materials and their quantum simulators (cold atoms in optical lattices, photonic systems etc). In our group, we try to extend the concept of Floquet engineering from single body properties to properties in interacting systems and their phase transitions. For example, we considered Mott insulators in strong laser fields and discovered that their magnetic properties can be modified. These modifications include the laser-induced chirality, Dzyaloshinskii-Moriya interaction, as well as spin current. In addition, using techniques developed in high-energy physics, we studied the steady state of strongly interacting fermions (holographic QCD) in circularly polarized lasers. Although some of the results obtained by holography are difficult to understand, we are trying to develop an understanding based on simple toy models that we can treat using conventional techniques.

Cooperations: In addition to the projects between the **mpipks** and MPI-CPfS, we initiated a number of projects with external collaborators.

- St. Andrews: Collaboration with Philip D. C. King and several members of his group on some experimental and theoretical findings regarding delafossite materials.
- Kyoto University: Collaboration with Yoshiteru Maeno and several members of his group on the experimental finding of the large diamagnetism in a current induced semimetal phase in the Mott insulator Ca_2RuO_4 .
- Osaka University: Collaboration with Kazuhiko Kuroki and several members of his group on the topological aspects of delafossite materials and the Mott insulator Ca_2RuO_4 . Collaboration with Koji Hashimoto and Keiju Murata on holographic Floquet states.
- Chuo University: Collaboration with Shunichiro Murata on holographic Floquet states.
- Ibaraki University: Collaboration with Masahiro Sato on ultrafast spintronics.

Max Planck Research Group: Strongly Correlated Light-Matter Systems

(since March 2017, Head: Dr. Francesco Piazza)

The research group "Strongly-Correlated Light-Matter Systems" was established in March 2017. It currently consists of two PhD students: Kieran Fraser (since August 2017) and Christian Johansen (since September 2018), and four postdocs: Jad Halimeh (since May 2017), Tomasz Wasak (since June 2018), Peter Karpov (since August 2018), and Bernhard Frank (since November 2018). In addition, Johannes Lang, so far a PhD student shared with Prof. Wilhelm Zwerger at the TU-Munich, will join as a postdoc in January 2019.

General topic.— Our research area lies at the border between condensed matter and quantum optics and deals with quantum many-body open systems.

Systems.— Our investigations are strongly related to ongoing experiments in hybrid light-matter systems. So far the focus has been mainly on neutral atoms coupled to nanophotonics structures like optical waveguides or cavities, allowing to enhance and control light-matter interactions at the quantum level. More recently, the research group is partially shifting the focus toward solid-state systems consisting

of strongly-correlated electrons coupled to quantum light, following recent experimental developments combining Van der Waals heterostructures with optical cavities.

Approach.— We develop non-equilibrium field-theoretical approaches tailored for the study of many-body phenomena in the above open quantum systems. These approaches are novel in the context of quantum optics and non-trivially extend methods typically used in condensed matter.

Goals.— We are interested in fundamental theoretical problems in many-body physics like collective phenomena and non-equilibrium phases. However, since our techniques are quantitatively reliable, we also concretely investigate hybrid light-matter devices for quantum technologies, in the context of ultraprecise metrology/sensing and quantum nonlinear photonic devices.

Quantum many-body systems of strongly interacting photons. A number of experimental platforms, such as atom-nanophotonics interfaces, Rydberg atomic gases, and circuit QED are now able to realise strong interactions between individual photons. One of the major questions that has emerged, and which is being actively investigated, is whether such systems might be capable of generating novel many-body states of light. However, progress on this front has been elusive, due to the associated challenge of solving an out-of-equilibrium, driven, open system. We recently made a significant step forward by developing a tailored theoretical formalism based on a non-equilibrium diagrammatic approach to describe the quantum many-body regime of interacting photons in optically dense media. Exploiting this new tool, we introduced and characterised the phenomenon of interaction-induced transparency (IIT), which consists in the appearance of a transparency window for strongly interacting photons due to nonlinear interference effects. In the context of nonlinear quantum optics, IIT constitutes a novel, genuine quantum many-body effect. From the more fundamental perspective of many-body physics, the IIT phenomenon is a non-equilibrium phase transition in the driven-dissipative steady state which has no analogue in condensed matter, as it stems from the dissipative and retarded nature of the polariton interactions. While so far we focused on optically-dense media made of neutral atoms, the formalism we developed is applicable to a wider class of materials. In particular, we are going to use it to study strongly interacting photons in solid-state platforms consisting of 2D semiconductors coupled to optical cavities (as for instance available in A. Imamoglu's lab at ETH-Zurich).

Crystalline, magnetic, and topological phases of atoms with light-mediated interactions. When the coupling between matter and light is strong enough for nonlinear optical effects to appear, one can think of photons as exchange bosons mediating interactions between the particles in the material. Recent experimental developments in tuning the light-matter coupling in presence of controlled boundary conditions for the electromagnetic field allowed to create photon-mediated interactions which can be shaped in space and also time. Typically, these interactions are long-ranged and possess a characteristic length scale set by the wavelength of the lasers used to pump photons into the system. This feature makes such interactions favour spatially ordered phases. This property has been exploited recently to achieve the first experimental realisation of a supersolid state of matter. The experiments were done in T. Esslinger's lab at ETH-Zurich using ultracold bosonic atoms inside two crossed optical resonators. A supersolid combines the superfluid nature — i.e. the phase coherence emerging from the spontaneous breaking of the continuous symmetry associated with number conservation — with the crystalline nature — i.e. the spatial order emerging from the spontaneous breaking of the continuous symmetry associated with momentum conservation. We developed a theoretical framework describing the supersolid phase created at ETH, showing that the translational invariance (and thus supersolidity) in this setup is actually always approximate and we studied the consequences for the collective excitations, in particular the Goldstone and Higgs modes. Inspired by the fact that light-matter systems are always driven-dissipative, we also recently revisited the concept of supersolidity in such open systems, highlighting the role played by the symmetries of the system-bath interactions. The physics of crystallisation with light-mediated interactions becomes even richer when fermionic matter is considered. We have shown that a crystalline phase of fermions coupled to photons propagating along an optical waveguide hosts a novel type of quasi-particle. The latter appears due to the quantum-optical nonlinearities, replacing the usual polaritons as low-lying excitations of a hybrid light-matter system. This novel object is a composite particle made of an optical soliton trapping a fermionic atom and carries a nontrivial topological quantum number. We are currently investigating the stability, mutual interaction and dynamics of such topological defects with particular attention to the role played by the drive and dissipation of the waveguide. The light-mediated interactions between atoms depend on the particular internal electronic transition addressed by the photons. By populating a selected number of hyperfine atomic states playing the role of a

spin degree of freedom it is possible to implement magnetic models with photon-mediated interactions. We recently demonstrated that neutral atoms inside an optical cavity can be used to implement spin models with a variety of interactions including both Heisenberg and Dzyaloshinskii-Moriya interactions. In particular, the antiferromagnetic domain-wall phase we predicted has been recently experimentally verified in B. Lev's lab at Stanford. In solid-state systems, optical cavities have also recently emerged as a tool to induce collective phenomena (like superconductivity and charge-density waves). Differently from coherent laser light, the strong light-matter coupling introduced by optical cavities allows to work in a regime where the quantum nature of light is important. Theoretical investigations so far have, however, not yet explored the effect of photon losses (inevitable due to imperfect mirrors) onto the light-induced collective phenomena and the non-thermal nature of the steady-states emerging in these systems. We are currently investigating this effect by employing tailored non-equilibrium quantum field theory methods.

Many-body dynamics of quantum open systems. We are also exploring scenarios for quantum many-body dynamics in open systems from a more fundamental perspective, inspired by - but independent of - a particular experimental setup. One important question that emerges in this context is how critical dynamics is modified by coupling the system to non-thermal baths. For instance, we studied the quench-dynamics of long-range Ising models in presence of longitudinal-field noise and found a novel universal dynamical critical regime where the system shows aging with peculiar exponents governed by the noise fluctuations. We also considered Ising models coupled to a lossy bosonic mode — an open version of the paradigmatic Dicke model for quantum light-matter interactions — and found that even though the losses induce a finite lifetime of all quasiparticle-excitations even at the critical point of the Dicke model, critical power-law dynamics still appears. Another topic of ongoing research in our group — which is also generally attracting a lot of interest in the condensed matter community — deals with open Floquet systems. Here the balance between the heating induced by the time-periodic drive in ergodic quantum systems and the cooling due to the bath should give rise to steady states whose properties are to a large extent yet to be explored.

Polarons in presence of drive and dissipation. The polaron — i.e. an impurity dressed by the excitations of the bath in which it is immersed — is a very powerful concept for the understanding of interacting systems at the border between few- and many-body physics. A polaron problem is defined by the type of bath in which the impurity is immersed. Investigations of this old problem both in theory and experiment have so far been restricted to the case where 1) the number of impurities is conserved and 2) the bath is in thermal equilibrium. In the context of quantum open systems however, it is natural to ask what happens when property 1) and/or 2) do not apply. This question is not only academically interesting but has recently become experimentally relevant. We are currently studying the scenario realised in A. Imamoglu's lab at ETH-Zurich, where tightly-bound excitons can be immersed in an electron gas in a 2D semiconductor. This constitutes a Fermi-polaron problem with the additional ingredient being that the excitons are very lossy and need to be optically re-pumped into the system — i.e. the property 1) does not apply. Another scenario which we are exploring is offered to us by the atom-waveguide setup discussed above, where the bath for the atom is made of the waveguide photons. This Bose-polaron problem is new in the sense that the waveguide photons are not in thermal equilibrium but rather continuously flow in and out of the waveguide — i.e. the property 2) does not apply. As the mostly employed variational methods do not work, we tackle this problems by extending the equilibrium diagrammatic approach to the Fermi/Bose polaron to include drive and dissipation by using a real-time Keldysh-functional-integral formulation.

External collaborations

Theory

- Darrick Chang, ICFO Barcelona, Spain
- Jan Chwedenczuk, University of Warsaw
- Farokh Mivehvar and Helmut Ritsch, ITP Innsbruck, Austria
- Matthias Punk, LMU Munich, Germany
- Richard Schmidt, MPQ Garching, Germany
- Wilhelm Zwerger, TU Munich, Germany

Experiment

- Tilman Esslinger's Lab, ETH Zurich, Switzerland

Max Planck Research Group: Fractionalization and Topology in Quantum Matter

(since September 2017, Head: Dr. Inti Sodemann)

The research group Fractionalization and Topology in Quantum Matter was established at the **mpipks** in September 2017. It currently consists of three PhD students (Oles Matsyshyn, Sebastian Mantilla, and Peng Rao) and one visiting scientist (Po-Yao Chang). We have also hosted two temporary visiting students (Snehasish Nandy and Jonah Herzog-Arbeitman).

Our work deals with the interplay of strong interactions and topology in quantum matter. Our studies fall within three broad categories: (a) quantum transport, in particular phenomena involving Berry's phase, (b) fractionalized and topological phases of matter, particularly quantum Hall and spin liquids, and (c) non-perturbative approaches to strongly interacting phases of gapless fermions. We now summarise some of the specific research projects and findings that we have had over the last year:

The shear sound of two-dimensional Fermi liquids. Classical liquids only have longitudinal sound waves, in contrast to classical solids which also have transverse sound. By using the bosonization approach to Landau Fermi liquids, we demonstrated the existence of an undamped shear sound mode in quantum Fermi liquids for sufficiently strong interactions. This shear sound mode is expected to appear in two-dimensional metals in which the quasiparticle mass is renormalised to about twice the bare mass.

Strongly enhanced Berry-dipole at topological phase transitions in BiTeI. A major open problem is the identification of useful measurable quantities to diagnose quantum phase transitions between topologically distinct states. By studying the giant-Rashba material bismuth tellurium iodine (BiTeI) which exhibits a pressure-driven phase transition between topological and trivial insulators in three-dimensions, we identified one such diagnostic: the Berry curvature dipole, which displays a giant enhancement accompanied by a change of sign across the transition. This effect could be probed in transport and optoelectronic experiments.

A cascade of phase transitions in an orbitally mixed half-filled Landau level. We assisted in the theoretical interpretation of a remarkable experiment that studied the fate of half-filled Landau levels in Zinc-Oxide (ZnO) two-dimensional electron systems by tuning a level crossing between a half-filled $N = 1$ and a half-filled $N = 0$. We identified a variety of correlated phases surrounding the level crossing, including an unexpected compressible phase in the $N = 1$ Landau level and a strongly anisotropic nematic-like phase at intermediate polarizations when the levels are near degeneracy, in addition to the known incompressible Moore-Read state at $\nu = 5/2$ and the compressible composite Fermi liquid.

Valley Stoner instability of the composite Fermi sea. We studied a two-component system of two-dimensional electrons at high magnetic fields at total filling factor $\nu = 1/2$ with anisotropic mass tensors as realized in Aluminum Arsenide (AIAs) quantum wells. Combining exact diagonalization and the density matrix renormalization group we demonstrated that the system undergoes a quantum phase transition from a gapless state in which both flavors are equally populated to another gapless state in which all the electrons spontaneously polarize into a single one, which is a form of itinerant Stoner transition from a two-component to a single-component composite Fermi sea. We pinpointed previously unidentified experimental evidence indicating the presence of the Stoner magnetic state of composite fermions in Aluminum Arsenide (AIAs) quantum wells by analyzing the Jain states surrounding $\nu = 1/2$.

Quantum oscillations in insulators with neutral Fermi surfaces. We proposed a fractionalized state of matter called the "composite exciton Fermi liquid" in SmB_6 and developed a theory for the de-Haas van Alphen effect for neutral fermions coupled to $U(1)$ gauge fields, completing some earlier work initiated while I was a postdoctoral researcher at MIT.

Collaborations

- Liang Fu, Department of Physics, Massachusetts Institute of Technology, USA.
- T. Senthil, Department of Physics, Massachusetts Institute of Technology, USA.
- Zheng Zhu, Department of Physics, Massachusetts Institute of Technology, USA.
- Jun Yong Khoo, Department of Physics, Massachusetts Institute of Technology, USA.
- Debanjan Chowdhury, Department of Physics, Massachusetts Institute of Technology, USA.
- Donna Sheng, Department of Physics and Astronomy, California State University, USA.
- Joseph Falson, Max-Planck-Institute for Solid State Research, Stuttgart, Germany.
- Jeroen van den Brink, Institute for Theoretical Solid State Physics, IFW Dresden, Germany

- Debaleena Nandy, Department of Physics, Harvard University, USA.
- Thierry Jolicoeur, Laboratoire de Physique Theorique et Modeles Statistiques, CNRS, Universite Paris-Sud, Universite Paris-Saclay, Orsay, France.
- Csaba Toke, Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary.

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 are currently one Master student (Tobias Becker), four PhD students (Manuel Alamo, Alexander Schnell, Martina Vlaho, Botao Wang), five postdoctoral researcher (Dr. Swetamber Das, Dr. Sanku Paul, Dr. Arko Roy, Dr. Nur Ünal, Dr. Ling-Na Wu), as well as one associated external member (Prof. Arnd Bäcker).

The interests of the group range from quantum signatures of regular and chaotic dynamics; over driven-dissipative quantum systems, and in particular ordering in their non-equilibrium steady states; to the quantum dynamics of isolated many-body systems of atomic quantum gases, where Floquet engineering and quench-based state tomography play a major role.

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. The minimal example systems are four-dimensional maps and three-dimensional billiards. In these systems we study power-law trapping, but it remains a challenge to identify its mechanism. In scattering systems with fully chaotic classical dynamics the quantum resonance eigenfunctions have fractal properties which depend on their decay rate. We stated a resonance eigenfunction hypothesis which provides a classical description of their average phase-space distribution based on conditionally invariant measures of the classical dynamics. The extension to scattering systems with partial escape is being developed. Finally, we are studying universal properties of the eigenstate entanglement entropy between quantum chaotic subsystems. The behaviors apply equally well to few- and many-body systems, e.g., interacting particles in quantum dots, spin chains, coupled quantum maps, and Floquet systems, as long as their subsystems are quantum chaotic and not localized in some manner. The progression from a lack of entanglement in the uncoupled limit to the entanglement expected of fully randomized states in the opposite limit is governed by a single scaling transition parameter.

Driven-Dissipative Quantum Systems. We are studying the properties of open driven quantum systems, such as Floquet systems (i.e. periodically driven systems) in contact with a thermal environment, systems driven out of equilibrium by coupling to several baths of different temperature, or pumped lossy photonic systems. One major theme of our work is ordering in non-equilibrium steady states. For example, we developed a theory for generalized forms of Bose condensation in pumped photonic systems coupling to a thermal environment, such as exciton-polariton gases. It describes lasing in the state with the largest effective gain and equilibrium-like ground-state Bose condensation on the same footing, as well as phases with a macroscopic occupation in multiple modes. And it explains experiments in the groups of Jacqueline Bloch and Stephan Reitzenstein. Other examples of our work include the investigation of basic concepts for Floquet engineering (i.e. the control by means of periodic driving) in open systems, an efficient description of open many-body localized systems in thermal environments exploiting their representation in terms of quasi-local integrals of motion, and the discovery that the competition between two baths of different temperature can induce Bose condensation even if both temperatures lie well above the equilibrium critical temperature.

Quantum Dynamics of Isolated Many-Body Systems in Atomic Quantum Gases. Ultracold atomic quantum gases are realized by trapping 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. Here one important focus of our work lies on the control of many-body systems by means of strong time-periodic forcing (Floquet engineering). For example, we proposed how to realize one-dimensional anyons in a shaken optical lattice, how to stabilize fractional Chern-insulator states, or how to implement local solenoid-type magnetic fields and use them for controlled quantized charge pumping along tailored paths in 2D (fractional) Chern insulators. Together with experimentalists from the groups of Bloch and Weld, we also investigated driving-induced interaction-dependent heating processes as well as their limitations by ergodicity breaking prethermalization. A second major theme of our work are measurement schemes that are based on pump-probe-type protocols, where the far-from equilibrium dynamics of a system is monitored after a sudden quench (an abrupt change in the Hamiltonian). Together with the experimental group of Klaus Sengstock, we reported the first direct measurement of the Chern numbers of a topologically nontrivial band structure. Recently, we also proposed schemes for measuring off-diagonal elements of the single-particle density matrix in an optical lattice as well for probing Floquet topological invariants.

Cooperations

- We have fruitful collaborations within the **mpipks** with
 - Dr. Markus Heyl on simulating disordered open quantum systems, measuring the single-particle density matrix in optical lattices, and on probing ergodicity breaking in driven quantum systems.
 - Prof. Roderich Moessner on statistical properties of eigenstates in single-particle and many-body systems.
 - Dr. Ivan Khaymovich on multifractal properties of eigenstates.
 - Prof. Holger Kantz on intermittency in Hamiltonian systems.
 - Prof. Eduardo Altmann (now University of Sydney) on classical and quantum aspects of open dynamical systems.
- as well as externally with the experimental groups of
 - Prof. Klaus Sengstock (U Hamburg) on characterizing topology by dynamics: Chern number from linking number (within the DFG Research Unit FOR 2414).
 - Prof. Immanuel Bloch (LMU Munich) on interaction dependent heating and atom loss in a periodically driven optical lattice (within the DFG Research Unit FOR 2414).
 - Prof. David Weld (UC Santa Barbara) on controlling and characterizing Floquet prethermalization in a driven quantum system.
 - Prof. Stephan Reitzenstein (TU Berlin) on pump-power-driven mode switching in a microcavity device and its relation to Bose-Einstein condensation.
- and with the theory groups of
 - Prof. Gediminas Juzeliunas and Prof. Egidijus Anisimovas (U Vilnius) on Floquet topological quantum systems.
 - Prof. Sergey Denisov (U Augsburg) on Floquet engineering in open quantum systems.
 - Prof. M. Haque (Maynooth University, Co. Kildare, Ireland) on multifractal properties of eigenstates.
 - Prof. S. Tomsovic (Pullman, Washington, USA) on entanglement in bipartite interacting systems.
 - Prof. A. Lakshminarayan (IIT Madras, Chennai, India) on entanglement in bipartite interacting systems.
 - Dr. S. C. L. Srivastava (VECC, Kolkata, India) on entanglement in bipartite interacting systems.
 - Prof. J. D. Meiss (University of Colorado, Boulder, USA) on dynamics in 4D symplectic maps.

- Dr. S. Anastassiou (University of Patras, Greece) on manifolds in 4D symplectic maps.
- Prof. S. Keshavamurthy (IIT Kanpur, Uttar Pradesh, India) on the phase-space dynamics of van der Waals dissociation.
- Prof. Tassos Bountis (Nazarbayev University, Astana, Kazakhstan) on manifolds in 4D symplectic maps.
- Prof. Haris Skokos (University of Cape Town, South Africa) on geometry of complex instability in galactic potentials.

1.11 Advanced Study Groups

Advanced Study Group 2016/2017: From Microscopic to Collective Dynamics in Neural Circuits (Convenor: Prof. Alessandro Torcini)

Scientific Aims, Procedures and Products The aim of the ASG was to analyze neural dynamics at a microscopic and macroscopic level in order to understand how the microscopic scale reflects on the macroscopic evolution and how the information generated at a microscopic level can be encoded in the population dynamics.

In particular, we focused, for its relevance for brain dynamics, on the so-called balanced regime [1–4]. Cortical neurons fire quite irregularly and with low firing rates, despite being subject to a continuous bombardment from thousands of pre-synaptic excitatory and inhibitory neurons. This apparent paradox can be solved by introducing the concept of balanced network, where excitation and inhibition balance each other and the neurons are kept near their firing threshold. In this regime spikes, representing the elementary units of information in the brain, are elicited by stochastic fluctuations in the net input current yielding an irregular microscopic activity, while neurons can promptly respond to input modifications.

Furthermore, we considered purely inhibitory networks [5,6]. Inhibition is a key aspect of neural dynamics playing a fundamental role for the emergence of neural rhythms and the implementation of various information coding strategies. Inhibitory populations are present in several brain structures and the comprehension of their dynamics is strategical for the understanding of neural processing.

One of the main transversal topic of study concerned the development of a mean-field theory for spiking neural networks able to capture exactly the microscopic dynamics [1,7–9]. Another one was the control of neural dynamics and the population coding strategies adopted in developing neural circuits [10–13] as well as the implementation of strategies to avoid anomalous neural synchronization [11,12,14]. A number of further related subjects in computational neuroscience have also been addressed during the course of the group’s activity together by the core members and the short term visitors.

The ASG brought together experts in statistical mechanics, nonlinear dynamics, applied mathematics and computational neuroscience in an effort to develop fruitful collaborations across disciplines. In order to stimulate discussions and interactions, 17 talks were given by the members and the visitors. Many collaborative projects have emerged from the ASG. So far there are twenty-one papers and preprints [1–21] that have resulted from work done at the ASG. 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 Personell The ASG was convened in two different periods. The first period was from June 15 to September 14, 2016, and the second period was from June 26 to August 26, 2017. The core, long-term members of the ASG were Prof. German Mato (Centro Atomico Bariloche, Argentina), Prof. Antonio Politi (Kings’ College, Aberdeen University, UK), Dr. Hugh Robinson (Cambridge University, UK), Prof. Marc Timme (TU Dresden, Germany). The group also benefited from 10 short-term visitors, including David Angulo Garcia (Aix-Marseille University, France), Christoph Kirst (The Rockefeller University, USA), Carlo Laing (Institute of Natural and Mathematical Sciences, Massey University, Albany, NZ), Erik Martens (Dept. of Applied Mathematics and Computer Science, Technical University of Denmark, Copenhagen, Denmark), Ernest Montbrió (Universitat Pompeu Fabra, Spain), Jan Nagler (Eidgenössische Technische Hochschule Zürich, Switzerland), Simona Olmi (INRIA, Nice, France), Robert Schmidt (Albert-Ludwigs-Universität Freiburg, Germany), Ekkehard Ullner (King’s College, University of Aberdeen, UK), Matteo di Volo (École Normale Supérieure, France). 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 The balanced state is typically associated to asynchronous dynamics, however this is not the only regime observable during spontaneous cortical activity. As a matter of fact, oscillations at different frequencies are typically observed in neural recordings at the global scale (e.g. EEG, LFP), thus indicating the emergence of collective dynamics.

We have found a novel mechanism for the emergence of collective oscillations (COs) in balanced spiking inhibitory networks in absence of any synaptic or delay time scale. COs can be triggered by microscopic irregular fluctuations, whenever the neurons will share a sufficient number of common inputs. Furthermore, for a sufficiently large in-degree the erratic spiking emissions can promote oscillatory dynamics over a broad range of frequencies [1].

Furthermore, we have shown that, contrary to the current expectations, even in the presence of a 10% dilution, the collective dynamics exhibited is characterized by a sizeable synchronization. The analysis of a suitable order parameter reveals that the macroscopic dynamics is highly irregular and remains such in the thermodynamic limit (i.e., for infinitely many neurons). The underlying form of synchronization is thereby different from the collectively regular dynamics observed in systems such as the Kuramoto model [2, 3].

Finally, we have identified a new mechanism for balancing in fully coupled excitatory-inhibitory heterogeneous neural networks with synaptic depression. In such a context, a transition is observable from asynchronous dynamics to COs. Furthermore, the balance is achieved due to the compensation of the increase of the coupling strength by the reduction of the average value of the phase response curve measured at the moment of the spike arrival and induced by almost synchronous dynamics [4].

We have clarified the mechanisms underlying a general phenomenon present in pulse-coupled heterogeneous inhibitory networks: inhibition can induce not only suppression of the neural activity, as expected, but it can also promote neural reactivation. In particular, for globally coupled systems, the number of firing neurons monotonically reduces upon increasing the strength of inhibition (neurons' death). However, the random pruning of the connections is able to reverse the action of inhibition, i.e. in a random sparse network a sufficiently strong synaptic strength can surprisingly promote, rather than depress, the activity of the neurons (neurons' rebirth). We have shown that this effect is observable whenever two sources of quenched disorder are present in the network: namely, a random distribution of the neural properties and a random topology [5]. In the context of pulse-coupled inhibitory networks with instantaneous synapses, we reported exact results for the firing rate, the coefficient of variation and the spike train spectrum for various synaptic weight distributions. Our results are not limited to stimulations of infinitesimal amplitude, but they apply as well to finite amplitude post-synaptic potentials, thus being able to capture the effect of rare and large spikes. The developed analytical methods are able to reproduce also the average firing properties of heterogeneous neuronal populations [6].

We have inferred the network topology given the correlations between neural signals. A focus was on linear time-continuous systems as characterizing large-scale brain activity close to some (experimentally defined) activity state. A core result is that there exists a principal limit of reconstructability: if the coupling strengths between recorded units (e.g. subareal activities) is above some level, inference of the physical connectivity structure is in general impossible, even in the limit of uncorrelated noise, linear systems of coupled one-dimensional units and infinitely long and arbitrarily exact time series recordings [15]

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Chapter 2

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2.1 The fate of a discrete time crystal in an open system

ACHILLEAS LAZARIDES AND RODERICH MOESSNER

The study of the non-equilibrium dynamics of quantum systems has been a most productive activity of late. One of our principal contributions consists of the prediction of a new form of spatiotemporal order in periodically driven systems. Originally christened π -spin glass [1], the phenomenon now goes under the name of Floquet discrete time crystal (DTC).

A priori, the main obstacle to observing interesting physics at long times in Floquet matter [2] is that a general ergodic system simply heats up maximally under driving, as its entropy increases due to the non-adiabatic nature of the perturbation [3,4]. This process may be frustrated robustly by introducing disorder which leads to a many-body localised (MBL) phase in static systems. Driving an MBL system leads to finite-energy-density long-time states [5–7] which may display non-equilibrium phases based on the notion of eigenstate order.

Eigenstate order in static systems describes the appearance of multiplets of eigenstates quasi-degenerate in energy. Analogously, in Floquet systems, the multiplets are quasi-degenerate in the corresponding quasi-energy. Since the periodic drive lowers time-translation invariance from continuous to discrete, the quasi-energy is conserved only modulo $2\pi/T$ (in units where $\hbar = 1$). This turns out to allow for some further types of eigenstate order.

In particular, in a Floquet Ising spin glass the quasienergy offset may be π . This new type of spatiotemporal order can further be generalised to more complex settings; for a parafermionic chain, which lacks the simple noninteracting limit of the Ising case, we find n -tuplets offset in quasienergy by $2\pi/n$ [8].

What all of these systems have in common is that they exhibit a subharmonic response to the driving. Like Bragg peaks signalling an increased magnetic unit cell, compared to the structural one, upon the onset of antiferromagnetic Néel order, this is encoded in the temporal Fourier transform. They thus break the residual discrete time-translation invariance by a further factor n , whence they are named discrete time crystals. For a brief review see Ref. [2].

This prediction immediately sparked activity aimed at the experimental confirmation of this new form of non-equilibrium order [9,10]. However, all experiments found a *temporally decaying* order parameter. This immediately poses the question of the stability of the spatiotemporal order in realistic environmental conditions. In addition, in this setting there is the obvious question about the role of decoherence – a concept of perennial interest in quantum physics.

Thus, motivated by its conceptual importance as well as its experimental relevance, we consider the effect of coupling to an external environment. We find, both analytically and numerically, that the DTC in disordered one-dimensional systems is destroyed at long times by *any* such natural coupling, even when the system is prevented from heating up in Floquet manner to infinite temperature by an external thermal bath [11].

Our study considers the evolution of the density matrix via a Lindblad equation describing coupling to a Markovian environment. We have concretely investigated two generic models of environmental decoherence as well as a model of an external thermal bath.

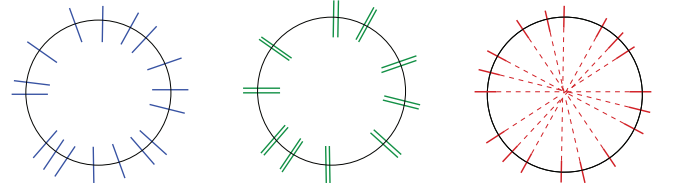


Figure 1: Floquet eigenstate order. The quasienergy axis is compactified into a circle on account of its periodicity with $2\pi/T$. Eigenstate quasienergies may be nondegenerate (left) or quasidegenerate in pairs for the 0-spin glass (middle), or separated by π/T for the π -spin glass (Floquet discrete time crystal, right).

The Floquet dynamics is provided by a binary drive, in which the period T is subdivided into two parts during each of which a time-independent Hamiltonian with random coefficients generates unitary evolution:

$$H(t) = \begin{cases} H_z & \text{if } 0 \leq t < T_z \\ H_x & \text{if } T_x \leq t < T = T_z + T_x \end{cases} \quad (1)$$

The model describing a chain of spins-1/2 represented by Pauli matrices σ_i^γ is [1]

$$H_z = \frac{1}{2} \sum_{i=1}^L h_i \sigma_i^z + \sum_{i=1}^{L-1} J_z \sigma_i^z \sigma_{i+1}^z, \quad (2)$$

$$H_x = \sum_{i=1}^{L-1} J_x \sigma_i^x \sigma_{i+1}^x + J_z \sigma_i^z \sigma_{i+1}^z$$

This leads to a unitary time-evolution operator over one period, $U := \exp(-iH_x T_x) \exp(-iH_z T_z)$. Crucially, in the DTC phase, its eigenstates come in the abovementioned n -tuples $|\omega_\alpha, A\rangle$ characteristic of eigenstate order, with $A = 1 \dots n$ and α labelling the multiplet. At long times, the density matrix of this sys-

tem acquires the visually simple form

$$\rho^{\text{BDE}} = \begin{array}{c|ccc|c} & \ddots & & & \\ \hline & \tilde{\rho}_{\alpha-1,\alpha-1} & 0 & 0 & \\ \hline & 0 & \tilde{\rho}_{\alpha,\alpha} & 0 & \\ \hline & 0 & 0 & \tilde{\rho}_{\alpha+1,\alpha+1} & \\ \hline & & & & \ddots \end{array} \quad (3)$$

This block-diagonal ensemble, in which off-diagonal terms between the different quasi-degenerate multiplets vanish, is the generalisation of the familiar diagonal ensemble in the absence of eigenstate order.

The most general equation for the possibly non-unitary evolution of a quantum density matrix is given by the Lindblad equation $\partial_t \rho = \mathcal{L}\rho$ with Lindblad operator

$$\mathcal{L}\rho = -i[H, \rho] + \sum_a \left(L_a \rho L_a^\dagger - \frac{1}{2} [L_a^\dagger L_a, \rho]_+ \right)$$

where $[\cdot, \cdot]_+$ is the anticommutator and the L_a arbitrary operators encoding the non-unitary part of the dynamics. In our work, we use this form with the time-dependent Hamiltonian of Eq. (1) and choices of Lindblad operators L_a appropriate to different types of environmental couplings.

We have studied a number of physically motivated forms of the Lindblad operators. Fig. 2 shows the temporal trace of an order parameter for coupling to a thermal bath at different inverse temperatures β , modelled by Lindblad operators of the form

$$L_{mn} = \Gamma_{mn} |m\rangle \langle n| \quad (4)$$

with $|m\rangle$ eigenstates of the instantaneous Hamiltonian, while $\Gamma_{mn} = 2\pi |V_{mn}| g(\epsilon_n)$ with V depending only on system properties and on the bath and the system-bath coupling. This is the standard form obtained by the Born-Markov approximation and for typical cases leads to a Gibbs state in the long-time limit for a time-independent Hamiltonian.

From these analyses, the following insights can be abstracted. Because DTC behaviour is a property of the Floquet states, not detectable by spatially and temporally local measurements, Lindblad operators preserving DTC are very restricted in their form. The most natural route to such a form is to express the Lindblad operators in the Floquet basis. The simplest choice then would be to restrict considerations to Lindblad operators which do not couple different multiplets $|\omega, A\rangle$ to each other at all. A less restrictive condition would be to allow them to couple Floquet states only to others selected based on the local operator that displays long-time subharmonic oscillations.

What both of these restrictions have in common is that the Lindblad operators need to ‘know’ about the details of the DTC spectrum, and the relation between its different multiplets. This leads to the conclusion that coupling to physical environments typically destroys

DTC, since in general the environment will not have this property. Thus while it is possible to write down Lindblad operators preserving the DTC, these do not appear to correspond to any natural physical processes.

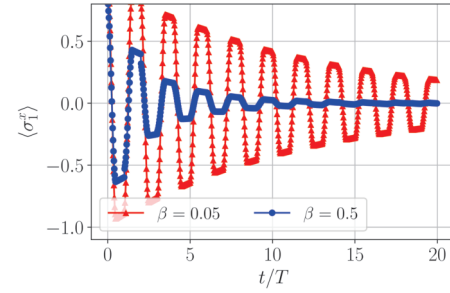


Figure 2: Real time plot of $\langle \sigma_1^x \rangle(t)$ using ‘thermal’ Lindblad operators for times $T_x = T_z = 1$. Such operators lead to thermal (Gibbs) steady states in the static case at inverse temperature β . The data displayed is for size $L = 5$.

This study signals a number of interesting further topics. The first is a detailed analysis of the dependence of these phenomena on gross system parameters – in particular, studying the influence of system dimensionality is a natural follow-on from recent studies of many-body localisation in higher dimension. This question is all the more pressing as one of the works studying the presence of time crystallinity was in fact undertaken on a three-dimensional system. [10] This ties in naturally with a second major question, namely how one can hope to stabilise time-crystalline behaviour for a long ‘intermediate’ time window, even if at asymptotically long times such order is completely lost. In particular, can one use the coupling to an environment to prolong, rather than curtail, the lifetime of subharmonic responses of the isolated system? There clearly remains much scope for exciting discoveries in both theory and experiment.

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2.2 Floquet multifractality

STHITADHI ROY, IVAN M. KHAYMOVICH, ARNAB DAS, AND RODERICH MOESSNER

Fractals are beautiful structures found in nature, whose complexity and elegance has always captured the imagination of scientists. They show up in seemingly unrelated phenomena at vastly different scales, for instance, from turbulent flows and brain dynamics to quantum physical systems at atomic and electronic scales. In the context of quantum condensed matter systems, fractal structures in electronic wavefunctions are commonly associated with critical wavefunctions at localisation transitions or in hierarchical and infinite-dimensional systems, the unifying feature being divergent localisation lengths in the former and exponentially growing site number with the distance in the latter [1]. Hence, realising (multi)fractality in an inherently short-ranged system without fine-tuning to criticality poses an interesting and important challenge.

Our search for robust multifractality in short-ranged systems takes us to non-equilibrium physics, specifically to that of periodically-driven (Floquet) disordered quantum systems. Such systems have generated many unexpected discoveries of late, such as periodic thermodynamic ensembles and the discrete time crystal [2, 3]. Robust multifractality in a Floquet system adds to the list of novel phases of quantum matter exclusive to them [5].

The ingredients are (1) a system with a single-particle mobility edge separating localised and delocalised eigenstates in energy, which is ubiquitous in systems with incommensurate bichromatic potentials, and (2) a time-periodic modulation which couples the delocalised and localised states separated in energy by an amount equal to the frequency of the modulation.

The central finding of this work is that such a hybridisation do not just delocalise localised states, but gives rise to a band of multifractal Floquet states. The latter are eigenstates of the corresponding time-evolution operator over a period, also known as the Floquet operator, denoted by U . The relevance of the eigenstates of U lies in the fact that they encode the full information about the stroboscopic dynamics of the system.

Our starting point is a variant of the one-dimensional Aubry-André Hamiltonian

$$H = \sum_x [J(\hat{c}_x^\dagger \hat{c}_{x+1} + \text{h.c.}) + Vv(x)\hat{c}_x^\dagger \hat{c}_x]. \quad (1)$$

It comprises a simple nearest-neighbour hopping term alongside a potential $v(x) = \cos(2\pi\kappa x + \theta)/[1 - \mu \cos(2\pi\kappa x + \theta)]$, quasiperiodic on account of its incommensurate wavevector, which we set to the golden mean, $\kappa = (\sqrt{5} + 1)/2$.

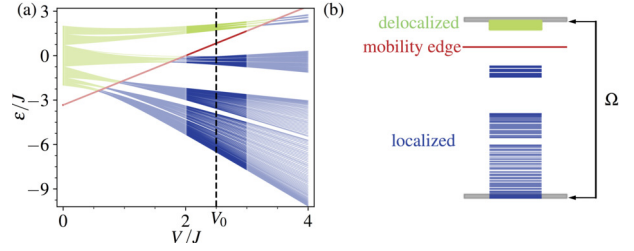


Figure 1: **Schematic of the coupling between localised and delocalised states via the periodic drive.** (a) The energy spectrum of the undriven Hamiltonian (1), where the colour shows the scaling of the inverse participation ratio with system size, with green corresponding to the delocalised states ($\sim L^{-1}$) and blue to localised states ($\sim L^0$). The red line denotes the mobility edge. (b) The energy levels corresponding to V_0 (denoted by the black dashed line in (a)) where a periodic drive with frequency Ω chosen to be slightly smaller than the bandwidth couples the delocalised and localised states approximately within the grey shaded windows.

The model exhibits a mobility edge at an energy, $\varepsilon_{\text{ME}} = 2\text{sgn}(V)(|J| - |V|/2)/\mu$ as shown in Fig. 1(a) [4]. We set $J = 1$ and $\mu = -0.6$ throughout. The system is driven by a time-periodic modulation of the amplitude of the quasiperiodic potential in the form of a square wave with frequency Ω , mean V_0 , and amplitude ΔV .

A common diagnostic for localisation properties of wavefunctions is their inverse participation ratio, $\text{IPR} = I_2 = \sum_x |\phi(x)|^4$ scaling with system size L as L^{-1} (L^0) for delocalised (localised) states in one dimension. The first signs of Floquet multifractality appear in the IPR scalings of the Floquet eigenstates. As Ω is chosen to be slightly smaller than the bandwidth of the spectrum of the static Hamiltonian (1), the drive primarily couples resonant states close to the edges of the undriven spectrum, leaving largely unaffected all the localised and delocalised states in between. These latter two, together with our newly discovered multifractal states, are evident in Fig. 2(a-c), which shows *three distinct* scalings of the IPR. In particular, the collapse of the data for different L , when the IPR is scaled with $L^{1/2}$ (Fig. 2(b)) betray the fractal nature of the states. A more complete characterisation of multifractality is via a generalised IPR and its scaling exponent τ_q ,

$$I_q(\phi) = \sum_{x=1}^L |\phi(x)|^{2q} \sim L^{-\tau_q}, \quad (2)$$

where $D_q = \tau_q/(q-1)$ is the *fractal dimension*. For delocalised (localised) states, $D_q = 1$ and $(0, q > 0)$, whereas any other behaviour of D_q implies multifractality. In our case, for the fractal states we find $\tau_q \approx (q-1)/2$ and hence $D_q \approx 1/2$ which provides a complete characterisation of the fractality.

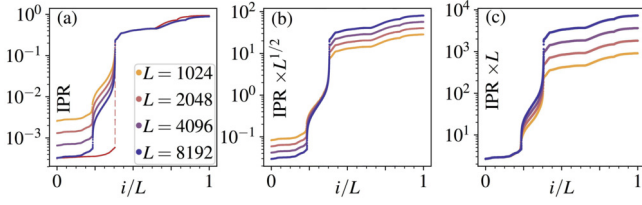


Figure 2: **Characterisation of Floquet multifractal states.** The inverse participation ratio (IPR), shown for the Floquet eigenstates sorted in increasing order of I_2 , for different system sizes L . The collapse of different segments of the data for different L , when the IPR is scaled with (a) L^0 , (b) $L^{1/2}$, and (c) L reflects the presence of localised, multifractal, delocalised states respectively. The data in red in (a) shows the IPRs of static eigenstates (for $L = 8192$) for reference. The system parameters are $V_0 = 2J$, $\Delta V = J/2$, and $\Omega = 2.74\pi J$, where the bandwidth of the undriven spectrum is $\approx 2.76\pi J$.

The mechanism underlying the Floquet generation of multifractality can be understood in a random matrix framework. A central ingredient is the coupling between localised states $\{|\psi_l\rangle\}$, via their Floquet-generated coupling to the delocalised states, $\{|\psi_d\rangle\}$. The leading effective matrix element coupling static localised states and determining a resulting Floquet eigenstate at quasienergy ω reads

$$M_{\psi_l, \psi_j} = \sum_{\psi_d} \frac{\psi_d(x_{l_i})v(x_{l_i})\psi_d^*(x_{l_j})v(x_{l_j})\Delta V^2}{(\omega - \varepsilon_{\psi_d} + \Omega)}. \quad (3)$$

Here, a localised eigenstate of the undriven Hamiltonian $|\psi_l\rangle = |x_{l_i}\rangle$ is approximated by a δ -function localised at $x = x_{l_i}$, and the primed sum denotes a sum over delocalised states near the top of the spectrum resonant with the localised ones at the bottom, as shown schematically in Fig. 1(b). This leads to a fully connected random matrix Hamiltonian within the localised states, with the undriven eigenenergies on the diagonal, and the M_{ψ_l, ψ_j} as the off-diagonal matrix elements. We note that the effective random matrix model characterised by the distribution, $P(M)$, of off-diagonal elements formally resembles the Rosenzweig-Porter random matrix ensemble, known to host fractal eigenstates with a certain fractal dimension $D_q = D$ [6].

This effective model allows us to connect the multifractality of the wavefunctions to the statistical properties of the Floquet-generated matrix elements M , which decay algebraically with system size, $\langle |M| \rangle_P \sim L^{-\gamma_1}$. Following [6] $\tau_q = (q-1)(2-2\gamma_1)$. Constructing $P(M)$ numerically yields $\gamma_1 \approx 0.78$, and hence $\tau_q \approx 0.44(q-1)$ in rather close agreement with the numerically obtained result. The underlying origin of multifractality is hence the non-trivial mixing of localised states mediated by the delocalised states as an effect of the Floquet drive, thus linking our fully short-range model to an effective long-ranged random matrix ensemble.

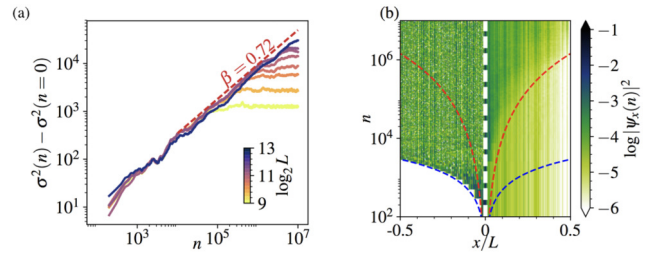


Figure 3: **Signatures of multifractality in wavepacket spreading.** (a) Subdiffusive behaviour in $\sigma^2(n)$ of multifractal states with exponent $\beta \approx 0.72$. (b) Local density $|\psi_n(x)|^2$ as a colour map over x and n , where $x < 0$ ($x > 0$) shows the ballistic (subdiffusive) dynamics due to delocalised (multifractal) states. The data for $x > 0$ corresponds to the case where the delocalised states have been projected out. The blue (red) dashed lines corresponding to ballistic (subdiffusive) dynamics indicate the difference between the two.

Having established the existence of Floquet multifractality, a natural question is what are its consequences on the dynamics of the system. We address this question via a simple process, the spreading of an initially localised wavepacket, $|\psi_0\rangle$. Wavepacket spreading is quantified by its variance $\sigma^2(n) = \langle \psi_n | \hat{x}^2 | \psi_n \rangle - \langle \psi_n | \hat{x} | \psi_n \rangle^2$, averaged over disorder, where $|\psi_n\rangle = U^n |\psi_0\rangle$ is the wavepacket after n driving periods. The presence of an extensive number of delocalised states in the eigenbasis of U leads to a ballistic leading behaviour $\sigma^2(n) \sim n^2$. In the presence of multifractal states, subleading behaviour emerges as $\sigma^2(n) \sim \lambda_1 n^2 + \lambda_2 n^\beta$. As a matter of principle, to accurately capture β , it is desirable to remove the dominant contribution of the delocalised states, which can be achieved in theory by projecting of the initial wavefunction onto subspace orthogonal to them. The (normalised) projected initial state $|\tilde{\psi}_0\rangle$, now has the leading contribution to the spreading from the multifractal states. The dynamics is in fact *subdiffusive* with $\beta \approx 0.72$, Fig. 3(a). That the spreading due to the multifractal is slower than that of the ballistic case is exemplified in Fig. 3(b).

We close by saying that while Floquet multifractality is an interesting theoretical direction, its observation is well within the reach of cold-atom experiments where incommensurate potentials as well as periodic modulations are quite the state of art [7].

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2.3 Dynamics and long-time behavior in static and periodically-driven many-body localized systems

TALÍA L.M. LEZAMA, JENS H. BARDARSON

Introduction. Many-body localization (MBL) is a general mechanism that prevents thermalization in closed quantum interacting disordered systems, resulting in an ideal insulator with vanishing conductivities at finite, or even infinite, temperatures [1]. As a result, systems exhibiting MBL are manifestly nonergodic, thereby violating the eigenstate thermalization hypothesis and providing examples where the framework of conventional statistical mechanics and thermodynamic phase transitions breaks down.

The MBL phase and the MBL-ergodic transition can be described in terms of the many-body eigenstates and their entanglement properties which can also be reflected in the dynamics of the system, for example, for non-equilibrium protocols such as quantum quenches and periodic driving. The MBL insulator is adiabatically connected to the Anderson insulator, just as the Fermi liquid to the Fermi gas [1, 4, 5]. The great difference between these two scenarios is that former can occur for highly-excited eigenstates, while the latter only for lowly-excited eigenstates. Distinctively from the Anderson insulator, the presence of interactions in the MBL phase gives rise to dephasing that results in a logarithmic growth of entanglement entropy [2] and a slow relaxation of local observables towards nonergodic stationary states at long times [3]. Dynamics deep in the ergodic phase is fast but starts slowing down when approaching the ergodic-MBL transition. In particular, for systems with extensive conserved quantities, the slow regime within the ergodic phase is characterized by zero DC conductivity and subdiffusive transport, as well as by a subballistic spreading of entanglement, and a power-law relaxation of autocorrelation functions [10].

One-particle density matrix occupation spectrum after a global quench. The analogy between many-body localization and Fermi-liquid physics [1, 4, 5] raises several questions, the most direct one being whether there is a finite-temperature analog by realizing an effective temperature. In a Fermi liquid the occupation spectrum is discontinuous only at zero temperature; any nonzero temperature leads to a smooth occupation spectrum.

In Ref. [6] we propose, by means of exact diagonalization and analytical arguments, that the long-time averaged one-particle density matrix (OPDM) obtained in the steady state after a quench from a local product state mimics occupation effects of temperature in a Fermi liquid, with the MBL eigenstates providing an analog to a zero-temperature Fermi liquid. The proposed protocol allows us to connect the OPDM occupations to experimentally relevant quantities as opposed to those obtained from exact eigenstates which generally are not accessible in experiments. In particular, we have introduced an OPDM occupation imbalance, which behaves similar to the density imbalance but with a slower relaxation towards the steady state, thereby capturing dephasing. We further show how the partial occupations in the steady state can be controlled by tuning the structure of the initial state and described by an effective temperature.

In Fig. 1 we show that in the many-body localized phase, the steady state reached at long times after a quench from a local product state has a smooth OPDM occupation spectrum \bar{n}_α with a highly nonthermal shape (with $\{\bar{n}_\alpha\}$ close to 1 and 0), in contrast to that obtained in the ergodic phase.

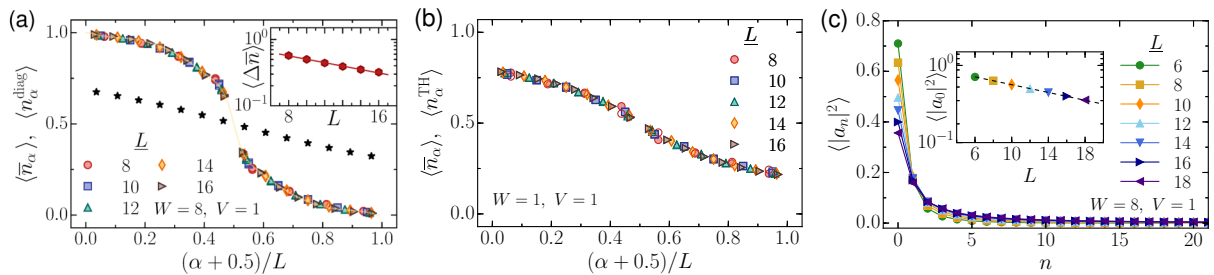


Figure 1: Infinite-time and disorder-averaged distribution of occupations as a function of system size L , for (a) strong, (b) weak disorder strengths. Additionally, (a) shows the diagonal-ensemble distribution in open symbols, the thermal ensemble (stars) and the inset the discontinuity as a function of L . Open symbols in (b) give the thermal distribution. (c) shows the disorder-averaged overlap between the initial state and the many-body eigenstates. Inset, disorder-averaged largest weight as a function of L . For further details we refer to Ref. [6].

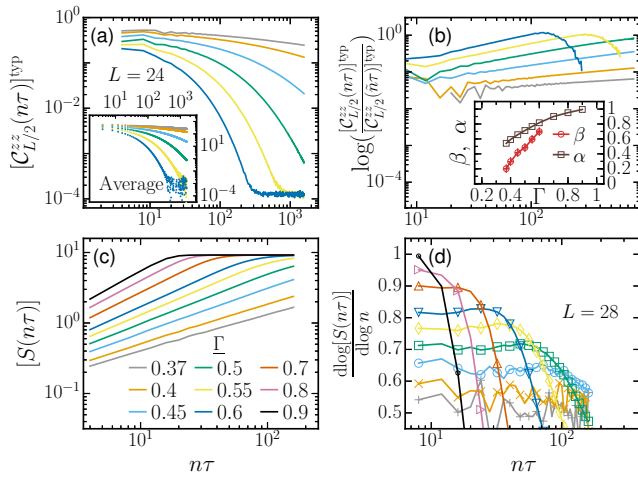


Figure 2: Stroboscopic time evolution of the disorder-averaged (a) autocorrelation function, (c) entanglement entropy. Inset in (b): Dynamical exponents as a function of disorder strength; the exponent β is extracted by fitting a linear function to the data points in (b), whereas α corresponds to the first data points in (d). For further details we refer to Ref. [11].

Dynamics in the ergodic phase of a periodically driven system. Floquet, or periodically-driven, quantum many-body systems are a central object of study in non-equilibrium physics. If the system is ergodic, it is to expect that an external forcing will drive it out of equilibrium, heating it up to an infinite-temperature or a fully-mixed state, as stated by variants of the eigenstate thermalization hypothesis applicable to Floquet systems [7]. There is a robust mechanism to prevent full heating inherent to periodic driving, which appears

when adding sufficiently strong disorder to a Floquet system. Such Floquet-MBL systems undergo an MBL-ergodic transition that can be tuned by the frequency or the amplitude of the drive [8].

The presence of slow dynamics on the ergodic side of the transition in Floquet systems without extensive conserved quantities, was conjectured but not seen before in microscopic models [9,10]. Under that premise, in Ref. [11] we study a model known to experience a Floquet-MBL transition which can be tuned by the disorder strength within a region of the frequency-amplitude space. In particular, we study the stroboscopic dynamics of two quantities: an autocorrelation function when the system is initially prepared in an infinite-temperature initial state, and the entanglement entropy starting from a product state. The model studied allows for an implementation of a Hadamard gate, thus enabling us to treat the system exactly and efficiently up to large system sizes and long times.

The main contribution of our work is the observation of such slow behavior while approaching the critical point. We summarize our main results in Fig. 2, where we observe a stretched-exponential decay of the return probability, $C_{L/2}^{zz}(t) \propto \exp(-\gamma n^\beta)$, and a subballistic spread of the entanglement entropy, $S(n\tau) \propto n^\alpha$ (see Fig. 2(a),(c)). Both quantities are expressed in terms of the stroboscopic time step n and the driving period τ , with dynamics characterized by a disorder-dependent exponent α and β , respectively.

Nonetheless, we further observe a flow of the associated exponents towards faster dynamics when studying larger system sizes and longer times (for further details we refer the reader to [11]).

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2.4 Effective potentials for dynamical quantum phase transitions in the Ising chain

DANIELE TRAPIN, MARKUS HEYL

Introduction

Quantum simulators have nowadays achieved experimental access to the real-time dynamics of closed quantum many-body systems due to the impressive progress in controlling matter at the quantum level within the last two decades [1]. Such quantum simulators have been realized on various experimental platforms such as ultra-cold atoms in optical lattices, trapped ions, and more, and have recently studied exotic dynamical phenomena inaccessible with conventional architectures. This includes the observation of particle-antiparticle production in lattice gauge theories [2], many-body localization [3,4], or discrete time crystals [5,6]. It is the central property of such nonequilibrium quantum states that they cannot be captured within a thermodynamic description. This, however, might not only be seen as an obstacle but rather as an opportunity to generate new quantum states beyond equilibrium constraints such as the principle of equal a priori probabilities in the microcanonical ensemble. A prominent example constitutes the celebrated time crystal, which cannot exist in equilibrium states.

From an alternative point of view the main challenge in the understanding of nonequilibrium quantum states is that now it is not sufficient to understand the properties of Hamiltonians alone. Instead, we have to characterize quantum time-evolution operators:

$$U(t) = \mathcal{T}e^{-i\int_0^t dt' H(t')}. \quad (1)$$

Here, \mathcal{T} denotes the time-ordering prescription and $H(t)$ the, in general, time-dependent Hamiltonian. Crucially, the propagator $U(t)$ contains one additional scale, which is time itself. Note that we use units such that $\hbar = 1$. However, it remains a central question how to extract general principles in time-evolution operators, i.e., quantum dynamics, and to which extent we can describe nonequilibrium quantum many-body states in a unified manner. The theory of dynamical quantum phase transitions (DQPTs) targets this characterization of quantum real-time evolution by lifting the notion of phase transitions to the time domain [8,9].

For concreteness, let's consider the nonequilibrium scenario of a so-called quantum quench, and let's prepare initially a system in the ground state $|\psi_0\rangle$ of an initial Hamiltonian H_0 . Then, at time $t = 0$ a parameter of the system is suddenly switched (quenched) such that the Hamiltonian H is now different from the initial one. As a consequence, the system evolves according to $|\psi(t)\rangle = U(t)|\psi_0\rangle$ with $U(t) = \exp(-iHt)$ since $H(t > 0) = H = \text{const.}$

Dynamical quantum phase transitions

The central object within the theory of DQPTs is the so-called Loschmidt amplitude [8,9]:

$$\mathcal{G}(t) = \langle \psi_0 | U(t) | \psi_0 \rangle = \langle \psi_0 | e^{-iHt} | \psi_0 \rangle, \quad (2)$$

which can be viewed as a matrix element of the time evolution operator $U(t)$ and thereby can serve the purpose of characterizing $U(t)$, or as a measure for how far the time-evolution drives the system away from its initial condition. On a formal level, $\mathcal{G}(t)$ has a structure very similar to equilibrium partition functions, with, however, one central difference in that $\mathcal{G}(t)$ in general assumes complex values due to the unitarity of quantum real-time evolution. As an important consequence of this formal equivalence, Loschmidt amplitudes $\mathcal{G}(t)$ can develop nonanalytic behavior in the same way as equilibrium partition functions at phase transitions. Concretely, the rate function $f(t) = -N^{-1} \log[\mathcal{G}(t)]$ for the Loschmidt amplitude can show singular behavior as the free energy density $f(\beta) = -(N\beta)^{-1} \log[Z(\beta)]$ corresponding to the partition function $Z(\beta)$ at inverse temperature β . Here, N denotes the number of degrees of freedom in the system. While free energy densities are nonanalytic as a function of an external control parameter such as temperature, $f(t)$ can exhibit singular behavior as a function of time. This is the definition of a DQPT. In Fig. 1 DQPTs occurring for quantum quenches in transverse-field Ising chains are shown.

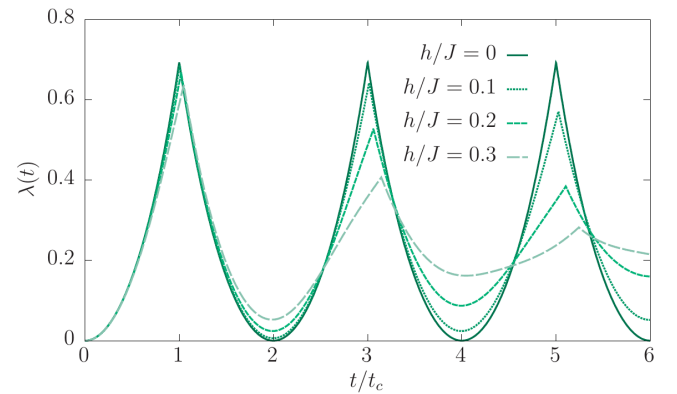


Figure 1: Dynamical quantum phase transitions for quantum quenches in the transverse-field Ising chain for various final transverse field strengths h .

Transverse-field Ising chain

In our work we explore further analogies between the equilibrium free energy density $f(\beta)$ and the rate function $f(t)$ for the paradigmatic Ising chain:

$$H = -J \sum_{n=1}^N \sigma_n^z \sigma_{n+1}^z - h \sum_{n=1}^N \sigma_n^x. \quad (3)$$

Here, σ_n^α denotes Pauli matrices with $\alpha = x, y, z$ and N the total number of lattice sites. In equilibrium this model undergoes a quantum phase transition from a magnetically ordered phase for $J < h$ to a disordered phase for $J > h$ [7].

In the following, we consider the Ising chain in a far-from-equilibrium scenario. The system is initially prepared in the ground state in the limit $J/h = 0$, which we denote by $|\rightarrow\rangle$. At time $t = 0$, the parameters are switched to the opposite limit, namely $h/J = 0$. Later on it is straightforward to generalize the results departing from this extreme case. It is known that after such a quantum quench the system experiences a periodic sequence of DQPTs with nonanalytic kinks in the rate function $f(t)$ [8], see for instance Fig. 1 where $\lambda(t) = 2\text{Re}[f(t)]$ is plotted. It is the main purpose of our work to explore to which extent a macroscopic description of $f(t)$ equivalent to a Landau theory is possible.

Effective potentials

For the considered quantum quench protocol, it is possible to write formally the Loschmidt amplitude as a conventional partition function [10]:

$$\mathcal{G}(t) = \langle \rightarrow | e^{iJt \sum_n \sigma_n^z \sigma_{n+1}^z} | \rightarrow \rangle = \frac{1}{2^N} \text{Tr} e^{-\mathcal{H}}, \quad (4)$$

where $\mathcal{H} = K \sum_n \sigma_n^z \sigma_{n+1}^z$ is a classical Hamiltonian with $K = -iJt$. The only difference to the equilibrium case is that now the couplings $K \in \mathbb{C}$ are complex. The partition function of the 1D Ising model is exactly solvable [7], which is also valid in the case of complex couplings.

In order to derive the targeted Landau theory from microscopics, let us use that:

$$\mathcal{G}(t) = e^{-Nf(t)} = \sum_s e^{\mathcal{H}(s)} = \int dM e^{-Nf(M,t)}. \quad (5)$$

Here, $\mathcal{H}(s)$ denotes the energy of a spin configuration $s = (s_1, s_2, \dots, s_N)$ with $s_n = \pm 1$ and $\exp[-Nf(M,t)] = \sum_s \exp[-\mathcal{H}(s)] \delta(M - \sum_n s_n)$ defines the analog of a free energy density $f(M,t)$ at a fixed magnetization M .

While thermodynamic potentials in equilibrium statistical physics obey a minimizing principle, here we find:

$$f(t) = \text{sp}_{m \in \mathbb{C}} f(m,t), \quad (6)$$

where sp stands for the saddle point taken over a set of complex magnetization density $m = M/N \in \mathbb{C}$. This is a consequence of the complex valued functions appearing in the above expressions. In the equilibrium limit where both $f(m,t)$ and m are real, the saddle point turns back into the minimization principle, allowing us to continuously connect to the equilibrium case. Further, from the exact solution of the Ising model we find that $f(m,t)$ admits an expansion:

$$f(m,t) = f_0(t) + \text{sign}(\theta) \alpha \tilde{m}^2(t) + \mathcal{O}(m^4(t)), \quad (7)$$

where $\tilde{m}(t) = U(t)m$, $f_0(t)$ is a time-dependent function and $U(t) = \exp[i\theta(t)]$ represents a rotation in the complex plane. From the exact solution of the model we observe that α is a time-independent constant and $\theta = (t_c - t)/t_c$ a linear function of the distance to the critical point in the vicinity of the DQPT at time t_c .

Consequently, one can interpret $f(m,t)$ as an effective potential for the DQPTs in the transverse-field Ising chain analogous to a Landau theory for equilibrium critical points. It will be a particularly interesting question for the future how these considerations can be extended to other systems and to explore to which extent effective potentials can be formulated from a macroscopic perspective without the need to compute them from a microscopic level.

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2.5 Real-time dynamics in lattice gauge theories

YI-PING HUANG AND MARKUS HEYL

Introduction

Gauge theories play an important role in physics ranging from the high-energy context [1] to models for quantum memories [2] and effective low-energy descriptions for condensed matter systems [3,4]. Today, synthetic quantum systems, such as realized in ultracold atoms in optical lattices or trapped ions, promise to provide a controlled experimental access to the unitary quantum evolution in lattice gauge theories, as demonstrated recently on a digital quantum simulator [5]. This has stimulated significant interest in the real-time dynamics of lattice gauge theories.

Gauge theories are characterized by strong local constraints enforced via Gauss' law. In the following we will consider lattice Hamiltonians in one dimension that can be cast in the form [6]:

$$H = -iw \sum_{x=1}^{L-1} (\psi_x^\dagger U_{x,x+1} \psi_{x+1} - h.c.) \quad (1)$$

$$+ m \sum_{x=1}^{L-1} (-1)^x \psi_x^\dagger \psi_x + J \sum_{x=1}^{L-1} L_{x,x+1}^2.$$

Here, ψ_x^\dagger (ψ_x) denotes the matter fermion creation (annihilation) operator on site x , where the presence of an electron (positron) is mapped to an unoccupied (occupied even) lattice site, allowing for a convenient incorporation of particles and antiparticles in a single fermion field. Accordingly, the second term in the above equation, representing the rest mass m , obtains a staggered sign. The gauge field degrees of freedom are represented by an electric field operator $L_{x,x+1}$ on the link between lattice sites x and $x+1$ with a conjugated operator $U_{x,x+1}$ obeying the commutation relation $[L_{x,x+1}, U_{x,x+1}] = U_{x,x+1}$. The first term in the above Hamiltonian corresponds to the creation and annihilation of particle-antiparticle pairs, and the third term reflects the energy stored in the electric field. Hamiltonians of the form in Eq. (2) can realize mainly the following two classes of lattice gauge theories. Within a Wilson lattice gauge theory formulation $U_{x,x+1} = \exp(i\varphi_{x,x+1})$ are complex phases and represent a continuous variable with $L_{x,x+1} = -i\partial/\partial\varphi_{x,x+1}$. This corresponds to the lattice Schwinger model, which is nothing but quantum electrodynamics in one dimension. Quantum link models provide an extension of Wilson lattice gauge theories using finite-dimensional Hilbert spaces for the gauge fields [7] by identifying $U_{x,x+1} = S_{x,x+1}^+$ and $L_{x,x+1} = S_{x,x+1}^z$ with quantum spin operators implying $2S+1$ states per link with S denoting the spin quantum number.

Experiment on a quantum computer

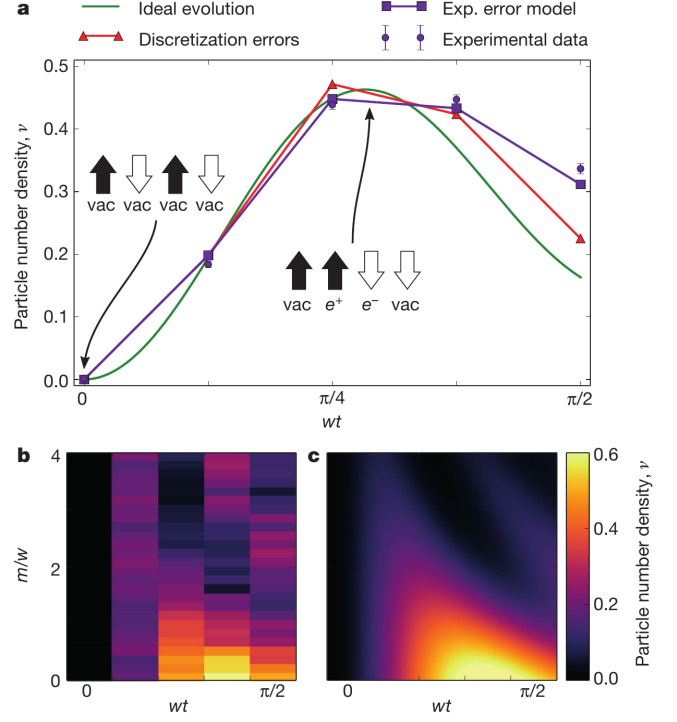


Figure 1: Measured particle-antiparticle production in the Schwinger model of quantum electrodynamics in one dimension on a small-scale quantum computer realizing four matter field sites [5]. **a** Dynamics of the particle number density ν for $m/w = 1/2$ and $J = w$ comparing experimental data to theoretically expected evolution including different error sources. The initial condition is the bare vacuum represented as a Néel state in the figure in a spin-1/2 language. **b** Experimentally measured ν in a color plot over various different values of m/w and compared to the ideally expected theoretical result in **c**.

In a recent experiment it has been shown that the nonequilibrium dynamics of lattice gauge theories can be synthesized on a trapped ion quantum computer by simulating the particle-antiparticle production in the Schwinger model of quantum electrodynamics in one dimension [5,8]. In that experiment the system was initialized in the bare vacuum $|\psi\rangle_0 = |1010\dots\rangle_\psi$, where matter is entirely absent, i.e., the ground state of H at $m \rightarrow \infty$. Through gauge invariance this also fixes the electric field configuration. Gauss' law requires that the generators $G_x = L_{x,x+1} - L_{x-1,x} - \psi_x^\dagger \psi_x - [(-1)^x - 1]/2$ fulfill $G_x = 0$ on every lattice site, when working in a so-called superselection sector without background charges. After this initialization the system is then time evolved for different masses and coupling strengths. The particle-antiparticle production in the dynamics is measured via the particle number density

$\nu(t) = L^{-1} \sum_{x=1}^L (-1)^x \langle \psi_x^\dagger(t) \psi_x(t) \rangle$. In Fig. 1 the resulting experimental data is shown for various parameter sets and also compared to the theoretically expected dynamics including different error models.

Localization dynamics

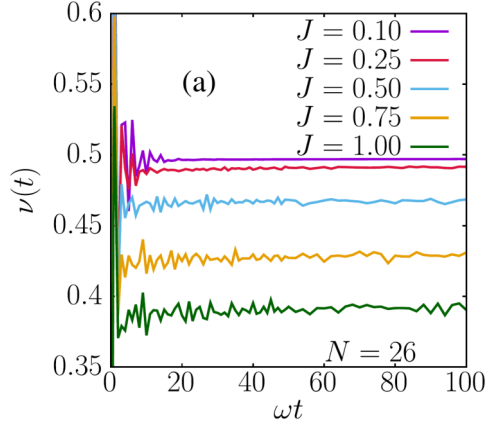


Figure 2: Dynamics of the matter field particle density $\nu(t)$ starting from a bare vacuum state for different values of coupling strength parameter J (measured in units of κ), $m = 0$, and a chain of length $L = 26$ [10].

When allowing for the inclusion of background charges, the dynamics of lattice gauge theories can be profoundly influenced and can lead to nonergodic behavior, although these systems are homogeneous and interacting. While nonergodic dynamics in systems without disorder has already been discussed in the context of disorder-free localization for instance [9], we have shown that the presence of superselection sectors in gauge theories associated with background charges provides a pristine mechanism for nonergodicity [10], whose origin can be conveniently tracked by lattice gauge theories of the form in Eq. (2). Practically, a superselection sector is defined by specifying a sequence

of charges q_x for Gauss' law such that $G_x = q_x \in \mathbb{Z}$ in a $U(1)$ gauge theory, instead of $q_x = 0$ as in the experiment discussed before. States of the form $|\psi\rangle_0 = \frac{1}{N^{1/2}} \sum_{q_x=0,\pm 1} |1010\dots\rangle_\psi \otimes |q_1 q_2 \dots\rangle$ represent a superposition over all superselection sectors involving at most one background charge. Taking such states as initial conditions for the dynamics, evolution can now become nonergodic even though the system is interacting and still homogeneous. For instance, the particle number density $\nu(t)$ of the matter fields does not approach the long-time value as expected for an ergodic system, as is shown in Fig. 2. For the specific case of vanishing rest mass $m = 0$, the only state at long times which is compatible with a thermal equilibrium state is one at infinite temperature. For the particle number density this implies $\nu(t \rightarrow \infty) = 1/2$. While this value is approached for small values of J , for larger J this is not anymore the case, indicating nonergodicity.

Outlook

The study of lattice gauge theories is not only motivated by the experimental advances in quantum simulators but also by fundamental theoretical questions, which have remained largely open until now. For instance, this concerns the influence of confinement onto nonequilibrium quantum real-time evolution. In this context also quantum link models are a particularly interesting class of systems to study since they can host physical phenomena, qualitatively different from Wilson's lattice gauge theory, such as crystalline confined and deconfined phases, existence of soft modes, deconfined Rokhsar-Kivelson points, and the realization of massless chiral fermions. Further, we have recently shown that an inherently nonequilibrium phenomenon can also occur in these quantum link models in that they can undergo dynamical quantum phase transitions in their real-time evolution [11]. All of these aspects make the study of the dynamics in lattice gauge theories a promising scope for future research.

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2.6 Symmetry-protected topological (SPT) phases and their transitions

RUBEN VERRESEN, RODERICH MOESSNER, AND FRANK POLLMANN

Topology is fundamental to characterizing quantum phases of matter in the absence of local order parameters [1]. A class of topological phases that currently receives a lot of attention are *symmetry-protected topological (SPT) phases* [2, 3], which are gapped quantum phases with short-range entanglement and a symmetry group G . The phases are distinct from a trivial phase (i.e., a phase smoothly connected to a simple product state) as long as certain symmetries are preserved. A characteristic feature of these phases are symmetry-protected gapless edge excitations. A celebrated example in one-dimensional systems is the Kitaev chain, which has non-abelian Majorana anyons at its boundaries [5]. Moreover, it is known that coupling stacks of such chains whilst preserving spinless time reversal symmetry produces eight distinct SPT phases [6, 7].

Conventional wisdom says topological edge modes require a bulk gap. Recently, there has been work on gapless phases hosting edge modes, but when their localization is exponential, it is attributed to gapped degrees of freedom (meaning there are exponentially decaying correlation functions) [8]. We indicate that this picture is at odds with the critical points between topological superconductors in the BDI class (noninteracting spinless fermions with time-reversal symmetry) [5]. It is of particular importance given the recent interest in the interplay between topology and criticality, since the bulk has no gapped degrees of freedom. In the following, we discuss how to identify a topological invariant in terms of a complex function that counts the edge modes in critical systems [9].

First we illustrate how a critical phase —without gapped degrees of freedom— can have localized edge modes by considering a concrete example. We decompose every fermionic site c_n, c_n^\dagger into two Majorana modes: $\gamma_n = c_n^\dagger + c_n$ and $\tilde{\gamma}_n = i(c_n^\dagger - c_n)$. The former is real ($T\gamma_n T = \gamma_n$ where T is complex conjugation in the occupation basis) and the latter imaginary ($T\tilde{\gamma}_n T = -\tilde{\gamma}_n$). These Hermitian operators anticommute and square to unity.

We define the α -chain Hamiltonian [10]:

$$H_\alpha = \frac{i}{2} \sum_n \tilde{\gamma}_n \gamma_{n+\alpha} \quad (\alpha \in \mathbb{Z}). \quad (1)$$

These *gapped* chains are illustrated in Fig. 1. For $\alpha = 1$, it is the Kitaev chain with Majorana edge mode γ_1 [5]. H_α has $|\alpha|$ Majorana zero modes per edge and can be thought of as a stack of Kitaev chains. The edge modes survive quadratic, T -preserving perturbations due to chirality: if *real* modes prefer to couple to their *left*, some remain decoupled at the left edge. This can be

quantified by a topological winding number counting edge modes, meaning each H_α represents a distinct phase of matter. The $2|\alpha|$ zero modes imply a $2^{|\alpha|}$ -fold degeneracy, with finite-size gap $\sim e^{-L/\xi}$ when the modes are exponentially localized.

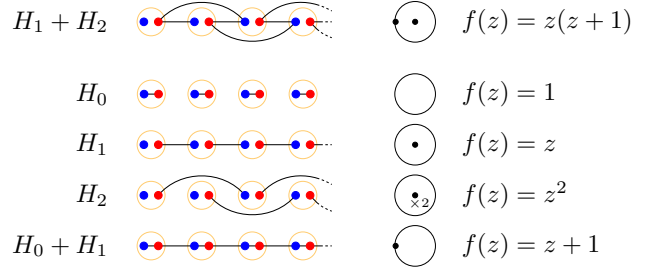


Figure 1: Representation of the critical Hamiltonian $H_1 + H_2$ with its edge mode (each fermionic site is decomposed into Majorana modes: γ (blue) and $\tilde{\gamma}$ (red), a bond signifies a term in the Hamiltonian). Also shown are the gapped Hamiltonians H_α ($\alpha = 0$ is trivial and $\alpha = 1$ is the Kitaev chain). $H_0 + H_1$ is the standard critical Majorana chain [9].

Consider now a critical point between the phases defined by fixed point Hamiltonians H_1 and H_2 , namely $H_1 + H_2$. Despite it being critical, Fig. 1 shows a localized Majorana edge mode. Nevertheless, there is no local operator \mathcal{O} with $\langle \mathcal{O}_n \mathcal{O}_m \rangle \sim e^{-|n-m|/\xi}$. Indeed, for periodic boundary conditions, shifting $\gamma_n \rightarrow \gamma_{n-1}$ (which one *cannot* smoothly implement in a local and T -preserving way) maps $H_1 + H_2$ to $H_0 + H_1$, the well-studied critical Majorana chain described by a CFT with central charge $c = \frac{1}{2}$.

We will now demonstrate that the edge mode is protected by a topological invariant. This invariant is similar to the winding number for gapped phases [5]. In short: we will associate to every chain a complex function $f(z)$ (illustrated in Fig. 2) whose number of zeros (minus poles) in the unit disk counts the edge modes.

We consider the full BDI class: chains of non-interacting spinless fermions with time reversal symmetry T (defined above). The aforementioned $\{H_\alpha\}_{\alpha \in \mathbb{Z}}$ form a basis for arbitrary translation invariant Hamiltonians in this class:

$$H_{\text{BDI}} = \frac{i}{2} \sum_{\alpha=-\infty}^{+\infty} t_\alpha \left(\sum_{n \in \text{sites}} \tilde{\gamma}_n \gamma_{n+\alpha} \right) = \sum_{\alpha} t_\alpha H_\alpha. \quad (2)$$

We take t_α to be non-zero for only a finite number of α (i.e. H is finite range). Time reversal symmetry forbids terms of the form $i\gamma_n \gamma_m$ and Hermiticity requires $t_\alpha \in \mathbb{R}$.

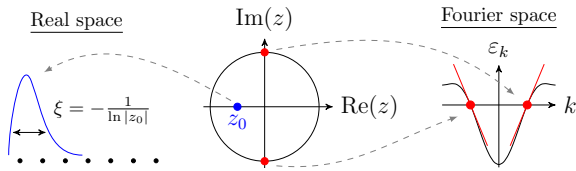


Figure 2: The middle figure shows the zeros of $f(z)$. The zero z_0 within the disk (blue) corresponds to an edge mode (per edge) with localization length $\xi = -\frac{1}{\ln|z_0|}$. Each zero on the unit circle (red) implies a massless Majorana field in the low-energy limit ($c = \frac{1}{2}$) [9].

H_{BDI} is determined by the list of numbers t_α , or equivalently, by its Fourier transform, $f(k) := \sum_\alpha t_\alpha e^{ik\alpha}$. It is efficiently diagonalized: if $f(k) = \varepsilon_k e^{i\varphi_k}$ (with $\varepsilon_k, \varphi_k \in \mathbb{R}$), then a Bogoliubov rotation over the angle φ_k diagonalizes H_{BDI} , with single-particle spectrum ε_k .

Using the above language, the invariant for gapped phases is simply the winding number of $f(k)$ around the origin: since ε_k is nonzero, the phase $e^{i\varphi_k}$ is a well-defined function from S^1 to S^1 . This fails when the system is gapless, but can be repaired using complex analysis. First, interpret the function $f(k)$ as living on the unit circle in the complex plane—abusing notation, write $f(z = e^{ik})$ —with *unique* analytic continuation

$$f(z) = \sum_{\alpha=-\infty}^{\infty} t_\alpha z^\alpha. \quad (3)$$

Now, f is a function $\mathbb{C} \setminus \{0\} \rightarrow \mathbb{C}$ with a pole at the origin when $t_\alpha \neq 0$ for some $\alpha < 0$. If it has no zero on the unit circle (i.e. the system is gapped), then *Cauchy's argument principle* says that the winding number defined above equals the number of zeros (N_z , including degree) minus the order of the pole (N_p) within the unit disk. If at least one zero lies on the unit circle, the aforementioned winding number breaks down—the quantity $N_z - N_p$, however, remains well-defined! Perturbing H_{BDI} smoothly moves the zeros of $f(z)$ around, and changing the support of t_α produces or destroys zero-pole pairs at the origin or infinity. Hence, by continuity, $N_z - N_p$ cannot change without affecting the number of zeros on the unit circle. This would change the bulk physics: every (non-degenerate) zero e^{ik_0} of $f(z)$ implies that $\varepsilon_k \sim k - k_0$, contributing a massless Majorana fermion (with central charge $c = \frac{1}{2}$) to the CFT (see Fig. 1).

Hence $\omega := N_z - N_p$ (strictly within the unit disk) defines a topological invariant, both for gapped and gapless chains. We now show its physical significance: if $\omega > 0$, it counts the Majorana zero modes which are exponentially localized on the boundary. Moreover, the localization lengths are given by the zeros of $f(z)$. Fig. 2 illustrates this, with the precise statement being:

If the topological invariant $\omega > 0$, then

1. each boundary has ω Majorana zero modes,
2. the modes have localization length $\xi_i = -\frac{1}{\ln|z_i|}$ where $\{z_i\}$ are the ω largest zeros of $f(z)$ within the unit disk,
3. the modes on the left (right) are real (imaginary).

If $\omega < -2c$ (where $c = \text{half the number of zeros on the unit circle}$), the left (right) boundary has $|\omega + 2c|$ imaginary (real) Majorana modes with localization length $\xi_i = \frac{1}{\ln|z_i|}$, with $\{z_i\}$ the $|\omega + 2c|$ smallest zeros outside the unit disk. For any other value of ω , no localized edge modes exist [9].

Note that in the gapped case c is zero, with $|\omega|$ correctly counting edge modes. At criticality, $2c$ counts the zeros on the unit circle, and if these are non-degenerate, the bulk is a CFT with central charge c . However, if $f(z)$ has a zero e^{ik_0} with multiplicity m , then $\varepsilon_k \sim (k - k_0)^m$, implying a dynamical critical exponent $z_{\text{dyn}} = m$.

In conclusion, we have shown that topology can protect exponentially localized, zero energy edge modes at critical points between one-dimensional symmetry protected topological phases. This is possible even without gapped degrees of freedom in the bulk, in contrast to recent work on edge modes in gapless chains. We presented an intuitive picture for the existence of these edge modes in the case of non-interacting spinless fermions with time reversal symmetry (BDI class of the tenfold way). The stability of this phenomenon relies on a topological invariant defined in terms of a complex function, counting its zeros and poles inside the unit circle. Moreover, we demonstrated that the topological edge modes of critical chains can be stable in the presence of interactions and disorder [9].

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2.7 Emergent locality in systems with power law interactions

DAVID J. LUITZ AND YEVGENY BAR LEV

Introduction. Recently, the spreading of local operators $\hat{A}_i(t)$ in the Heisenberg picture has attracted significant attention since it is a local probe for the spreading of quantum information in many-body systems. Local operators typically become increasingly nonlocal under the complex quantum many-body dynamics, and the locality can be probed by a commutator with another local operator $[\hat{A}_i(t), \hat{B}_x]$ at a distance $x - i$. Since the commutator itself is an operator, it is useful to consider its norm

$$C_x(t) = \|[\hat{A}_i(t), \hat{B}_x]\|, \quad (1)$$

which is strictly zero if the operator $\hat{A}_i(t)$ contains no terms at the position x in real space of the probing operator \hat{B}_x . For systems with short range interactions, Lieb and Robinson have derived the bound $C_x(t) \leq c \exp \lambda(t - x/v)$ in Ref. [1] with constants c and λ and the Lieb-Robinson velocity v .

There are many physical systems with interactions decaying as a power law in distance $\propto r^{-\alpha}$ for which Lieb-Robinson bounds typically don't hold. Naively one expects superballistic information spreading and it was shown that the causal region becomes at most logarithmic $t \propto \log x$ in Ref. [2]. Subsequently this was improved to the prediction of an algebraic light-“cone” $t \propto r^\xi$ for $\alpha > 2d$ in d dimensions [3]. It is currently an open question how tight these bounds are and how universal information spreading is in long range interacting systems. We have studied information spreading in two generic long range interacting spin chains in Ref. [4]. Using a powerful numerically exact method for calculating $C_x(t)$ that we introduced in Ref. [5], we could reach system sizes twice as large compared to the previous state of the art, allowing us to reach the conclusion that for $\alpha > 1$, the causal region is asymptotically confined within a linear light cone with power law leaking of information outside of the light cone with the same exponent α as given by the interactions. We show that asymptotically,

$$C_x(t) \sim C_x^\infty(t) + A \frac{t}{x^\alpha}, \quad (2)$$

where A is a constant and $C_x^\infty(t) \equiv \lim_{\alpha \rightarrow \infty} C_x(t)$, which constitutes the main result of our work. It implies that up to logarithmic corrections, the “light-cone” is linear for $\alpha > 1$ and scales as $t \sim x^\alpha$ for $\alpha < 1$.

Long range interacting spin chain. We study information spreading in the spin 1/2 XXZ chain

$$\hat{H} = \sum_{i=1, j \neq i}^L \frac{1}{|i-j|^\alpha} \left(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+ + \Delta \hat{S}_i^z \hat{S}_j^z \right) \quad (3)$$

where L is the size of the system and we set the anisotropy parameter $\Delta = 2$ to break the conservation of the total spin. The total z -projection of the spin is still conserved, and throughout this work we work in subsectors with smallest positive magnetization. The model is nonintegrable for all *finite* α , but reduces to integrable models in the $\alpha \rightarrow 0$ and $\alpha \rightarrow \infty$ limits. For $\alpha < 1$, the energy becomes superextensive, invalidating standard thermodynamics.

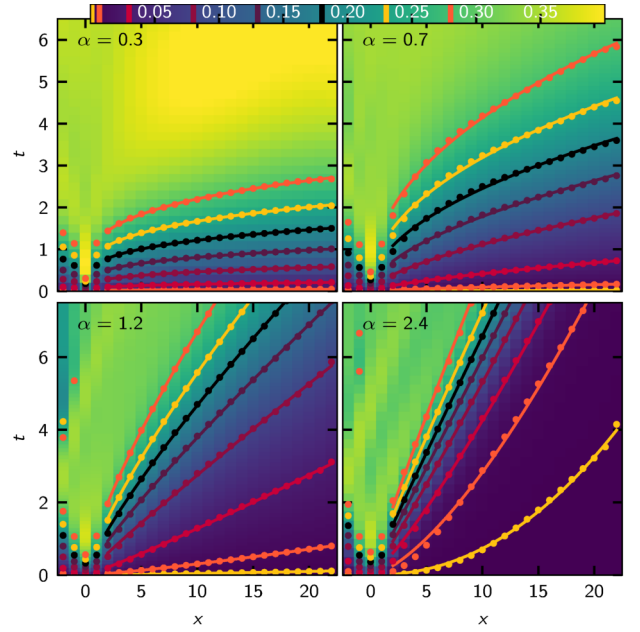


Figure 1: Spreading of the out of time order correlator $C_x(t)$ for various interaction exponents α . The points correspond to discrete contour lines for various thresholds θ indicated in the colorbar, the solid lines are power law fits to these contours. Here, we use open boundaries and $L = 25$.

To calculate $C_x(t)$ in Eq. (1) we use the normalized Frobenius norm, $\|\hat{O}\|_F = \sqrt{\mathcal{N}^{-1} \text{tr}(\hat{O}^\dagger \hat{O})}$, where \mathcal{N} is the Hilbert space dimension. We set $\hat{A}_i(t) = \hat{S}_i^z(t)$ and $\hat{B}_{i+x} = \hat{S}_{i+x}^z$ (other choices yield the same results), for which $C_x(t)$ reduces to,

$$C_x(t) = \sqrt{\frac{1}{8} - \frac{1}{\mathcal{N}} \text{tr}(\hat{S}_i^z(t) \hat{S}_{i+x}^z \hat{S}_i^z(t) \hat{S}_{i+x}^z)}. \quad (4)$$

To maximize the available distances, x , in a system of a finite size, we set $i = 3$, namely a short distance from the left boundary of the system, and restrict our observations to positive x [5].

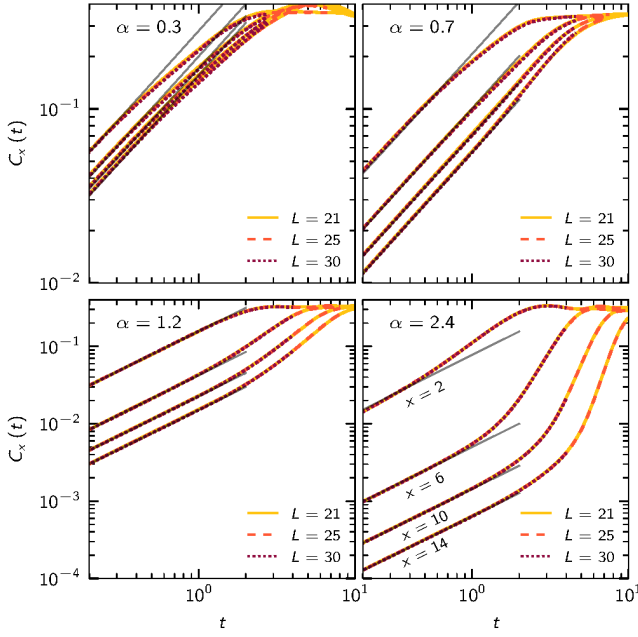


Figure 2: Temporal growth of $C_x(t)$ at distances $x = 2, 6, 10,$ and 14 (lines order from left to right) for different interaction exponents $\alpha = 0.3, 0.7, 1.2$ and 2.4 and system sizes $L = 21, 25$ and 30 (indicated by different line styles). The gray solid lines are linear fits $C_x(t) \sim t$ to the initial temporal growth.

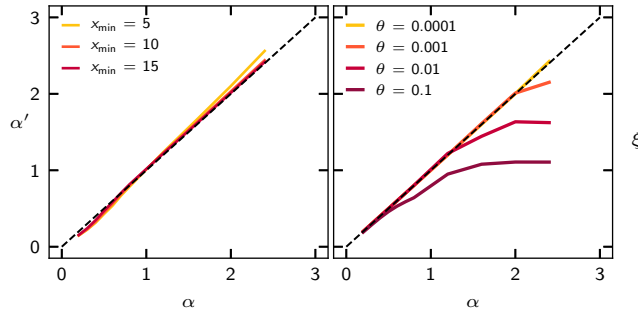


Figure 3: *Left:* Exponent α' of the power law spatial tail of $C_x(t_0)$ versus the interaction exponent α for different fit windows $[x_{\min}, L - i_0]$ and fixed time $t_0 = 1$. *Right:* Exponent ξ of the power law shape of the contour obtained from solving $C_x(t) = \theta$ for different thresholds θ . The dashed lines in both panels corresponds to $\alpha' = \alpha$ and $\xi = \alpha$ respectively. The system size is $L = 30$.

Results. We computed $C_x(t)$ using a massively parallel code based on the method we introduced in Ref. [5] for various ranges of the power-law interaction, $0 < \alpha < 3$, limiting the propagation to times where $C_x(t)$ saturates in the entire system. In Fig. 2 we show the initial temporal growth of $C_x(t)$ at fixed distances x from the spreading operator, which corresponds to vertical cuts in Fig. 1. For all values of α we find that the initial temporal growth is linear in time.

We have also analyzed the long distance spatial tail of $C_x(t)$, which is of the form $C_x(t) \propto 1/x^{\alpha'}$ and we show

the exponent α' in the left panel of Fig. 3 as a function of the interaction exponent α using different fit windows. Our results clearly show that the exponent $\alpha' = \alpha$ for all considered α . In the right panel of Fig. 3, we analyze the exponent ξ of the power law contours $t_\theta(x)$ defined by the solution of $C_x(t) = \theta$ for various θ . We find that for small thresholds θ , corresponding to the tails of $C_x(t)$, the exponent of the contour corresponds to the interaction exponent α , confirming that the asymptotic form of $C_x(t)$ is given by t/x^α .

Conclusion. We have studied information spreading, as embodied by the out-of-time-order correlation function, $C_x(t)$ (1) in a one-dimensional generic spin-chain with power-law decaying interactions, $r^{-\alpha}$. We have shown that for all α , sufficiently far from its saturation value, $C_x(t) \sim t/x^\alpha$, namely it increases linearly in time (see Fig. 2) and has a power-law decaying tail, with an exponent α (see Fig. 3). This behavior corresponds to the leading order in (t/x^α) expansion of the commutator in Eq. (1), indicating that the effect of the long-range part of the Hamiltonian could be understood perturbatively. We have confirmed that similar behavior persists for other models and other local operators taken in (1), as long as they are generic (results shown in the appendix of [4]).

Counterintuitively, the behavior of $C_x(t)$ for $C_x(t) \ll 1$ yields sublinear “light-cones”, $t \sim x^\alpha$, with suppressed causal regions for $\alpha > 1$. This could be already seen from the contour lines which correspond to the lower thresholds in the bottom panels of Fig. 1.

The overall behavior of $C_x(t)$ we obtain is presented in Eq. (2), and constitutes the central result of our work. It shows that for $\alpha > 1$ the effect of the long-range part of the Hamiltonian is rather limited, resulting in a transient behavior where the front which corresponds to the short-range part is “catching up” with the slower long-range part. From Eq. (2) and using the LR bound, one can obtain the asymptotic shape of the “light-cone”, which including the first logarithmic correction is,

$$t \sim \begin{cases} \theta x^\alpha & \alpha < 1 \\ x/v - \lambda^{-1} \log(\lambda x^\alpha) & \alpha > 1 \end{cases}, \quad (5)$$

namely faster than ballistic, for $\alpha < 1$, and almost linear for $\alpha > 1$, with a finite LR velocity.

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2.8 Localization of Rydberg electrons through an environment

PERTTU LUUKKO, MATT EILES, ANDREW HUNTER, ALEXANDER EISFELD AND JAN M ROST

Rydberg atoms ideally interface with an ultracold environment. Their (small) energy scales and large extensions match energies and mean interatomic distances realizable in dilute ultracold gases, giving rise, e.g., to new Rydberg systems such as ultralong range molecules with a large dipole moment consisting of a Rydberg and a ground state atom. Surprisingly, such molecules thrive when increasing the gas density such that thousands of atoms fill the Rydberg orbital volume. Despite the classical non-integrability of the system, the molecular wavefunctions localize on classical Kepler ellipses of the unperturbed Rydberg atom. The hydrogenic electron problem separates in many different coordinate systems due to its high symmetry. This leads to high degeneracy of N^2 states in each Rydberg excitation manifold N with energy $E_N = -(2N)^{-2}$. For that reason hydrogenic wavefunctions for a given energy E_N are a priori not well localized since they can be a superposition of many different eigenstates from the same manifold N . What breaks these degeneracies naturally are residual interactions with the ionic core or perturbations from the environment.

The most “natural” environment is another charged particle. If it is an electron tightly bound to the ion, this effective two-body system forms a new core for the Rydberg electron preserving the atomic character of the entire system, e.g., a Rydberg excited multi-electron atom. An antiproton can adopt the same role, e.g., for antiprotonic helium. However, an electron as well as the antiproton can polarize the Rydberg electron in a molecular type of binding if the distance R of the ion and the negatively charged particle is comparable to the Rydberg orbit, $R \sim N^2$ [1]. In this case a molecular type of binding emerges which breaks the degeneracy of the Rydberg electronic states through the additional negative particle and leads to localization through polarization, see Fig.1. Molecular binding through an additional electron describes doubly excited atomic states, where the two electrons polarize each other and localize on classical orbits [2].

Of course, electron localization differs here from electron localization in condensed matter systems since it refers to the body-fixed system only: A molecule may have angular momentum and tumble about its internuclear axis R in space, averaging out the Rydberg electron localization in the lab fixed frame. Can one suppress the molecular tumbling motion? This is achieved with so called pendular states by applying external fields preventing full rotation [3]. There is a more natural way of transient localization in the sense that the

tumbling motion becomes so slow that it virtually is absent on the (already long) time scales of Rydberg dynamics.

This can be achieved by weakening the forces at work, i.e., by removing charge from the three-body system under discussion: Removing one positive and one negative charge from the antiprotonic helium leaves a (singly charged) ion, a (Rydberg) electron and a neutral atom. Now, the presence of the ground state atom breaks the degeneracy of the Rydberg electron polarizing and thereby localizing it and leading to a very weakly bound long range molecule, a so called trilobite [4]. For typical Rydberg excitations of $N \sim 50$ in an ultracold gas of ^{87}Rb atoms the rotational constant $B = 1/(MR^2) \propto N^{-4}$ of the ensuing molecule is with $B \approx 3\text{ kHz}$ several orders of magnitude smaller than for a conventional polar molecule of similar dipole moment (e.g., KrB with $B \approx 1\text{ GHz}$) [5]. Hence, the Rydberg electron of a trilobite molecule is indeed transiently localized in the lab frame over many Rydberg electron periods of $T_e = N^3 \approx 3\text{ ps}$.

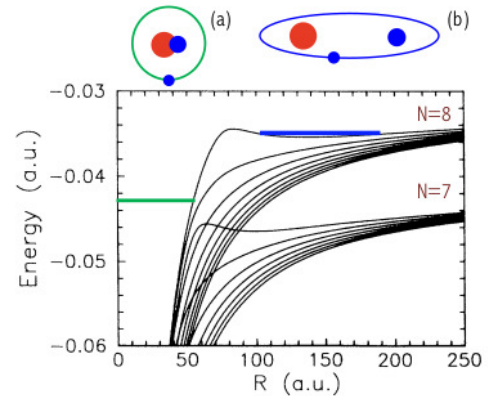


Figure 1: Sketch of the atomic (a, green) and molecular (b, blue) binding mechanism for a doubly charged ion (red) with a Rydberg electron (small blue with green or blue orbit) and an additional negatively charged particle (blue, here an antiproton). The potential energy curves show the electronic energy as a function of distance R between the ion and the antiproton in the Rydberg manifolds $N = 7, 8$. If N is large enough the polarizability of the Rydberg electron through the antiproton is sufficiently large for a shallow minimum to emerge in the top potential curves of each manifold N giving rise to the molecular binding mechanism (b). The respective total energies of the two binding mechanisms are indicated with horizontal lines in green and blue.

Since this electronic Rydberg time scale, although slow compared to ground state electron dynamics, is much faster than any other time scales of the atoms involved, it is reasonable to view for this kind of transient Rydberg electron dynamics all atoms as frozen, i.e., the

ion and the ground state atom(s) at fixed positions in space. Considering the Rydberg atom as immersed in its natural environment, an ultracold gas of ground state atoms, this poses the question how dense the gas may be before the polarization of the Rydberg electron is lost and therefore its localization destroyed. Naively one expects that this happens as soon as several ground state atoms are within reach of the Rydberg electron since the resulting electronic state should be a superposition of trilobite wavefunctions with different (randomly located) ground state atoms. This is indeed the case, as one can see in Fig. 2. However, if the gas density is further increased, the dipole moment of the Rydberg electron increases again indicating that more ground state atoms localize the electron, an effect certainly counterintuitive on a first glance. The corresponding wavefunction is highly structured spatially in all three dimensions which is attributed to two different mechanisms [6]: The possibility to create diatomic trilobites comes from the fact that for a certain density ρ , it is highly likely to find several gas atoms within the volume of the cubed wavelength which is characteristic for the Rydberg wave function. Such clustering of atoms in a random gas is akin to the famous birthday paradoxon stating the surprisingly low number of 23 people in a room it takes to have a probability of more than 50% that two of them have birthday on the same day of the year.

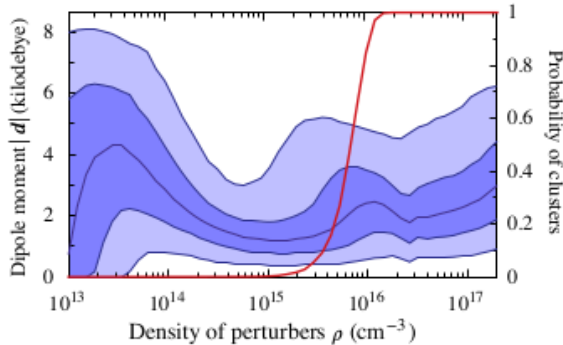


Figure 2: Probability distribution of the dipole moment of the $N = 50$ trilobite state as a function of the atom density ρ . The black line shows the median value and the edges of the two shaded regions denote the 5th, 25th, 75th, and 95th percentiles. The red line shows the probability that a snapshot of a random gas sample contains at least one cluster where three atoms are located within 300 a.u. of each other. The values are estimated from an ensemble of 10^4 snapshots of the atom locations.

In the example of Fig. 3, there is a cluster of three atoms (yellow) which form a “superatom” with triple interaction strength on which the wavefunction localizes like a regular diatomic trilobite. Since the latter has cylindrical symmetry, there is degeneracy in the azimuthal angle ϕ about the molecular axis. This symmetry is broken by the residual interactions with the (single) gas

atoms. They act as perturbers on the otherwise integrable azimuthal motion and the trilobite wavefunction can localize also in ϕ on a periodic orbit of the *unperturbed* system due to perturber induces scarring [7], which is a semiclassical scarring phenomenon, different from the well known scarring about integrable tori or unstable periodic orbits.

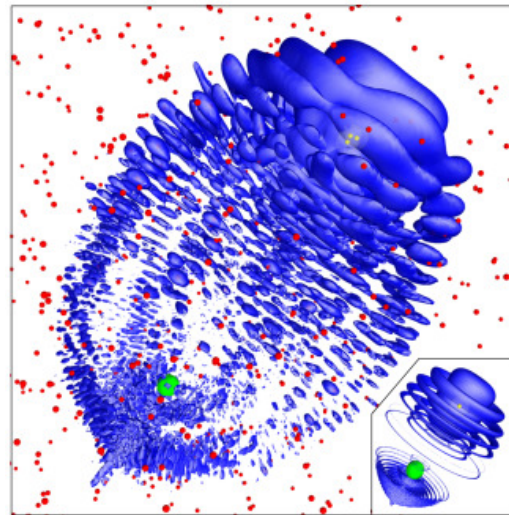


Figure 3: Electron density of the polar trilobite state at an atomic gas density of $\rho = 10^{16} \text{cm}^{-3}$. The electron density is visualized using a contour surface (in blue) that contains 42% of the total probability mass. Small red spheres denote the locations of the perturbing atoms. For visibility, their radius is approximately twice the electron-atom scattering length. The electron density is localized around the highlighted cluster of three atoms (in yellow) and the Rydberg core is shown in green. For comparison, the inset shows an equal visualization of the ordinary trilobite state [4] with $N = 30$ and a single atom at $R = 1232$ which is does not show localization in the azimuthal angle. Adapted from [6], where more details can be found.

In summary, immersed in a structured or random environment a Rydberg excitation with its high local density of states towards the ionization threshold $N \rightarrow \infty$ offers surprisingly rich perspectives for hybrid quantum systems with interesting properties which can be influenced via the environment.

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2.9 Electronic interference with single strong XUV laser pulses

SAJAL GIRI, QICHENG NING, ULF SAALMANN AND JAN M ROST

Short intense VUV light pulses interacting with matter create electron wave packets. Owing to dynamical conditions often several electron bursts with well defined time-delays are produced during a single pulse leading to unexpected interference phenomena. More formally, they can be understood in terms of virtual and real photon exchange with the illuminated target. The former leads to transient Stark shifts in the electronic energies following the time-dependent pulse envelope, while the latter leads to the coexistence and interaction of states dressed with a different number of photons. In the first example we reveal a parameter regime where a single Gaussian laser pulse acts like a double pulse giving rise to two electron ionization bursts. This happens if the electron orbital is weakly bound and therefore suffers considerable dynamic Stark shifts and if the intrinsic time scale of the bound electron state is too slow to follow the change of the pulse envelope. In this case a peak in the photo electron spectrum appears at low energies. Figure 1 demonstrates that the spectrum (black dashed-dotted line) is created from the coherent contributions of two electron bursts with amplitude $A_{\uparrow\downarrow}(E)e^{i\varphi_{\uparrow\downarrow}(E)}$ created at the maximal derivatives of the pulse envelope during its rise ($t = -T/2, A_{\uparrow}$) and fall ($t = T/2, A_{\downarrow}$). The two bursts are separated by the pulse length T . The rising and falling half pulses for themselves would create almost the same spectrum separately (red and blue dashed line in Fig. 1 and black circles for their sum) but the coherent superposition of the full spectrum $P_E = A_{\uparrow}^2 + A_{\downarrow}^2 + 2A_{\uparrow}A_{\downarrow} \cos(\varphi_E)$ has an oscillating part with the phase difference $\varphi_E = \varphi_{\uparrow}(E) - \varphi_{\downarrow}(E)$ approximately given by $\varphi_E \approx -ET + \int_{-T/2}^{+T/2} E_g(t) dt + \pi$, where $E_g(t)$ is the Stark shifted bound state during the pulse. Due to the strong energy dependence of the spectrum P_E , the oscillations akin to Stueckelberg oscillations become only visible, if P_E is normalized to the sum of the ionization probabilities from the two half pulses (inset of Fig. 1), for details see [1]. Hence, in the parameter regime of ionization due to light pulse derivatives, a single laser pulse can act as a pump and probe separated in time by the pulse width. This “zero photon” (low energy) photo ionization is almost completely separated for large enough photon energy from the standard single photo ionization peak in the spectrum, located at $E = E_g(0) + \omega_0$.

The second example involves in addition to dynamic Stark shifts also the absorption of photons. More precisely, we will consider a scenario where two bound states have an energy difference, resonant with the central laser frequency ω_0 of a Gaussian light pulse with

vector potential

$$\mathcal{A}_{\beta}(t) = A_{\beta} g_{\beta}(t) \cos(\phi_{\beta}(t)), \quad (1a)$$

$$g_{\beta}(t) = \exp(-2 \ln 2 t^2 / T_{\beta}^2), \quad (1b)$$

whose frequency drifts linearly in time

$$\omega_{\beta}(t) = \frac{d}{dt} \phi_{\beta}(t) = \omega_0 + \frac{4 \ln 2}{\beta + 1/\beta} \frac{t}{T^2}, \quad (1c)$$

controlled by a dimensionless chirp parameter β . The Fourier-limited pulse ($\beta = 0$) is characterized by carrier frequency ω_0 and length T . Any chirp stretches the pulse in time to $T_{\beta} = [1 + \beta^2]^{1/2} T$ which implies a reduced peak amplitude of $A_{\beta} = [1 + \beta^2]^{-1/4} A_{\max}$, leaving the pulse energy unchanged.

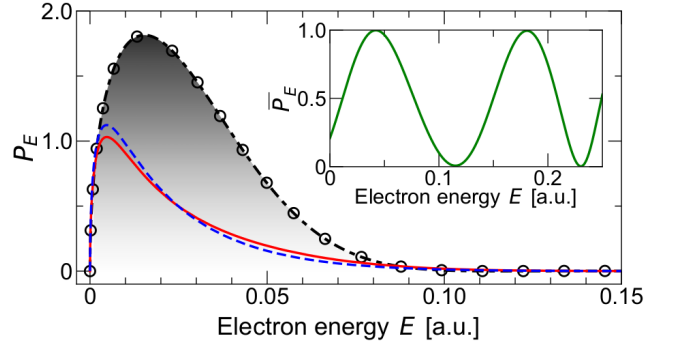


Figure 1: Nonadiabatic electron spectrum for ionization of an electron weakly bound with energy $E_g = -0.0277$ a.u. exposed to a laser pulse of peak amplitude $F = 0.5$ a.u., frequency $\omega_0 = 0.314$ a.u. and a Gaussian pulse envelope of width $T = 51$ a.u. (dashed-dotted) and combined from the sequence of a rising and falling half-pulse with $T/2 = 25.5$ a.u. (open circles) with $T/2$ measured between the maximum of the electric field amplitude $F(t)$ and its maximal derivative. The contribution from the 1st electron burst $A_{\uparrow}^2(E)$ (solid, red) and the 2nd one $A_{\downarrow}^2(E)$ (dashed, blue) are also shown. The inset reveals Stueckelberg oscillations [2] of the normalized spectrum, $\bar{P}_E \equiv P_E / [2A_{\uparrow}^2(E) + 2A_{\downarrow}^2(E)]$.

Solving the Schrödinger equation numerically including the light-matter coupling term $\mathcal{A}_{\beta}(t) \hat{p}$ for a model atom with a single active electron restricted to the two lowest states shows upon driving with a chirped laser almost perfect rapid adiabatic passage (Fig. 2d). The two lowest states have energies of $E_0 = -24.2$ eV and $E_1 = -8.6$ eV, respectively, corresponding to a transition energy of $\Delta = E_1 - E_0 = 15.6$ eV with E_0 close to the binding energy of helium.

With a resonant carrier frequency $\omega_0 = \Delta$ (Fig. 2), the uncoupled dressed states with energies $E_0 + \omega_{\beta}(t)$ and E_1 would cross. The laser coupling, however, pushes them apart (Fig. 2a), and thereby suppresses

(non-adiabatic) transitions. Consequently, only one adiabatic state is occupied for all times. Yet, this enables a transition since the adiabatic state changes its character. The sign of the chirp β does not play any role.

However, without restriction to the two lowest levels E_0, E_1 , reversing the chirp for our single-active electron Helium has a dramatic consequence for ionization [3], which is now possible: while the negative chirp leads to a similar effect as in the pure two-level system, namely a nearly complete exchange of the two bound states apart from small losses to the continuum (Figs. 2b,e), the system almost fully ionizes under positive chirp (Figs. 2c,f).

As for standard adiabatic passage, the chirp locks the

two bound states into a linear combination $|\psi_{\text{ini}}(t)\rangle = \text{sign}(\beta)|0\rangle \exp[iE_0(t)] + |1\rangle \exp[iE_1(t)]$. The standard strong field ionization dynamics [4]

$$|\psi(t)\rangle = -i \int dt' \hat{U}(t, t') \mathcal{A}_\beta(t') \hat{p} |\psi_{\text{ini}}(t')\rangle, \quad (2)$$

can be solved analytically with the (Volkov) propagator $\hat{U}(t, t')$ if we fix the vector potential at maximal field strength A_β and neglect the chirp in the frequency which changes the photon energy maximally by $|\delta\omega/\omega_0| < 0.03$ for our parameters.

At resonance $k^2/2 = E_0 + 2\omega_0 = E_1 + \omega_0$ and in leading order of the electron-photon coupling parameter $\lambda = A_\beta k/\omega_0$ the ionization probability reads $P_{\text{ion}}^{\text{res}} \equiv |\langle k|\psi(t \rightarrow \infty)\rangle|^2 \propto |\text{sign}(\beta) \langle k|0\rangle \lambda^2/2 + \langle k|1\rangle \lambda|^2$.

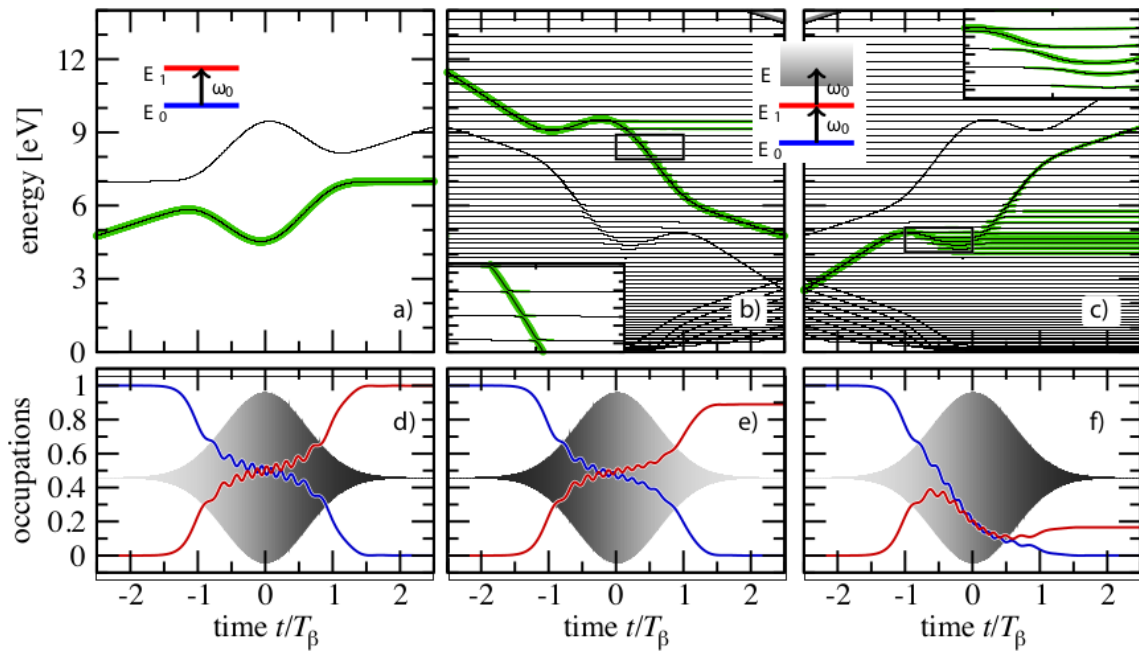


Figure 2: Dressed-state description of adiabatic passage to the continuum. Panels **a, d**: two-level system with positively chirped pulse. Panels **b, e** and **c, f** two levels coupled to a continuum with negative and positive chirp, respectively. Upper row: Time-dependent energy levels (black lines) and corresponding occupations (green lines with the thickness corresponding to the occupation probability). The dense set of lines in **b, c** represents the discretized continuum. Lower row: Occupation probability of the two lowest field-free states. The gray-shaded areas show the envelope (with the brightness gradient illustrating the frequency chirp) of the driving laser pulse.

Obviously, ionization is suppressed for negative chirp $\beta < 0$ if $\langle k|0\rangle \lambda/2 = \langle k|1\rangle$ due to destructive or constructive interference of the lower bound state $|0\rangle$ dressed with two photons ($\propto \lambda^2$) and the higher bound state $|1\rangle$ dressed with one photon ($\propto \lambda$).

In summary, ultrashort timespans are not only of interest in tunneling ionization and streaking scenarios (for our contributions to this topic, see [5, 6]), but also when the dynamics depends in a more subtle way on specific instants in time during the pulse. They can be often defined by stationary phase approximations in time [7] and give rise to interfering electron wavepackets.

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2.10 Reservoir engineering with Rydberg atoms

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Quantum simulators offer an alternative to numerical solutions of open quantum system problems. In many situations it is essential to simulate the thermalization of the target system, which means in particular that the simulator evolves towards a Boltzmann distribution of its eigenstates. We use a highly controllable setup based on Rydberg atoms. The system part consists of resonant dipole-dipole-interacting Rydberg states; the environment is formed by laser-driven atoms with a strong dissipation channel. Appropriate choice of the laser parameters allows us to prepare a Boltzmann distribution of the system's eigenstates. By tuning the laser parameters and system-environment interaction, we can change the temperature associated with this Boltzmann distribution, and also the thermalization dynamics.

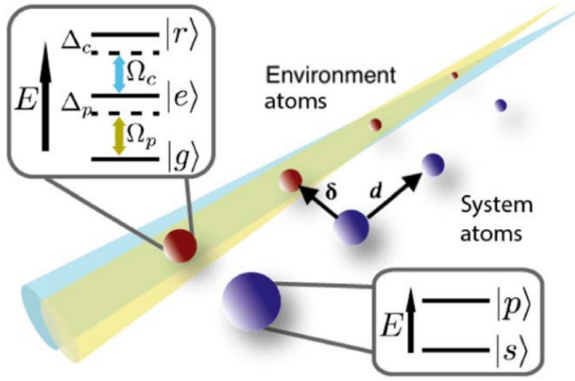


Figure 1: Conceptual sketch of the setup. A “system” of dipole-dipole interacting Rydberg atoms is coupled to a laser-driven atomic “environment”, which is dissipative through its coupling to the electromagnetic continuum. The boxes show the relevant states and laser parameters for system and environment atoms.

The basic setup, introduced in Ref. [1], is sketched in figure 1. Dipole-coupled Rydberg atoms constitute our system of interest. There are many possibilities for the geometry of the system atoms. Here, as concrete examples, we present results for the dimer and longer equidistant linear chains. The system atoms are in two different Rydberg states. We consider one atom prepared in a Rydberg p-state $|p\rangle$ and the other atoms are prepared in a Rydberg s-state $|s\rangle$. Resonant dipole-dipole interactions lead to collective eigenstates. To provide the thermalization of these eigenstates, we use a driven dissipative atomic environment. The effective temperature scale of the Boltzmann distribution of eigenstates is determined by the system interaction strength rather than the ‘ambient’ temperature of the ultracold environment.

Hamiltonian and equations of motion: The system part is given by the Hamiltonian

$$\mathcal{H}_{\text{sys}} = \sum_{n \neq m} W_{nm} |\pi_n\rangle \langle \pi_m|, \quad (1)$$

where a single $|p\rangle$ excitation localized at atom n is written as $|\pi_n\rangle = |s \cdots s p s \cdots s\rangle$. The resonant dipole-dipole interaction $W_{nm} = C_3 / (\mathbf{R}_n - \mathbf{R}_m)^3$, where \mathbf{R}_n is the position of atom n and C_3 is a state-dependent coefficient.

The environment for the Rydberg system is provided by laser-driven atoms, which are placed at a distance δ from a given system-atom. Two laser beams address the environment atoms. The first, with Rabi frequency Ω_p and detuning Δ_p , couples the ground state $|g\rangle$ of an environment atom to an intermediate state $|e\rangle$ which is coupled to a continuum of electromagnetic modes, thereby inducing radiative transitions (spontaneous emission) with decay rate Γ_p to the ground state of the environment atom. The second laser, with Rabi frequency Ω_c and detuning Δ_c , couples the intermediate state $|e\rangle$ to a Rydberg state $|r\rangle \neq |p\rangle, |s\rangle$. The Rydberg states $|r\rangle$ of the environment atoms introduce interactions both between the environment atoms and between the environment atoms and system atoms. The environment atoms interact with each other via van der Waals interaction $V^{(rr)}$. The interactions between environment and system atoms are state-dependent, $\mathcal{H}_{\text{int}} = \sum_{n,\alpha} \bar{V}_{n\alpha} |\pi_n\rangle \langle \pi_n| [|r\rangle \langle r|]_{\alpha}$, where $\bar{V}_{n\alpha} = V_{n\alpha}^{(pr)} + \sum_{m \neq n} V_{m\alpha}^{(sr)}$ denotes the overall interaction of a specific environment atom α with the entire system if the latter is in the state $|\pi_n\rangle$. Here, $V_{n\alpha}^{(pr)}$ ($V_{n\alpha}^{(sr)}$) indicates the interaction between the $|r\rangle$ state of environment atom α with a $|p\rangle$ ($|s\rangle$) excitation at system atom n . The interactions $V_{n\alpha}^{(pr)}$ and $V_{n\alpha}^{(sr)}$ increase drastically with decreasing distance and are therefore strongest for adjacent environment and system atoms.

We emphasize that the tunability of the environment arises through its composition of a finite part, the laser-driven three-level atoms, and an infinite part, the photon bath. By tuning the parameters of the lasers addressing the environment atoms, the dynamics within the finite part can be controlled. This in turn affects the system dynamics.

This system dynamics is governed by the many-body Lindblad master equation for the density matrix, $\dot{\hat{\rho}} = -i[\hat{H}, \hat{\rho}] + \sum_{\alpha} \mathcal{L}_{\hat{L}_{\alpha}}[\hat{\rho}]$. The Hamiltonian consists of three terms: $\hat{H} = \hat{H}_{\text{agg}} + \hat{H}_{\text{EIT}} + \hat{H}_{\text{int}}$, which describe the evolution of the aggregate, the background gas of three-level atoms, and the Rydberg-Rydberg interactions, re-

spectively [1]. The super-operator $\mathcal{L}_{\hat{L}_\alpha}[\hat{\rho}]$ describes the spontaneous decay of the background atom α from level $|e\rangle$, thus $\mathcal{L}_{\hat{\delta}}[\hat{\rho}] = \hat{O}\hat{\rho}\hat{O}^\dagger - (\hat{O}^\dagger\hat{O}\hat{\rho} + \hat{\rho}\hat{O}^\dagger\hat{O})/2$ and the decay operator is $\hat{L}_\alpha = \sqrt{\Gamma_p}\hat{\sigma}_{ge}^{(\alpha)}$, with $\hat{\sigma}_{kk'}^{(\alpha)} = [|k\rangle\langle k'|]_\alpha$ acting on atom α only.

Thermalization: In our setup there are four easily tunable parameters that determine the properties of the environment: the Rabi frequencies Ω_c and Ω_p and the detunings Δ_c and Δ_p . We have found that, depending on the values of these parameters, we can obtain very different dynamics, ranging from Markovian to non-Markovian [2]. To see if it is possible to find parameters that lead to thermalization, we performed many dynamical calculations which solved the master equation of the system, starting from a non-thermal initial state. We characterize the closeness to a thermal state by the trace distance $D(\rho_S(t_f), \rho_{T_{\text{eff}}}^{\text{th}}) = \frac{1}{2}\text{Tr}\{|\rho_S(t_f) - \rho_{T_{\text{eff}}}^{\text{th}}|\}$, which measures the distinguishability of a given state of the system $\rho_S(t_f)$ from the target thermal state $\rho_{T_{\text{eff}}}^{\text{th}}$. The state $\rho_S(t_f)$ is obtained by time-propagation and by tracing out the environment atoms [3].

For the case of a dimer, with dipole-dipole interaction W , such parameter scans are shown in Fig. 2 for a target temperature $T = 1.2W$. As an additional constraint we required that the thermal state is reached within $2\ \mu\text{s}$. One sees that there are indeed large regions in parameter space (yellow) where this is possible [3]. We have seen that for each point (for which thermalization occurs) we obtain a different thermalization *dynamics*.

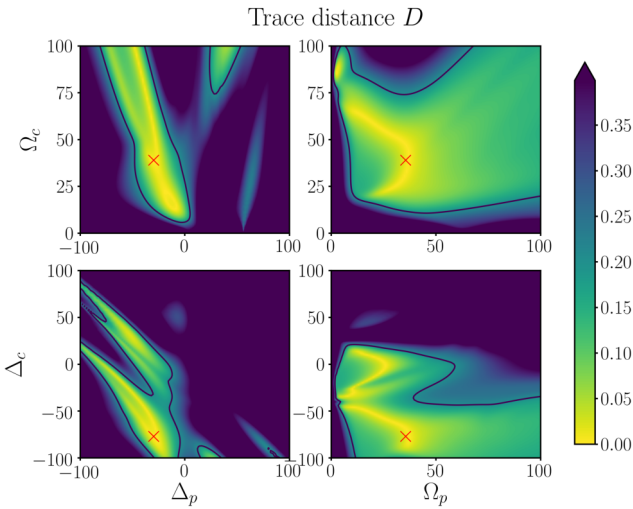


Figure 2: Parameter scan for a Rydberg dimer. The cost D is evaluated after $2\ \mu\text{s}$. The cross marks the common point of the 2D cross-sections: $(\Omega_p, \Omega_c, \Delta_p, \Delta_c) = (37.1, 40.1, -26.6, -74.7)$, which has $D = 6 \times 10^{-5}$. The solid lines mark the contour defined by $D = 0.2$.

For each panel we performed simulations for $100 \times 100 = 10^4$ points. Such a huge number of simulations is only possible for the dimer, not for larger systems.

Therefore we investigated the use of Gaussian process regression to estimate the parameter landscape [4]. Indeed, we found that with only 1000 calculations we can quite accurately reconstruct the relevant regions of the complete four-dimensional parameter-space. We then applied this approach to larger aggregates. An example is shown in Fig. 3 for a tetramer. Also here we can find parameters that lead to thermalization, with different thermalization dynamics.

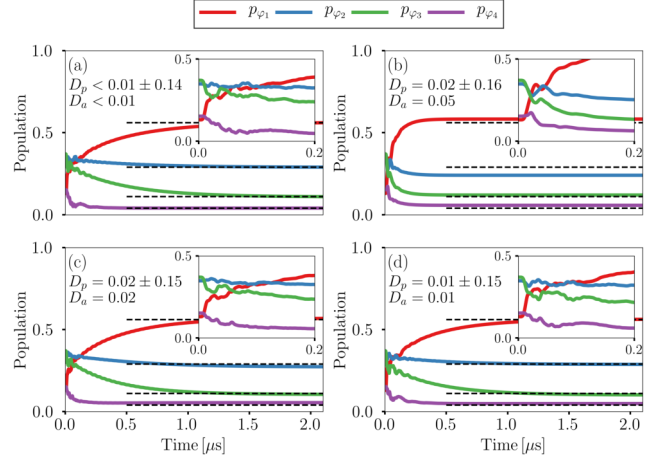


Figure 3: Tetramer eigenstate-population dynamics for different sets of laser parameters (for details see Ref. [4]). Each set of parameters was chosen from predictions of the Gaussian process regression (GPR). The population in the j th lowest energy eigenstate $|\varphi_j\rangle$ is denoted by p_{φ_j} . The target thermal state populations are also shown (dashed lines). D_p is the predicted error of the GPR and the actual error is D_a . The inset is a zoomed-in display of the first $0.2\ \mu\text{s}$ from the respective subplot.

Conclusions: We use reservoir engineering to transform a typically non-thermal environment into a thermal environment with controllable temperature, such that the system relaxes to a corresponding mixture of its eigenstates. Using Gaussian process regression we can find laser parameters that provide thermalization (and even obtain information about the complete parameter landscape), without the need to perform expensive scans of the full parameter space. Our scheme thus provides the essential feature required for simulation of an open quantum system approaching thermal equilibrium. To accurately simulate a particular target open system, further details of the specific dynamics will need to be engineered; our scheme also offers considerable flexibility that could be used to obtain various kinds of system dynamics.

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2.11 Collective optical properties of molecules on surfaces

XING GAO, ALEXANDER EISFELD

When molecules are assembled into an aggregate, their mutual dipole-dipole interaction leads to electronic eigenstates that are coherently delocalized over many molecules. Knowledge about these states is important to understand the optical and transfer properties of the aggregates. We demonstrate that by using electromagnetic fields, that vary over the size of a few molecules one can obtain detailed information about the eigenstates, even those that are inaccessible with traditional far-field techniques.

Our setup is motivated by the increasing number of experiments where aggregates are created on dielectric surfaces. For example, in Ref. [1, 2] far field absorption spectra of two-dimensional aggregates of the organic semiconductor PTCDA on a KCl surface show clear indications of excited state wavefunctions that are coherently delocalized over tens of molecules. For this system the temperature dependence of the superradiance behaves anomalously at low temperatures. This was theoretically traced back to optically dark states at the bottom of the excited state manifold [2]. However, a direct confirmation of this theoretical prediction is missing. As we will show below, near field excitation grants access to this relevant state.

Hamiltonian of the aggregate: For each monomer in the aggregate we take two electronic states into account: the ground state $|g\rangle_n$ and the first excited state

$|e\rangle_n$, where the index n labels the monomers. The transition dipole between these two states is denoted by $\vec{\mu}_n$. Initially, the aggregate, which consists of N molecules (monomers), is in the total ground state $|g_{\text{agg}}\rangle = |g\rangle_1 \cdots |g\rangle_N$. For linear absorption we are interested in states with one excitation. Using as a basis state $|m\rangle = |e\rangle_m \prod_{n \neq m}^N |g\rangle_n$ the excited state Hamiltonian for the system is written as

$$H_{\text{ex}} = \sum_m \varepsilon_m |m\rangle \langle m| + \sum_{m \neq n} V_{mn} |m\rangle \langle n|. \quad (1)$$

Here ε_m is the excitation energy for the monomer m and V_{mn} is the transition dipole-dipole interaction, which to a good approximation can be written as $V_{mn} = \frac{1}{R_{mn}^3} (\vec{\mu}_m \cdot \vec{\mu}_n - 3(\vec{\mu}_m \cdot \frac{\vec{R}_{mn}}{R_{mn}})(\vec{\mu}_n \cdot \frac{\vec{R}_{mn}}{R_{mn}}))$ with \vec{R}_{mn} the distance vector from monomer m to n and $R_{mn} = |\vec{R}_{mn}|$. From the time-independent Schrödinger equation $H_{\text{ex}}|\phi_\ell\rangle = E_\ell|\phi_\ell\rangle$ one obtains the N eigenenergies E_ℓ with corresponding eigenstates

$$|\phi_\ell\rangle = \sum_{m=1}^N c_{m\ell} |m\rangle. \quad (2)$$

The coefficients $c_{m\ell}$ depend on the arrangement of the molecules in the aggregate.

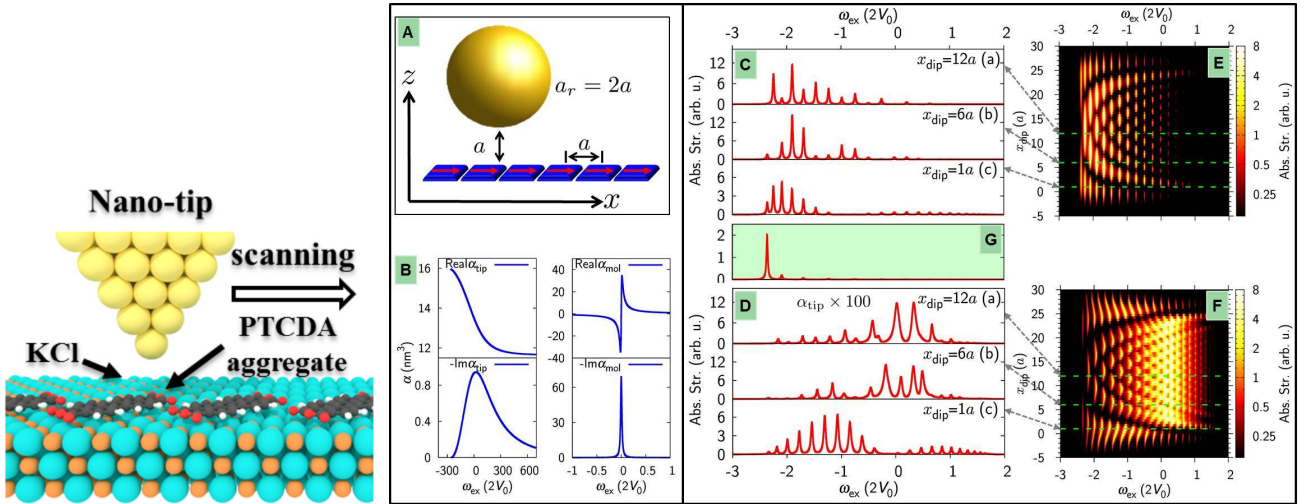


Figure 1: Left: Basic setup: A metallic tip is used to create a localized dipole field which excites the collective eigenstates of an molecular aggregate on a dielectric surface. For each tip position one can record an absorption spectrum. Right: Dependence of the spectra on the tip position for the example of a linear chain of 25 molecules. Panel A shows the arrangement used in our calculations; the tip is modeled by a gold nano-sphere. In panel B the used polarizabilities for the tip (α_{tip}) and the molecules (α_{mol}) are shown. The spectra in the top row (panels D and F) are calculated with these parameters. For the spectra shown in the bottom row (panel D and F) the tip polarizability has been multiplied by a factor 100. Panel G shows the corresponding far field spectrum.

Spectra for spatially varying electromagnetic fields: The space and time dependence of the electric field of a monochromatic light source with frequency ω is given by $\vec{E}(\vec{r}, t) = \text{Re}\{\vec{E}(\vec{r})e^{i\omega t}\}$. Note the explicit dependence of the electric field on the position \vec{r} . In the following we use the term *far-field* spectra, to refer to the situation when the electric field variation is so small over the extent of the aggregate (or more precisely over the extent of the coherent size of the eigenstates of the aggregate) that one can take the field equal for all molecules, i.e. $\vec{E}(\vec{R}_m) = \vec{E}$ for all m .

Absorption spectra for fields that vary over the extent of the aggregate (but have only a small variation over the extent of a single molecule) can be approximately written as $\sigma(\omega) = \sum_{\ell} \mathcal{A}_{\ell} \delta(\omega - E_{\ell})$ with the *absorption strength* for a transition to the state ℓ given by

$$\mathcal{A}_{\ell} = \left| \sum_{m=1}^N c_{m\ell} \vec{\mu}_m \cdot \vec{E}(\vec{R}_m) \right|^2 \quad (3)$$

Here, crucially we have made use of the assumption that there is no overlap between the electronic wavefunctions of the monomers, as is justified for typical molecular aggregates [5].

As a concrete example for an electric field distribution we use the field from a Hertzian dipole. Such a field could, for example, stem from a tapered metallic tip. In recent years it has been shown that such setups can be used for spectroscopy [3]. In Fig. 1 our basic setup is discussed. Here a Hertzian dipole with dipole moment \vec{d} , located at \vec{R}_{dip} creates an electromagnetic field. In the near field zone this field can be written as $\vec{E}(\vec{R}_{\text{dip}} + \vec{r}) = \frac{3\hat{r}(\hat{r} \cdot \vec{d}) - \vec{d}}{r^3}$. Here with \vec{r} we denote the spatial position relative to \vec{R}_{dip} and \hat{r} and r are the corresponding direction and magnitude, respectively. This near-field formula is appropriate for our situation since the wavelength (> 400 nm) is much larger than the distance between tip and aggregate ($r \lesssim 10$ nm). For aggregate molecules that are far away from the tip the electric field strength is quite small, so that deviations from the ideal dipole field do not matter.

Effect of the tip: To include the interaction of the tip with the molecules we use local field theory [5], which relates the induced dipole moment $\vec{P}_m(\omega)$ of particle m to the total field at its position which consists of the external field $\vec{E}_m^{\text{ext}}(\omega) = \vec{E}(\vec{R}_m)$ and the 'internal' fields $\vec{E}_{mn}^{\text{int}}$ produced by all other particles n :

$$\vec{P}_m(\omega) = \overset{\leftrightarrow}{\alpha}_m(\omega) \left(\vec{E}_m^{\text{ext}}(\omega) + \sum_{n \neq m}^N \vec{E}_{mn}^{\text{int}}(\omega) \right) \quad (4)$$

The field contribution $\vec{E}_{mn}^{\text{int}}$ originates from a dipole moment at particle n and is given by $\vec{E}_{mn}^{\text{int}}(\omega) = -\overset{\leftrightarrow}{T}_{mn} \vec{P}_n(\omega)$ in which the transfer tensor $\overset{\leftrightarrow}{T}_{mn}$ between

m and n is $\overset{\leftrightarrow}{T}_{mn} = \frac{1}{R_{mn}^3} \left(\overset{\leftrightarrow}{I} - 3 \frac{\vec{R}_{mn} \otimes \vec{R}_{mn}}{R_{mn}^2} \right)$, which corresponds to the point dipole-dipole interaction for V_{nm} as given below Eq. (1). We use the same form for the interaction between molecules and tip. Solving the coupled system of equations for given external fields one can obtain the induced dipole moments \vec{P}_m of all particles. In our setup the external field stems solely from the nano-tip and thus $\vec{E}_0^{\text{ext}} = 0$, since the index 0 stands for the tip. Finally the linear absorption spectrum is obtained from $\sigma(\omega) = -\text{Im} \sum_{m=0}^N \vec{P}_m(\omega) \cdot \vec{E}_m^{\text{ext}}(\omega)$

Spectra: As an instructive example we consider the case of a linear chain of identical molecules (i.e. ϵ_m and μ_m are the same for all molecules). The molecules are arranged in a line, chosen to be the x-axis, and are equidistantly spaced by a distance a and aligned in parallel. We use a as the unit for distance; thus the monomeric positions are $\vec{R}_m = (ma, 0, 0)$. This situation is also sketched in panel A of Fig. 1. It is well known that for this arrangement only states at the edge of the 'exciton' band absorb in the *far-field* limit, as can be also seen in panel G. To simulate the near field spectra we model the tip as a spherical metal particle as sketched in panel A, with the polarizability given in panel B. One then obtains the spectra shown in panels C and E. It is clearly visible that now also peaks at higher energies contribute to the spectra. In panel E scans along the x direction are shown. We have found for aggregates with length $\lesssim 10$ that one can reconstruct the corresponding coefficients c_{nk} for each eigenstate, by using Gaussian process regression. Finally, to get a feeling for the effect of molecule-tip interaction, in panels D and F we show spectra where the polarizability of the tip is multiplied by 100.

This example shows that one now has access to otherwise optically forbidden states. For the case of two-dimensional aggregates, relevant for the experiments of Ref. [1, 2] we found that one can also identify the dark state at the bottom of the exciton band [5].

Conclusions: We have shown that near fields, stemming from metallic nanotips, reveal information about eigenstates of molecular assemblies that are inaccessible by conventional spectroscopy. For small systems sizes we are already able to reconstruct the full information about the eigenfunctions. For larger systems we plan to use neural networks for this task. It could even be possible to extract parameters of the underlying Hamiltonian of the aggregate in this fashion.

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2.12 Quantum optical networking via polariton exchange interactions

M. KHAZALI, C. R. MURRAY AND T. POHL

Introduction The vanishing optical nonlinearity in vacuum dictates that photons lack mutual interactions. However, the ability to mediate synthetic photon-photon interactions, and thus generate strongly correlated quantum states of light, would open up interesting perspectives for both fundamental and applied quantum optics. Motivated by this, significant efforts are now being devoted to the design of material systems featuring large optical nonlinearities at the few photon level [1]. Coupling light to strongly interacting atomic ensembles under conditions of electromagnetically induced transparency (EIT) provides one approach to achieving uniquely long-ranged effective photon interactions [2]. Here, EIT supports the lossless propagation of single photons in the form of dark-state polaritons, while the atomic interactions can block the formation of nearby polaritons, resulting in nonlinear phenomena at the level of individual light quanta. However, as a direct consequence of this blockade mechanism, the emergent photon interactions are intrinsically dissipative in character, which is detrimental for many perspective applications.

To overcome this obstacle, new concepts are being explored that go beyond initial blockade ideas and allow for coherent effective polariton interactions. This has been achieved through alternative light-matter coupling schemes [3] or the use of excitation-exchange interactions [4]. By mapping photons onto Rydberg polaritons composed of highly excited states and featuring dipolar exchange interactions, one can induce an unusual effective interaction that yields a symmetry protected phase shift of $\pi/2$ during a photon collision.

Here, we extend this process to higher dimensional multi-geometries geometry, as depicted in Fig.1. Surprisingly, we find that the effective photonic exchange reactions are even more effective between spatially separated rails as compared to previously realised one-dimensional geometries. As a first application, we demonstrate how one can exploit this effect in simple 3D networks for realising a symmetry protected π -phase gate with integrated optical feedback and record-breaking gate fidelities.

Dual-rail dynamics We consider two transversally separated channels A and B, formed from tightly focussed free-space optical modes that are incident on separate atomic ensembles, both of which are collectively prepared in the ground state $|g\rangle$. A single photon propagating in channel A is first stored in its respective ensemble as a stationary spin wave excitation in the Rydberg s-state $|s\rangle$. Subsequent to this storage, the resulting spin wave excitation is transferred to the Rydberg

p-state $|c\rangle$ via a microwave π -pulse, which we term the P-polariton. The state $|c\rangle$ is not optically coupled from this point on, such that the P-polariton remains stationary. A second photon in the adjacent optical channel B then propagates through its respective ensemble as a polariton under conditions of EIT with the state $|s\rangle$, which we term the S-polariton. Here, the photon resonantly couples the $|g\rangle - |p\rangle$ transition with a collectively enhanced coupling G , while a second classical field continuously drives the $|p\rangle - |s\rangle$ transition with a constant Rabi frequency Ω . The states $|s\rangle$ and $|c\rangle$ then interact via a dipolar interaction $V(r) = C_3/r^3$ that results in a coherent exchange of the excitations across the separated channels.

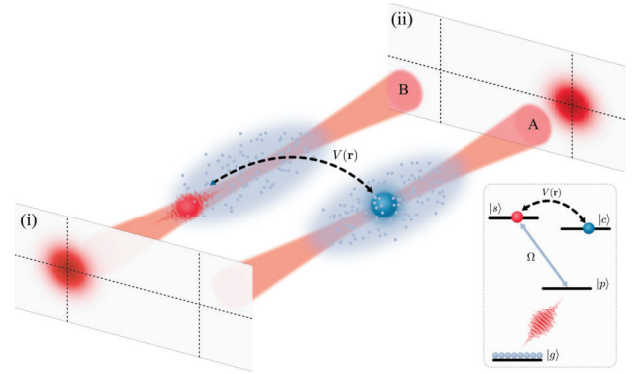


Figure 1: Multi-channel setting in which Rydberg mediated photon exchange is considered. A stored Rydberg spinwave (blue) in channel A interacts with a propagating Rydberg polariton (red) moving in the adjacent channel B via a dipolar exchange interaction. Panels (i) and (ii) show the transverse photonic density before and after interacting with the stored Rydberg spin wave. Each channel overlaps with a separate atomic ensemble, whose constituents possess the internal level structure shown in the inset. The optical coupling of these atoms required to achieve EIT is also shown.

To examine the influence of channel separation L on the exchange dynamics, we define the exchange efficiency η as the probability for the polaritons to swap channels during a collision. We plot η in Fig.1(a) for both vanishing and finite widths of the two optical channels. Remarkably, the exchange efficiency is not maximal for a 1D geometry ($L = 0$), but rather benefits from a finite transversal channel separation between the channels. The emergence of this counter-intuitive behaviour can be understood from the effective equation governing the polariton dynamics. For a 1D geometry, the coupling coefficient describing coherent spin exchange is vanishing for small longitudinal separation z . This simply reflects the conditions of Rydberg blockade, and the fact that photon hopping becomes a far off-resonant process under such conditions. However, a

finite transversal separation L constrains the propagating S-polariton to only experience partial blockade as it interacts with the stored P-polariton. Correspondingly, the hopping coefficient is non-vanishing for small z , and this contribution leads to a larger integrated hopping amplitude relative to the 1D situation.

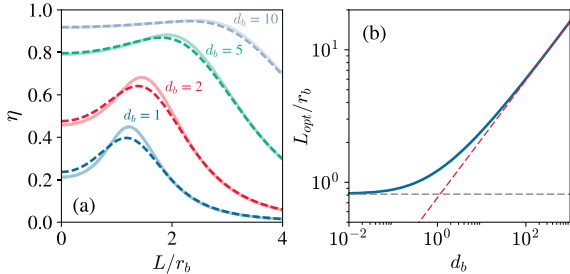


Figure 2: (a) Exchange efficiency as a function of the channel separation L for various indicated blocked optical depths. Solid lines indicate the idealised scenario of zero channel width, while the dashed lines show the behaviour when each channel is described by a Gaussian transverse mode with a beam waist of $0.2z_b$. (b) Optimal channel separation as a function of the blocked optical depth for zero channel width shown in blue. The grey dashed shows the limiting value of L_{opt} for small d_b , while the red dashed line shows the power law scaling of L_{opt} in the limit of large d_b .

To further analyse the optimal geometry, we determine the optimal channel separation L_{opt} by maximising the efficiency with respect to L , which we plot as a function of the blocked optical depth in Fig.2(b). In the low- d_b limit, we find that L_{opt} is roughly set by the blockade radius, consistent with the fact that the propagation dynamics is governed by polariton blockade in this regime. In the large- d_b limit however, we find that the optimal separation obeys a power law scaling $L_{\text{opt}} \propto d_b^\alpha$, with a numerically determined exponent of $\alpha \approx 0.44$ [Fig.2(b) red line]. This scaling is similar to that of the hopping radius, consistent with a crossover to polariton exchange dominated dynamics. Qualitatively, L_{opt} increases with d_b due to the competition between the dissipative and coherent components of the effective polariton interaction. Specifically, while the loss rate and hopping coefficient increase linearly with d_b , their asymptotic scaling at large transversal separations shows that losses can be suppressed relative to the hopping by increasing L .

Multi-rail gate operation When the propagating and stored polaritons exchange spin states during a collision, they acquire a robust phase shift of exactly $\pi/2$ that originates from the symmetries of the underlying effective Hamiltonian [4]. Compared to alternative methods for generating large conditional phase shifts based on the polariton blockade [5], this mechanism is independent of the precise experimental parameters, and is therefore ideally suited for implementing high-fidelity photon-photon phase gate operations. However, most practical applications demand a phase shift

of π . Achieving this with the current setting therefore requires the involved polaritons to interact and exchange spin states exactly twice. In Fig.3, we show a simple photonic network capable of achieving this. Building on the dual-channel setting of Fig.1, the envisioned network naturally employs integrated feedback from the output of channel A into the input of a third channel C, so as to engender a second collision between the involved polaritons.

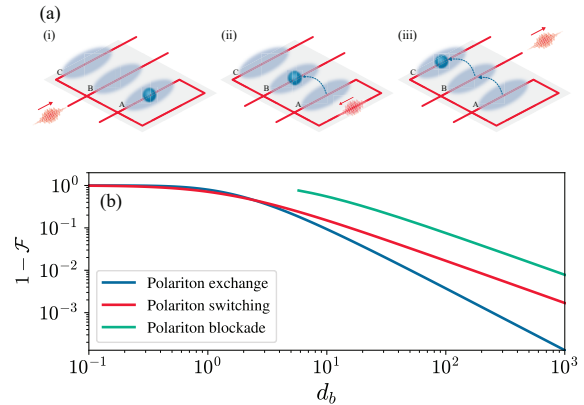


Figure 3: (a) Schematic of the optical network for realising a π -phase gate based on polariton exchange interactions. (i) A stationary polariton is initially prepared in channel A, while a second propagating polariton traverses channel B. (ii) Following a successful exchange interaction, the stationary polariton is left in channel B while the propagating polariton exits channel A and is redirected to the input of channel C with the feedback loop shown. (iii) The propagating polariton entering channel C then interacts for a second time with the stationary polariton remaining in channel B and exits the network as shown. (b) π -phase gate performance for different interaction mechanisms. The blue line shows the gate performance of the optimised network shown in (a). The red line shows the corresponding performance for a gate based on coherent polariton switching [Ref. [3]], while the green line shows the optimal performance for a dispersive π -phase gate based on polariton blockade [5].

Conclusion In conclusion, we have studied the propagation dynamics of interacting Rydberg polaritons in multi-channel optical networks subject to coherent mutual exchange interactions. While we have focussed on the simplest application of the considered setup, the general setting of photons hopping in multiple spatial dimensions could provide a powerful platform for complex quantum optical networks.

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2.13 Universal properties of stochastic entropy production

ÉDGAR ROLDÁN AND FRANK JÜLICHER

Irreversibility and entropy production. Processes that operate away from thermodynamic equilibrium are fundamentally irreversible and are associated with the production of entropy. An important example are biological systems which always operate far from equilibrium. When thermodynamics is applied at mesoscopic scales where energy changes of the order of $k_B T$ become relevant, thermodynamic quantities exhibit fluctuations and can be described by stochastic processes. Here k_B denotes Boltzmann's constant and T temperature. An important example is entropy production, which fluctuates at mesoscopic scales. The second law of thermodynamics demands that entropy production is positive on average. However stochastic entropy production of an individual mesoscopic system can transiently become negative due to fluctuations. This raises the question of what are the statistical properties of the records of entropy production such as infima and suprema of entropy changes. We have recently discovered that the extreme-value statistics of entropy production of irreversible stochastic processes such as the distributions of infima obey universal laws. These results stem from the Martingale property of the exponential of stochastic entropy production.

Stochastic entropy production in mesoscopic systems. We study a nonequilibrium stochastic process of a mesoscopic system, whose dynamics is described by trajectories of coarse-grained state variables $\mathbf{X}(t) = \{\mathbf{q}(\tau), \mathbf{q}^*(\tau)\}_{\tau=0, \dots, t}$. Here the variables $\mathbf{q}(t)$ and $\mathbf{q}^*(t)$ represent the n and n^* degrees of freedom that are even and odd under time reversal, respectively. The stochastic entropy production associated with the trajectory $\mathbf{X}(t)$ is given by

$$S_{\text{tot}}(t) = k_B \ln \frac{\mathcal{P}(\mathbf{X}(t))}{\mathcal{P}(\tilde{\mathbf{X}}(t))} . \quad (1)$$

Here \mathcal{P} denotes the steady-state path probability, and $\tilde{\mathbf{X}}(t) = \{\mathbf{q}(t - \tau), -\mathbf{q}^*(t - \tau)\}_{\tau=0 \dots t}$ denotes the time-reversed trajectory corresponding to $\mathbf{X}(t)$. For a steady state, $\langle S_{\text{tot}}(t) \rangle = \langle v_S \rangle t$, with $\langle v_S \rangle \geq 0$.

Martingale theory for entropy production. We have recently shown that for nonequilibrium steady states, the exponential of the negative stochastic entropy production is a so-called *martingale* process [1]. A martingale is a stochastic process without drift. The martingale property of the stochastic variable $e^{-S_{\text{tot}}(t)/k_B}$ implies that the average

$$\langle e^{-S_{\text{tot}}(t)/k_B} | \mathbf{X}(\tau) \rangle = e^{-S_{\text{tot}}(\tau)/k_B} , \quad (2)$$

for any $t \geq \tau$, where the average is taken over trajectories with common past history $\mathbf{X}(\tau)$. For $\tau = 0$, Eq. (2) implies Jarzynski's equality $\langle e^{-S_{\text{tot}}(t)/k_B} \rangle = 1$, if $S_{\text{tot}}(0) = 0$, see Fig. 1. The martingale property can also be used to obtain generalizations of such expressions and holds for first-passage times and general stopping times of entropy production [1]. A stopping time \mathcal{T} is the stochastic time at which the entropy production first satisfies a certain condition.

Stopping-time and extreme-value statistics. Using martingale theory, we have derived universal relations for the distributions of entropy-production stopping times \mathcal{T} , for which entropy production at the stopping time equals $S_{\text{tot}}(\mathcal{T}) = s$. Analogously, we define conjugate stopping times \mathcal{T}' associated with \mathcal{T} , for which $S_{\text{tot}}(\mathcal{T}') = -s$. Examples of such stopping times are first- and second-passage times with finite mean, and waiting times of stochastic entropy production. We have shown that such stopping times obey generalized fluctuations theorems. The *stopping-time* fluctuation theorem reads [1, 2]

$$\frac{P_{\mathcal{T}}(t; s)}{P_{\mathcal{T}'}(t; -s)} = e^{s/k_B} . \quad (3)$$

Here, $P_{\mathcal{T}}(t; s)$ is the probability density of the stopping time \mathcal{T} , and $P_{\mathcal{T}'}(t; -s)$ is the probability density of the conjugate stopping time \mathcal{T}' , see Fig. 2a. Remarkably, Eq. (3) implies that the stopping-time distributions $P_{\mathcal{T}}(t; s)$ and $P_{\mathcal{T}'}(t; -s)$ have the same shape but can have different amplitudes, i.e.

$$P_{\mathcal{T}}(t|s) = P_{\mathcal{T}'}(t| -s) , \quad (4)$$

where $P_{\mathcal{T}}(t|s) = P_{\mathcal{T}}(t; s) / \int_0^\infty dt' P_{\mathcal{T}}(t'; s)$ and $P_{\mathcal{T}'}(t| -s) = P_{\mathcal{T}'}(t; -s) / \int_0^\infty dt' P_{\mathcal{T}'}(t'; -s)$.

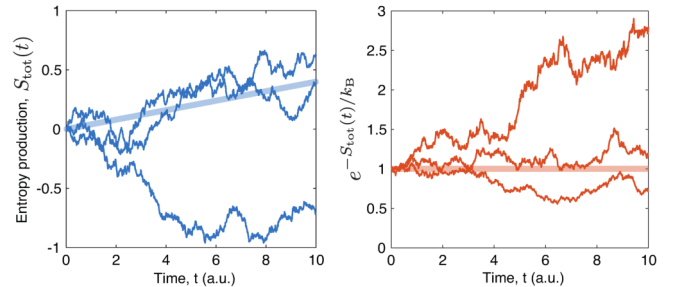


Figure 1: Sample traces of stochastic entropy production $S_{\text{tot}}(t)$ (left, thin lines) and exponentiated negative entropy production $e^{-S_{\text{tot}}(t)/k_B}$ (right, thin lines) as a function of time t . For a non-equilibrium steady state, the average entropy production $\langle S_{\text{tot}}(t) \rangle \geq 0$ (left, thick line) increases with time whereas the martingale $e^{-S_{\text{tot}}(t)/k_B}$ obeys $\langle e^{-S_{\text{tot}}(t)/k_B} \rangle = 1$ (right, thick line).

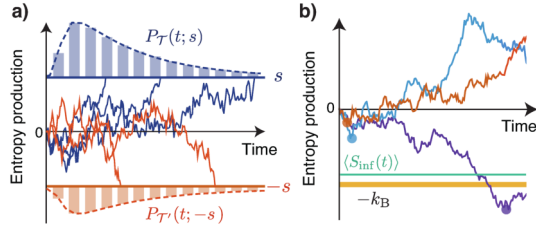


Figure 2: Illustration of the stopping-time fluctuation theorem (a) and the infimum law (b). (a) Traces of stochastic entropy production that first cross a positive (negative) absorbing boundary located at s ($-s$) before reaching another boundary located at $-s$ (s) are shown in blue (red). The first-passage-time distributions ($P_{\mathcal{T}}(t; s)$, blue bars; $P_{\mathcal{T}'}(t; -s)$, red bars) have the same shape [see Eqs. (3) and (4)]. (b) Traces of stochastic entropy production and their corresponding infima (circles). The average finite-time infima (green line) is always greater or equal than $-k_B$ (yellow line), see Eq. (6).

In addition to stopping-time statistics, it is important to understand the extreme-value statistics of entropy production, and in particular how much can $S_{\text{tot}}(t)$ be reduced against the average tendency to increase entropy. We have investigated the statistics of finite-time infima $S_{\text{inf}}(t) \equiv \inf_{0 \leq t' \leq t} S_{\text{tot}}(t')$ of entropy production. We showed, using of the martingale property of $e^{-S_{\text{tot}}(t)/k_B}$, that the statistics of infima of entropy production obey universal laws. The cumulative distribution of the finite-time infima of entropy production obeys

$$\text{Pr}(S_{\text{inf}}(t) \leq -s) \leq e^{-s/k_B} . \quad (5)$$

This result implies a fundamental lower bound for the average infimum of stochastic entropy production:

$$\langle S_{\text{inf}}(t) \rangle \geq -k_B . \quad (6)$$

This infimum law (6) and the inequality (5) hold for any nonequilibrium steady state, including both discrete and continuous stochastic processes [1], see Fig. 2b.

Universal entropy fluctuations of Langevin systems.

An important example of nonequilibrium steady states are mesoscopic systems described n slow degrees of freedom $\vec{X} = (X_1(t), X_2(t), \dots, X_n(t))^T$ in contact with a thermal bath at temperature T . The fluctuating dynamics of such systems can be described by the Ito Langevin equation

$$\frac{d\vec{X}}{dt} = \mu \cdot \vec{F} + \vec{\nabla} \cdot \mathbf{D} + \sqrt{2\mathbf{D}} \cdot \vec{\xi} . \quad (7)$$

Here $\mu = \mu(\vec{X}(t))$ and $\mathbf{D} = \mathbf{D}(\vec{X}(t))$ are state-dependent mobility and diffusion tensors, which obey the Einstein relation $\mathbf{D} = k_B T \mu$, and $\vec{F} = -\vec{\nabla} U(\vec{X}(t)) +$

$\vec{f}(\vec{X}(t))$ is the force at time t , with U is a potential and \vec{f} is a non-conservative force. The term $\vec{\xi}(t)$ is a n -dimensional Gaussian white noise with covariance matrix equal to the identity matrix. For the systems described by (7) in nonequilibrium stationary conditions, the entropy production rate obeys the following Itô stochastic equation [3]

$$\frac{dS_{\text{tot}}}{dt} = v_S + \sqrt{2k_B v_S} \cdot \xi_S . \quad (8)$$

The evolution of $S_{\text{tot}}(t)$ given by (8) is driven by the dynamics of $\vec{X}(t)$ described by (7) via the entropic drift

$$v_S = k_B \frac{\vec{J} \cdot \mathbf{D}^{-1} \cdot \vec{J}}{P^2} . \quad (9)$$

Here $P = P(\vec{X}(t))$ is the probability distribution to find the system in a configuration $\vec{X}(t)$ at time t , which obeys the Smoluchowski equation $\partial_t P = -\vec{\nabla} \cdot \vec{J}$ with $\vec{J} = \mu \cdot \vec{F} P - \mathbf{D} \cdot \vec{\nabla} P$ the instantaneous probability current. Entropy fluctuations are governed by the one-dimensional Gaussian white noise $\xi_S = \vec{\xi} \cdot \mathbf{D}^{-1/2} \cdot \vec{J} / \sqrt{\vec{J} \cdot \mathbf{D}^{-1} \cdot \vec{J}}$ that obeys $\langle \xi_S(t) \rangle = 0$ and $\langle \xi_S(t) \xi_S(t') \rangle = \delta(t - t')$. Equation (8) can be simplified by introducing the dimensionless entropic time [3]

$$\tau = \frac{1}{k_B} \int_0^t v_S(\vec{X}(t')) dt' . \quad (10)$$

Performing the random-time transformation $t \rightarrow \tau$ in Eq. (8) we obtained a Langevin equation for steady state entropy production at entropic times

$$\frac{1}{k_B} \frac{dS_{\text{tot}}}{d\tau} = 1 + \sqrt{2} \eta(\tau) , \quad (11)$$

where $\eta(\tau)$ is Gaussian white noise with $\langle \eta(\tau) \rangle = 0$ and $\langle \eta(\tau) \eta(\tau') \rangle = \delta(\tau - \tau')$. Equation (11) implies that all properties of S_{tot} that are invariant under the transformation $t \rightarrow \tau$ are generic. Moreover, the distribution of such generic properties can be found from the statistics of a drift-diffusion process with constant drift k_B and diffusion coefficient k_B^2 . Our work demonstrates that martingale theory provides a unifying framework to describe the statistics of extrema, stopping-time and other universal properties of stochastic entropy production in non-equilibrium steady states. Our theory will provide novel insights in the fluctuations of entropy production in mesoscopic devices and active systems.

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2.14 Spontaneous division of active droplets

RABEA SEYBOLDT, CHRISTOPH A. WEBER AND FRANK JÜLICHER

Liquid droplets can spatially organize chemical reactions. Phase separated droplets create a chemically distinct environment due to the composition difference with their surrounding. This difference implies that droplets can concentrate reactants for chemical reactions thereby affecting the kinetic parameter such as mobilities or reaction rates. Thus intracellular droplets provide microreactors for biochemical reactions. We have shown that chemical reactions between the droplet components driven by an external fuel reservoir may give rise to novel phenomena that are not present in classical phase separated systems. For example, such active droplets can control their nucleation and size [3], position colloidal particles inside droplets [4], and droplets can spontaneously divide [1,2]. The physics of active droplets can be studied using irreversible nonequilibrium thermodynamics of phase separating systems.

Dynamics of chemically active droplets. The local concentration c of droplet material D obeys

$$\partial_t c + \nabla \cdot (cv) = -\nabla \cdot j + s(c), \quad (1)$$

where $\nabla \cdot (cv)$ accounts for advection with the fluid-flow v , j is the diffusive flux and $s(c)$ denotes a source term due to chemical reactions [1,2]. The Ginzburg-Landau free energy

$$F = \int d^3r \left[-\frac{a}{2}c^2 + \frac{b}{4}c^4 + \frac{\kappa}{2}(\nabla c)^2 \right], \quad (2)$$

describes interactions between droplet material D and solvent S and leads to phase separation in two coexisting phases with concentrations $c \approx c_+^{(0)}$ and $c \approx c_-^{(0)}$. We denote the droplet phase with $-$, and the bulk phase with $+$. The gradient term is related to the surface tension of the droplet. Using linear response theory, the diffusive flux is given by $j = m\nabla\delta F/\delta c$. In a

minimal model, the chemical reaction $S \rightleftharpoons D$ leads to a chemical reaction flux $s(c)$ which describes the production and degradation of droplet material. We consider the case where the chemical reactions are driven and maintained away from equilibrium by an external energy source. The concentration c_∞ far from the droplet is set by the chemical reaction with $s(c_\infty) = 0$ defining the supersaturation $\epsilon = (c_\infty - c_+^{(0)})/\Delta c$, where $\Delta c = c_-^{(0)} - c_+^{(0)}$.

Droplet shape changes can couple to hydrodynamic flows. In the Stokes limit where inertial effects are neglected, force balance equation reads, $0 = \partial_\beta(\sigma_{\alpha\beta}^{\text{eq}} + \sigma_{\alpha\beta}^{\text{d}})$. Here, $\sigma_{\alpha\beta}^{\text{eq}}$ and $\sigma_{\alpha\beta}^{\text{d}}$ denote the equilibrium and dissipative stress tensors, respectively. The force balance together with the incompressibility condition, $\partial_\alpha v_\alpha = 0$, determine the flow field v and pressure P for a given concentration field. We can describe the influence of hydrodynamic flows in the system by a (dimensionless) viscosity $\eta w/(\gamma\tau)$, where η is the viscosity, γ is the surface tension of the droplet, and w and τ are a characteristic length and time scales.

Chemical reactions drive droplet division. Fig. 1 shows an example of spontaneous droplet division obtained as numerical solutions of the dynamic equations. In the presence of chemical reactions droplets can reach a spherical shape of stationary size that is set by the balance of the fluxes created by the reactions inside and outside the droplet [3]. Furthermore, we find that droplets can undergo a shape instability by which they spontaneously elongate and subsequently divide into two daughter droplets Fig. 1. Droplets may undergo several cycle of growth and divisions [1,2].

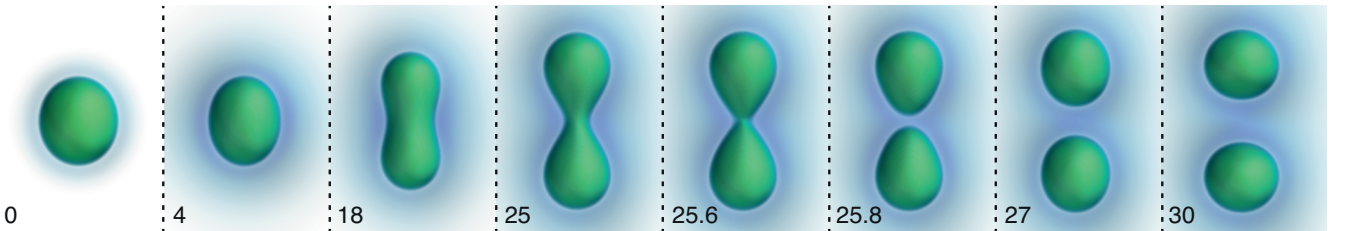


Figure 1: Sequence of shapes of a dividing droplet at different times as indicated. The droplet (green) and the surrounding concentration field (blue-white) are shown. The color code for the concentration is given in Fig. 2A.

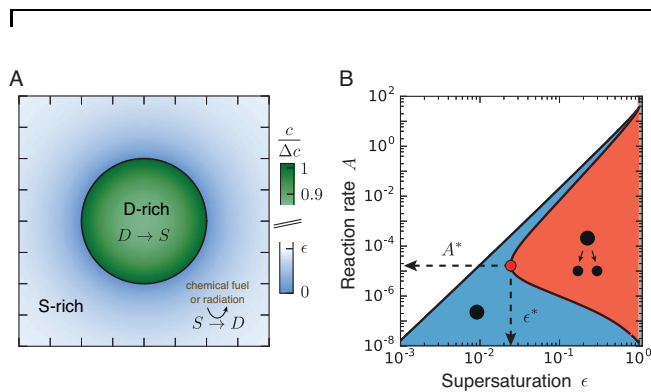


Figure 2: A: Concentration field of a chemically active droplet at stationary size, described by an effective droplet model. Chemical reactions $B \rightarrow A$ create a sink of droplet material B in the droplet, and reactions $A \rightarrow B$ create a supersaturation ϵ of droplet material in the A-rich phase outside. B: Stability diagram of stationary droplets as a function of reaction amplitude A and supersaturation ϵ for dimensionless viscosity $w\eta/(\gamma\tau) = 1000$. The stationary solution can be stable (blue) or unstable (red) with respect to shape perturbations of the $l = 2$ mode. For small supersaturation and large reaction amplitudes, no stationary radius exists (white).

Shape instability of chemically active droplets. We investigate the stationary state and its stability using an effective droplet model valid in the limit of a sharp interface. This model is suited to calculate the droplet shape as a function of time. An example of a stationary spherical droplet is given in Fig. 2A. Concentration gradients create stationary diffusive fluxes of droplet material that balance the changes in concentration due to the chemical reactions in both phases. These stationary diffusive fluxes can trigger a droplet shape instability: A deformation of the droplet pushes the interface into the concentration gradient, so that the gradient increases and more material flows towards the interface, increasing the deformation. The surface tension of the droplet counteracts this deformation by perturbing diffusive fluxes and generating hydrodynamic flows. The resulting dynamical behavior may be explored with a linear stability analysis of a shape deformation of the droplet and the corresponding concentration field. A stability diagram in Fig. 2B shows the different dynamical regimes as a function of the supersaturation ϵ and the reaction amplitude $A = s(c_-^{(0)})\tau/\Delta c$. For large reaction amplitudes, no stationary droplets exist (white region). For smaller reaction amplitudes

and sufficiently large supersaturation, the droplet can be stationary (blue region). For intermediate reaction amplitudes and large supersaturation, the droplets undergo a shape instability and can divide. For small reaction amplitudes, the stationary fluxes become small, and hydrodynamic flows can prevent the instability and stabilize the spherical shape of the droplet. Thus for increasing reaction rate amplitude the instability shows reentrance behavior. The instability is thus most prominent for an intermediate value A^* of the reaction amplitude and the supersaturation ϵ^* , which are strongly influenced by the viscosity and the surface tension of the droplet. For colloidal or biological systems of droplets with a small surface tension, realistic reaction rates could allow micron-sized active droplet to divide spontaneously.

Chemically active droplets as a model for protocells.

These droplets may provide a simple model for protocells at the origin of life [1]. Living systems today consist of cells that grow and divide. Cells take up material that is metabolized by dissipative chemical reactions to achieve growth which leads to the release of waste products. Furthermore, cells are able to divide, thereby creating more cells. Our simple model of chemically active droplets incorporates many of these fundamental properties and thereby represents a primitive protocell. The droplet material D corresponds to the nutrients taken up by a protocell. The solvent S represents the surrounding multi-component fluid which coexists with the protocell. Components of the surrounding fluid are converted under energy input into nutrients D during growth, while metabolic processes produce waste components by converting D to S. The energy required could for example be supplied by chemical fuels or radiation. Our work has shown that chemically active droplets can undergo cycles of growth and division reminiscent of living cells. Living cells possess information carrying molecules such as DNA that are copied imperfectly which provides variability for evolutionary processes. Such information carriers are lacking in our model but are fundamentally required for the evolution and the formation of complex cells and organisms. However, our simple model shows that life-like behaviors can emerge from simple physical mechanisms that provide a starting point for the formation and the evolution of cellular structures.

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2.15 Micro-phase separation in the three-dimensional organization inside cell nuclei

LENNART HILBERT, FRANK JÜLICHER, VASILY ZABURDAEV

Three-dimensional organization of DNA in the cell nucleus. The cell nucleus contains the genome, which is the genetic information required to establish cell type and function. In different cell types and in different functional situations, different parts of the genome are being selectively accessed and transcribed into messenger RNA, which in turn is translated into proteins that establish cell function. In this sense, the cell nucleus can be seen as the central, DNA-based information storage system of the cell.

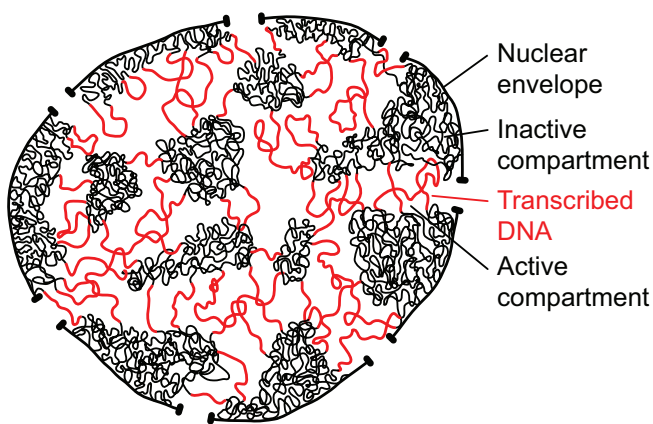
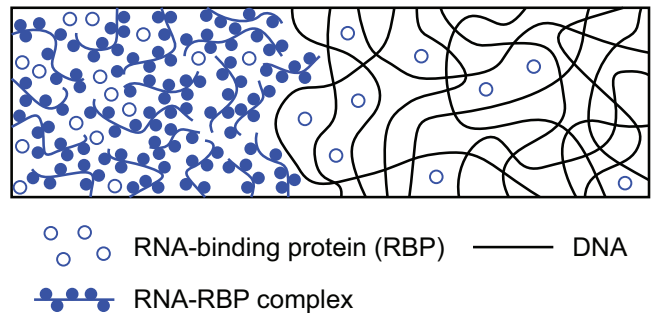


Figure 1: **Segregation of DNA into the active and inactive nuclear compartments.** Transcribed DNA is unfolded and localizes to the active nuclear compartment. Not transcribed DNA is compacted and localizes to the inactive nuclear compartment.

Across a wide range of different organisms and cell types, a consistent three-dimensional organization of DNA in the cell nucleus can be seen, which dynamically adjusts to the selective transcriptional access to the genome (see Figure 1). Specifically, the nucleus is subdivided into an active and an inactive compartment. The greater part of the genome is not accessed, relatively compact, and localized within the inactive compartment of the nucleus. The parts of the genome that are accessed for transcription are three-dimensionally unfolded and localized to the active compartment. This three-dimensional organization pattern dynamically adjusts, meaning that changes in which genes are transcribed are dynamically reflected in changes in this organization to fit the new gene expression patterns. Despite the wide conservation of this organization, it is still unclear how this general pattern is established by transcription, and how it might contribute to regulation and function in the biological cell.

1) Segregation of RNA-RBP complexes from DNA



2) Retention of transcribed DNA among RNA-RBP complexes

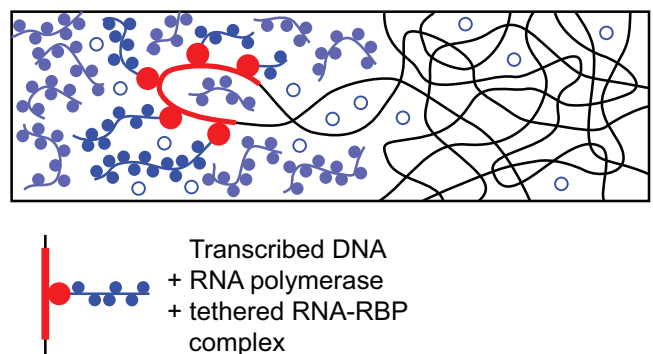


Figure 2: **Suggested macromolecular mechanisms of spatial organization of DNA by transcription.** (1) RNA-binding proteins segregate from DNA upon the binding of RNA transcripts. (2) RNA transcripts are tethered to the transcribed DNA, resulting in co-segregation with the RNA-protein phase.

Active micro emulsion theory of DNA organization by transcription. In collaboration with Vastenhout lab (MPI-CBG), we found that two key macromolecular mechanisms can describe the spatial organization of DNA by transcription (see Figure 2). The first macromolecular mechanism that we propose is a segregation between DNA and RNA-protein complexes. As long as the RNA-binding proteins, which are numerous present in the cell nucleus, are not bound by RNA, they are free to intermix with DNA. Upon the addition of RNA transcripts by the process of transcription, RNA-protein complexes form and segregate from DNA into a separate liquid phase. The second macromolecular mechanism that we propose follows quite directly from the first one. The completion of a transcript from the transcribed DNA sequence takes several minutes. During this time, the RNA transcript is physically tethered to the DNA template and recruits RNA-binding proteins. In consequence, the DNA-RNA-protein complex formed during transcription co-segregates with the RNA-protein phase.

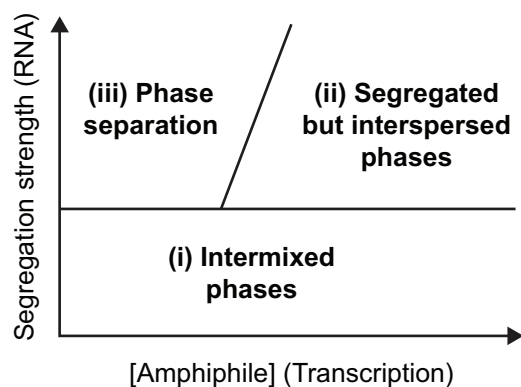


Figure 3: **Micro emulsion phase diagram for different levels of RNA and transcriptional activity in the cell nucleus.** Transcriptional activity is proportional to the amount of amphiphiles in the system; increasing RNA levels in the nucleus lead to higher segregation strength of the RNA-binding proteins. Main regions of spatial organization are indicated with (i) to (iii).

The above macromolecular mechanisms suggest a strong analogy between DNA organization by transcription and the organization that emerges in conventional micro emulsions. Conventional micro emulsions consist of two liquid phases that spontaneously separate from each other, for example hydrophilic and a hydrophobic liquids. In micro emulsions, however, an additional amphiphile with valencies for both phases stabilizes an interspersed pattern that forms between both the phases [2]. In the case of DNA organization in the cell nucleus, DNA and RNA-protein complexes take the role of the two segregating phases. Amphiphiles are formed during the transcription process, where RNA transcripts are tethered to the accessed region of DNA for several minutes (see Figure 3).

To explore the active micro emulsion concept, we implemented a simulation model as well as super-resolution microscopy imaging of DNA, RNA, and transcriptional activity in pluripotent zebrafish embryo cells. We could, in simulation as well as experiments, obtain matching organizational patterns in different regions of the micro emulsion phase diagram (see Figure

4). Together with live cell microscopy data and simulations on the dynamics of the establishment of DNA organization with transcriptional onset, these results are fully in line with the active micro emulsion model.

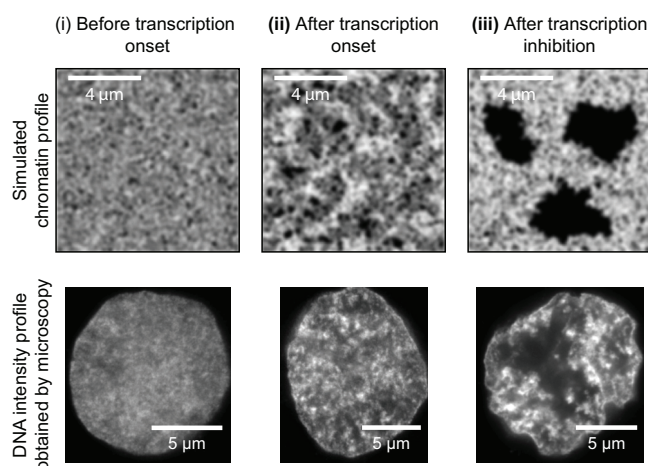


Figure 4: **DNA organization in different regions of the active micro emulsion phase diagram.** Simulated chromatin density profiles and STED super-resolution microscopy sections through pluripotent zebrafish embryo cells both show DNA organization in agreement with an active micro emulsion model of DNA organization by transcription.

Recent research, including our work described above, has provided a set of generally applicable physical mechanisms that drive the three-dimensional organization of DNA in the cell nucleus. It still remains unclear how the resulting organization can contribute to function and regulation of the biological cell. Also, our investigation points out that the combination of phase separation with active catalytic processes can result in unexpected spatial patterns that cannot occur in classical systems. We are continuing our work along both axes, exploring the regulatory relevance and physical implications of the active micro emulsion model of DNA organization by transcription.

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2.16 Modeling lifespan of *C. elegans* dauer larvae

XINGYU ZHANG, VASILY ZABURDAEV

Dauer larvae of *Caenorhabditis elegans* worms may consume ethanol. Dauer larva represent a special developmental stage of *C. elegans* worm that can resist multiple environmental stresses such as drought, high or low temperatures, and lack of nutrients. It was believed that dauers are almost completely isolated from the surrounding environment and entirely depend on their internal energy sources to support the minimum of physiological activity that is required to keep them alive for approximately 4 weeks [1,2].

However, recent findings of Kurzchalia lab (MPI-CBG) suggest that dauers can take up and utilize ethanol provided to the surrounding liquid medium as an external carbon source. In their experiments, the traces of radioactively labeled ethanol were detected in trehalose, amino acids and lipids, suggesting that ethanol has been fully incorporated into the metabolism of worm and can be used as an external energy source. In agreement with this observation, the lifespan of dauers in media containing ethanol is extended in a concentration dependent manner. The lifespan increases when small amounts of ethanol are supplied, but starts to decrease when the ethanol concentration becomes too high. At the optimal concentration of ethanol (~ 1 mM) the lifespan of dauers is approximately twice longer than that of the dauers without ethanol. Moreover, ethanol, by helping to accumulate more trehalose, also enhances the survival of dauers during desiccation. However, if the ethanol provides a practically unlimited source of energy, why larvae still die? Inevitably, in all conditions, the death of the dauer is preceded by the deterioration of mitochondria, but no other details hint at the mechanism regulating its lifespan.

Mathematical model for metabolism of dauers. To identify the mechanism of how the lifespan of *C. elegans* dauer is regulated and altered by the supplied ethanol, we developed a theoretical model based on the known metabolic pathway of dauers. This model takes the supplied ethanol concentration as an input and the lifespan of dauer is its output. As a result, different assumptions and models that link metabolism of dauer to its lifespan can be investigated.

The model can be formalized as a system of differential equations describing the chemical reaction network illustrated in Figure 1. Without external ethanol, the lipids provide the main energy resource for dauers. We used the mitochondrial activity as an indicator of dauers being alive. For simplicity, we combined both energy production pathways into a general “Energy production” term and grouped several steps of ethanol consumption as an “Acetate” component. The continuing process of energy production sustains the mito-

chondrial activity while low levels of energy production would damage mitochondria. Without external ethanol, the initial storage of lipids determines the lifespan. When lipids are depleted, energy production is reduced, leading to the damage of mitochondria and death of worms. This, however, should not happen when an external source of ethanol is provided because it is metabolized by dauers to replenish the lipid storage. Therefore, there should exist an additional mechanism that limits the lifespan as observed in experiments. Such a mechanism could be the accumulation of a toxic compound(s) derived from ethanol that can damage mitochondria while there is sufficient energy turnover. We assumed that the potential source of toxicity is the fatty acid component of the metabolic pathway. Importantly, already within this very simple model, we could consider most of the experimental situations investigated in this work.

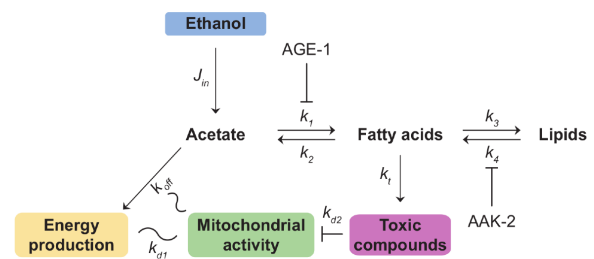


Figure 1: Simplified model of the metabolism of *C. elegans* dauer larvae. Normally lipids are converted into acetate through the fatty acids and participate in energy production. Energy production keeps mitochondria in a healthy state. Toxic compounds may be produced from fatty acids and damage mitochondria. External ethanol provides an additional source of acetate that influences the whole metabolic pathway.

First, we checked if this model was able to recapitulate the basic result that the dauer lives longer with supplied ethanol but still dies later on. The result is shown in the Figure 2. It is clear that without ethanol worms consume the stored lipids. When lipids are depleted, the acetate concentration and energy production decreases, and ultimately mitochondria deteriorate and the larva dies (see top panel of Figure 2). With external ethanol, worms can increase the lipid storage and produce energy, but start to accumulate toxic compounds. When the concentration of toxic compounds reaches a certain threshold, mitochondria start to get damaged and after some time the larva dies.

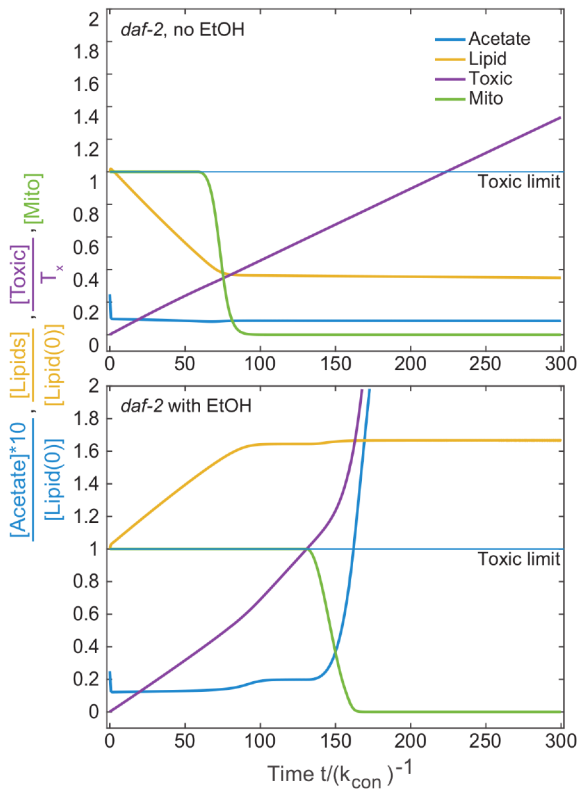


Figure 2: Results of the model for the lifespan of the dauers without (top panel) and with (bottom panel) external ethanol. In case of no ethanol, the initial amount of lipids determines the lifespan of the worm. With external ethanol, lipids are accumulated and there is always sufficient amount of energy. However, fatty acids lead to the production of toxic compounds that accumulate and irreversibly damage mitochondria.

Thus the model reproduces the observed (two-fold) increase in the lifespan of dauer in the presence of ethanol. To further test our model, we considered the survival of very short living dauers (7-8 days) of *aak-2* strain. The dauers from this strain deplete the energy storage very fast, enter a starvation-like state, and die prematurely. The model confirms that a higher rate of lipolysis leads to premature mitochondrial deterioration because the energy reserves are rapidly depleted. However, ethanol addition only partially rescues the mitochondria, because the combination of fast fatty acid synthesis and fast lipolysis makes the rate of toxic build-up higher. That way, although the dauers may have enough energy, they pass the damage threshold early on and die prematurely as seen in the experiments.

We also asked whether the model could explain the extremely extended survival (almost triple the lifespan of wild-type) of *age-1* strain on ethanol in comparison to

other dauers. Because the energy production should not be limiting when ethanol is provided, we postulated that the damage threshold may be reached much later in *age-1* dauers on ethanol. This is possible if the rate of toxic build-up is lower. Such an effect can be achieved if the rate of fatty acids synthesis is low. Then the acetate can be used for energy production without build up of fatty acids and consequently of toxic products. Indeed, the model can recapitulate the increase of the lifespan in *age-1* strain with ethanol in agreement with data. Importantly, the model predicts that because of ethanol present in unlimited amounts, worms do not need to store it as lipids. To experimentally test this prediction, we measured the incorporation of radioactive ethanol into lipids in *age-1* strain. Indeed, consistent with the model, *age-1* dauers accumulated significantly lower amount of labeled lipids compared to the wild-type animals.

Our model hints to a mechanism that determines the lifespan of dauers even in the presence of an unlimited source of energy. Specifically, an accumulation of toxic compound(s) resulting from fatty acid metabolism is in agreement with several experimental observations. In its current state, our mathematical model only suggests the possibility of such a mechanism, as all the parameters used in the model still need to be confirmed by experiments. At the same time, there are several relevant processes (e.g. detoxification, mitochondria recovery, etc.) that can be added to the model. In our future work, we will transform the model so as to capture quantitatively observations from experiments. Further, we will experimentally address those components whose behavior in terms of the model remains unclear.

Taken together, our study [3] provides insights on how dauer larvae utilize environmental sources of energy while maintaining a homeostatic balance through fine regulation of the metabolic mode. This could, on one hand, lead to a better understanding of the survival strategies and the stress resistance in worms and other animals, while on the other hand may provide new mechanisms of how organisms can cope with a surplus of energy underlying the development of metabolic syndrome in higher organisms, including humans.

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2.17 Scaling and universality of clone dynamics during tissue development

STEFFEN RULANDS

Tracing cell fate Biological systems, being highly structured and dynamic, function far from thermodynamic equilibrium. This is particularly evident in embryonic development where, through large-scale cellular self-organization, highly complex structures emerge from a group of genetically identical, pluripotent stem cells. To achieve the stereotypic ordering of organs and tissues, the fate of embryonic stem cells and their progeny must be tightly regulated, such that the correct number and type of cells is generated at the right time and place during development. Mechanisms regulating such cell fate decisions are at the centre of research in stem cell and developmental biology. To understand how complexity at the microscopic scale translates into coherent collective behaviour at the macro-scale, statistical physics provides a useful theoretical framework. But, given the complexity of embryonic development, can such concepts be applied to study cellular behaviour?

At the cellular scale, the patterns of cell fate decisions during embryonic development are reflected in the time-evolution of individual developmental precursor cells and their progeny, which together constitute a *clone*. While the dynamics of individual clones may be complex statistical ensembles of clones may provide robust (predictive) information about the relationship between different cell types and mechanisms regulating cellular behaviour. In mammals, where live-imaging of developing embryonic organs is typically infeasible, efforts to resolve clonal dynamics have relied on cell lineage tracing studies using transgenic animal models [1]. In this approach, the activation of a reporter gene allows individual cells to be marked with a fluorescent reporter. As a genetic mark, this label is then inherited by all progeny of a marked cell, and allows clone sizes and cell compositions to be recorded at specific times post-labelling. Lineage tracing studies therefore provide a ‘two-time’ measure of clonal dynamics in the living embryo. Given that clone sizes are not constrained by tissue size, and the ambiguity arising from clone merger and fragmentation due to forces exerted on the clones by the surrounding tissue (Fig. 1A,B), to what extent can information on cell fate behaviour be recovered?

Scaling behaviour of size distributions To address this question, our collaborators labelled the earliest precursors of the heart, cells expressing the gene *Mesp1* (Fig. 1C), and quantified the surface area (SA) covered by each fluorescent cluster in a given heart compartment at different developmental time points [2]. From the SAs, we then determined their distributions in each

heart region. Although cardiac development involves complex cell fate decisions, with regional and temporal variations in proliferation, we found that the resulting cluster size distribution was remarkably conserved: After rescaling the SA of each cluster by the ensemble average for each compartment at a given time point, the resulting rescaled size distributions perfectly overlapped (Fig. 1D).

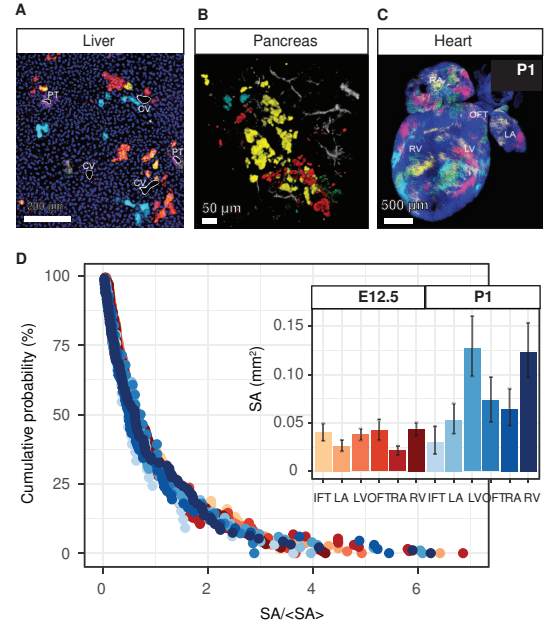


Figure 1: (A)-(C) Illustration of clone fragmentation in mouse during the development of liver (A), pancreas (B), and heart (C). (D) Cluster size distributions for mouse heart collapse onto a scaling form. Sizes were rescaled by the regional and temporal averages (inlay).

This result implies that, despite the complex and variable histories of clones, the resulting SA distribution is fully characterized by the average alone, the defining property of scaling. Formally, the frequency $f(x, t)dx$ of a cluster with a SA between x and $x + dx$ at time t post-labelling acquires the statistical scaling form, $f(x, t) = \Psi(x/x(t))$.

The distribution of cluster sizes, $f(x, t)$, is the result of different sources of variability, including growth by cell division, fragmentation and merger. Formally, the time evolution of the cluster size distribution can be cast (symbolically) as a sum of operators L that describe the effect of these contributions on the time evolution,

$$\partial_t f(x, t) = L_g[f(x, t)] + \varphi L_f[f(x, t)] + \mu L_m[f(x, t)] + \dots$$

where the parameters, φ , μ and so on, characterize the relative strength of these processes against that of growth.

Renormalisation of the cluster dynamics To investigate the origin of scaling, we questioned what determines the long-term, large-scale dependence of the cluster size distribution. In statistical physics this question is typically answered by successively coarse-graining the dynamics and monitoring changes in the relative contributions of different processes. Under this renormalization, when a cell divides, cluster sizes are rescaled by the resulting increase in tissue size, $x \rightarrow x/(1 + \delta X) \equiv \rho$. Simultaneously, time is rescaled in such way that the total rate of merging and fragmentation events remains constant in this process. After repeated rounds of dynamic renormalization, the kinetic equation converges to a self-similar (critical) form, where the fluctuations in cluster sizes are dominated solely by a balance between merger and fragmentation events, while the influence of other processes becomes vanishingly small,

$$\partial_\tau f(\rho, \tau) \approx \varphi' L_f[f(\rho, \tau)] + \mu' L_m[f(\rho, \tau)].$$

Here, φ' and μ' are rescaled parameters and ρ and τ are rescaled sizes and time, respectively. Intuitively, this means that, as the organ grows, different sources of variance contribute to the cluster size distribution by different degrees (Fig. 2A). Crucially, in the long term, contributions relating to cell fate behaviour (for example, cell division or loss) become dominated by merger and fragmentation processes, resulting in information on the former becoming erased. Therefore, while cell fate decisions affect the mean cluster size, the shape of the distribution is determined entirely by merger and fragmentation events (Fig. 2A), leading to the emergence of scaling behaviour observed in heart development.

Comparison to experimental data These results suggest not only that the cluster size distribution is entirely determined by its average (scaling), but also that the shape of the distribution is independent of the biological context (universality). The form of the scaling function relies on the dependence of the merging and fragmentation rates on cluster size. In a uniformly growing tissue, clone merger and fragmentation events are the result of the slow diffusive motion of clusters originating from random forces exerted by the surrounding tissue. In this case, the resulting scaling form is well-approximated by a log-normal size dependence. This analysis provides an explanation for the observed scaling behaviour of labelled cluster sizes of mouse heart, where the distribution indeed follows a strikingly log-normal size dependence (Fig. 2B). To further challenge the universality of the scaling dependences, we used a similar genetic labelling strategy to trace the fate of early developmental precursors in mouse liver

and pancreas as well as the late-stage development of zebrafish heart. In all cases, cluster size distributions showed collapse onto a log-normal size dependence. As merging and fragmentation are emergent properties of cell fate decisions, deviations from the scaling form can inform on structural properties of organ formation. As an example, in the developing pancreas, acinar cells initiate from precursors localized at the tips of a complex ductal network and aggregate as cohesive cell clusters, thereby suppressing clonal fragmentation. This results in a departure from scaling behaviour of the cluster size distribution (Fig. 2B, inlay).

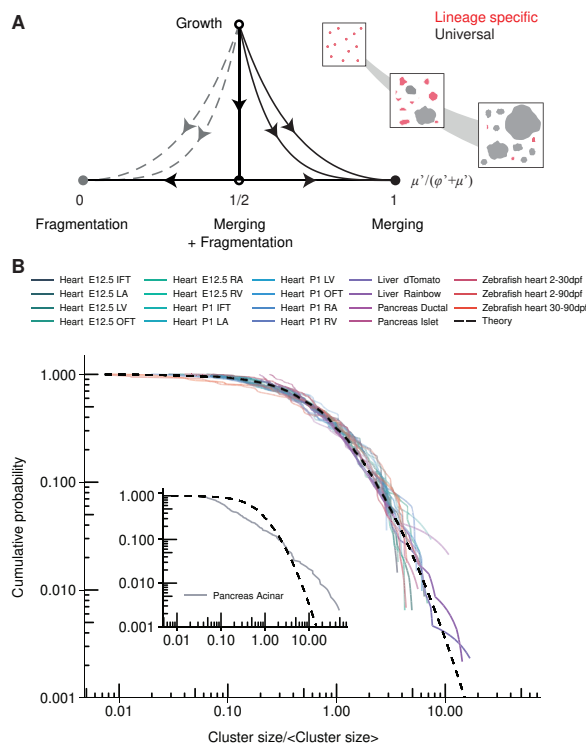


Figure 2: (A) Sketch of the renormalization flow. (B) Cluster size distributions from different organs and species collapse onto the universal master form predicted by the theory (dashed line).

Summary In recent years, there has been a growing emphasis on genetic lineage tracing as a tool to resolve the proliferative potential and fate behaviour of stem and progenitor cells. We have shown that the collective cellular dynamics in tissue growth and turnover lead to universal clone dynamics, where cluster size distributions become independent of the fate behaviour of cell populations. These findings identify quantitative strategies to unveil cell fate-specific information from such experiments. At the same time, by highlighting the unexpected emergence of core concepts of statistical physics in a novel context, this study provides a model of how the cellular dynamics of living tissues can serve as a laboratory for statistical physics.

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2.18 Collective oscillations in epigenetic DNA modifications

BAHAREH KIANI AND STEFFEN RULANDS

Epigenetic DNA modifications The regulation of cell fate relies on a multitude of molecular processes. Historically, emphasis has been placed on genes, their expression and translation to proteins, and their interplay in gene regulatory networks. In recent years, it has become clear that there are additional, *epigenetic*, layers of regulation: dynamic changes in the way the DNA is folded, modifications to the protein complexes the DNA is wrapped around or chemical modifications of the DNA itself (Fig. 1A). DNA methylation is the primary layer of epigenetic regulation. Methyl groups are attached to cytosines (C) when positioned next to a guanine (G) on the DNA (CpG). In mammalian embryonic development, the segregation of lineages giving rise to differentiated cell types is associated with large-scale changes in DNA methylation. Following fertilization, global loss of DNA methylation from both the maternal and paternal genomes is tightly linked with the acquisition of naïve pluripotency in the inner cell mass of the blastocyst, i.e. the capability of embryonic stem cells to generate any cell type in the adult body [2]. During the transition towards a state where cells are primed for differentiation, de-novo methylation results in a global gain of this epigenetic mark [2]. The patterns of DNA methylation established during this period are associated with the assignment of different cell types and lack of DNA methylation leads to an early death of the embryo. In adult, alterations in DNA methylation or mutations in the enzymes driving methylation are one of the hallmark markers of cancer. But in which way is DNA methylation involved in cell fate assignment during early embryonic development?

Heterogeneous DNA methylation in embryonic stem cells To answer this question, we started with an in vitro system for embryonic cells primed for differentiation, namely embryonic stem cells cultured in serum conditions. Using single-cell bisulfite sequencing we were able to measure DNA methylation in single cells with the resolution of single base pairs. We found surprising heterogeneity in global DNA methylation levels between cells (ranging between 17 and 86 percent in a set of functionally relevant regions). Nevertheless, gene expression patterns were similar across cells and, in particular, global DNA methylation was not correlated to the expression of genes that are thought to drive (de-) methylation [1]. We therefore hypothesised that this autonomous heterogeneity could be the result of an oscillatory process, where cells cycle between a lowly and a highly methylated state.

Collective oscillations in DNA methylation during exit from pluripotency But could such a genome-

wide collective oscillation of DNA methylation occur under biological conditions?

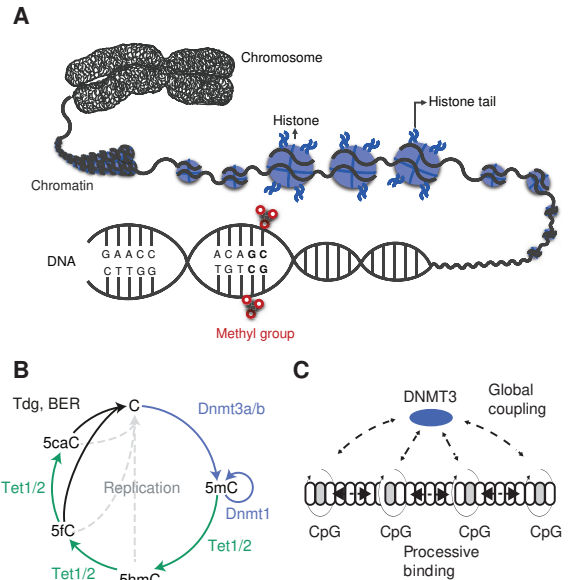


Figure 1: (A) DNA methylation affects cytosines in a CpG context. (B) The biochemistry of DNA methylation is cyclic in case of co-expression of Dnmt3 and Tet genes. (C) Global feedback via active degradation of DNMT3 proteins and local coupling via DNMT3 processivity can lead to synchronisation of DNA methylation states.

To answer this questions we followed a theoretical approach. The biochemistry of DNA methylation turnover not only involves de-novo methylation via DNMT3 enzymes. The process of methylation can also be reverted by a sequence of chemical reactions involving TET enzymes and, ultimately, excision and repair of the DNA (Fig. 1B). Therefore, if both, genes from the Dnmt3 and the Tet family, are co-expressed DNA methylation turnover is a cyclic process involving many protein binding and unbinding events. Importantly, the “phase” of single CpGs is coupled via processive binding of DNMT3s and global feedback via control of their active degradation [1] (Fig. 1C).

Starting with with a full stochastic dynamics governing single CpGs we performed strong disorder renormalisation and found that, on the genome-scale, the dynamics of a coarse-grained phase variable Θ_i is governed by a heterogeneous Kuramoto equation,

$$\dot{\Theta}_i = \tilde{\omega}_i + \tilde{\kappa}_i \sum_j \tilde{\kappa}_j \sin(\Theta_j - \Theta_i), \quad (1)$$

with intrinsic renormalised frequencies, $\tilde{\omega}_i$, and effective coupling strengths, $\tilde{\kappa}_i$. With this we predicted genome-wide synchronised oscillations if the average

coupling strength between CpGs or its variance exceeds a threshold given by the statistical weight of the dominant intrinsic frequency, $g(\tilde{\omega}_0)$,

$$\langle (\tilde{\kappa} - \langle \tilde{\kappa} \rangle)^2 \rangle + \langle \tilde{\kappa} \rangle^2 \geq \frac{2}{\pi a g(\tilde{\omega}_0)}. \quad (2)$$

This condition can indeed be fulfilled under biologically relevant conditions.

Experimental validation of global oscillations in DNA methylation To test the model predictions and obtain more direct evidence for genome-scale DNA methylation oscillations, we considered an *in vitro* “2i release” experiment in which cells were transferred from so-called 2i conditions, where the genome is globally demethylated, to primed serum culture conditions, where cells upregulate the expression of Dnmt3 genes. Cells were collected for whole-genome bisulfite sequencing over a subsequent time course of 10 hours. We reasoned that the transfer of cells between the two

conditions might synchronize their entry into an oscillatory phase, allowing direct evidence for oscillations to be acquired from population-based measurements. We detected evidence for rapid oscillations in the mean methylation rate over different genomic domains, with a period of approximately 2-3 hr (Fig. 2A,B). Spectral analysis confirmed enriched oscillations in these regions and the whole genome ($p = 1e - 51$). Using a computational reconstruction of the developmental time of single cells we observed genome-wide oscillations in DNA methylation during the loss of pluripotency in mouse embryos ($p = 2e - 4$, Fig. 2C). By parallel sequencing of the methylome and gene expression products over time we found that these oscillations were paralleled by oscillations in short-lived gene products (RNAs) (Fig. 2D). Using existing genomic heterogeneities in DNMT3 binding affinities we found agreement between theoretical predictions on frequency and amplitude variations and experimental measurements both *in vitro* and *in vivo* [1].

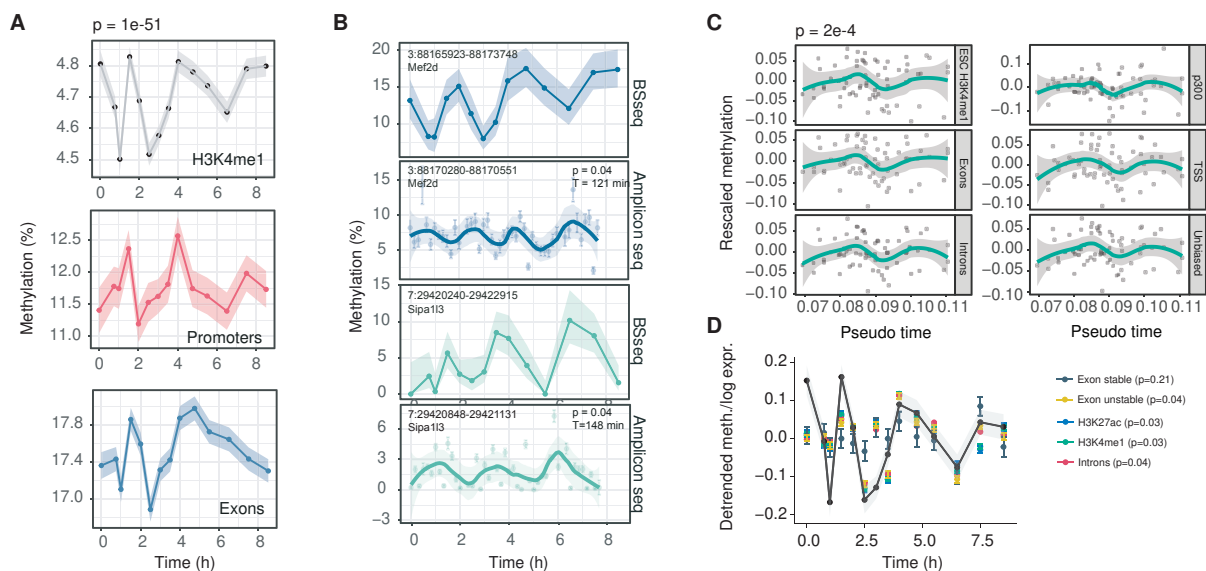


Figure 2: Collective oscillations in DNA methylations were experimentally observed by (A) whole-genome bisulfite sequencing for average methylation levels in different functional regions of the genome and (B) both whole-genome bisulfite sequencing and Amplicon sequencing for single genome regions, and (C) single-cell methylome and transcriptome sequencing of cell taking from mouse embryos for statistically inferred developmental times of cells. (D) Oscillations in global DNA methylation are associated with parallel oscillations in short-lived transcripts.

Summary We showed that during the loss of pluripotency, co-expression of enzymes required for DNA methylation turnover, DNMT3s and TETs, promotes cell-to-cell variability in this epigenetic mark. Using a combination of single-cell sequencing and methods from non-equilibrium physics, we show that this variability is associated with coherent, genome-scale oscillations in DNA methylation. Analysis of parallel single-cell transcriptional and epigenetic profiling pro-

vides evidence for oscillatory dynamics both *in vitro* and *in vivo*. These observations provide insights into the emergence of epigenetic heterogeneity during early embryo development, indicating that dynamic changes in DNA methylation might influence early cell fate decisions. This work shows that the combination of novel methods in single-cell genomics and non-equilibrium physics can yield mechanistic insight into cell fate decision making.

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2.19 Phase separation in concentration gradients

FRANK JÜLICHER AND CHRISTOPH A. WEBER

Liquid droplets inside living cells. Biological function inside cells is attained by the spatial-temporal organisation of biomolecules and the control of their chemical reactions. For this purpose the interior of the cell is divided into compartments, referred to as organelles. While some organelles have a membrane, such as mitochondria, others are not enclosed by a membrane; they are called non-membrane bound compartments or biomolecular condensates. Many of these membrane-less organelles have been found to exhibit properties reminiscent of liquid droplets [1]. In contrast to passive emulsions, these cellular droplets exist in the non-equilibrium environment of living cells. For instance, actively maintained concentration gradients can spatially organize these droplet-like organelles [2].

To understand the positioning of condensed phases (e.g. droplets) we have studied how concentration gradients of a regulator component affect phase separation of two components. The concentration profile of a regulator molecule can be influenced by an external field such as gravitation, electric or magnetic fields [3], or by boundary conditions [4].

Positioning of condensed phases by regulator gradients. We have investigated how regulator concentration gradients affect a mixture which undergoes phase separation [5]. If the regulator gradients are generated by external fields, the corresponding stationary states are inhomogeneous thermodynamic states and can thus be addressed by a minimisation of the free energy.

To this end, we have studied a simple ternary model [6] accounting for the demixing of two components, A and B , and a regulator component R that interacts with the other components and thereby affects phase separation between A and B . The spatial distribution of the regulator component R is influenced by an external potential $U(x)$. The free energy density of the system involves this external field, entropic contributions and interactions between the components i and j , which are captured by the mean-field interaction parameters χ_{ij} . We considered an incompressible system where the molecular volumes are constant and equal for all components. The interaction parameter between A and B , χ_{AB} , determines the tendency of A and B to phase separate. To ensure that R acts as a regulator we chose these interaction parameters such that the regulator R does not demix from A or B . For simplicity, we have considered a one dimensional system of size L in the absence of boundaries and with periodic boundary conditions.

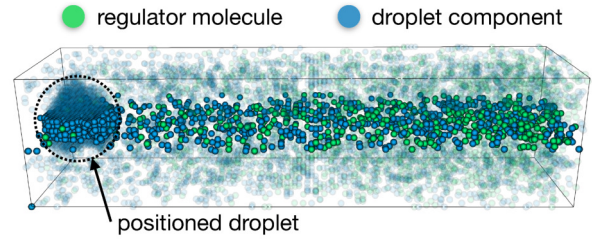


Figure 1: Snapshot of a positioned droplet (majority component is shown by blue spheres) in a regulator gradient (green spheres). These results are obtained by Monte-Carlo simulations with flux boundary conditions for the regulator molecules at the right and left most boundary. This non-equilibrium system also shows a discontinuous behaviour of the order parameters. We currently investigate the qualitative differences to thermodynamic equilibrium studied in Ref. [5].

To find the equilibrium states we determined the concentration profiles $c_i(x)$ of all components $i = A, B, R$ by minimising the total free energy. Minimisation leads to two coupled Euler-Lagrange equations that we have solved numerically and studied analytically. We found two extremal profiles of the phase separating component A and two corresponding profiles of the regulator component R (the profile of B follows from incompressibility). In the first case, the phase separating material A can be accumulated at larger regulator concentration and correlates (+) with the concentration of the regulator material. In the second case, the A -material accumulates at smaller regulator concentrations corresponding to an anti-correlation (−) with respect to the regulator profile. The free energies of the correlated and the anti-correlated states, F^+ and F^- , are different for most interaction parameters. The free energies only intersect at one point $\chi_{BR} = \chi_{BR}^*$. At this point the minimal free energy exhibits a kink. This means that the system undergoes a *discontinuous phase transition* when switching between a spatially anti-correlated (−) and a spatially correlated (+) solution with respect to the regulator. Consistently, the corresponding order parameters jump at the threshold value χ_{BR}^* .

Our analysis shows that the occurrence of this novel discontinuous phase transition solely relies on the existence of the position-dependent profile of the regulator and the interactions of the regulator molecules with the liquid condensed phases. To test whether the discontinuous nature of the transition is also preserved if the regulator gradient is driven by boundary conditions we are employing Monte Carlo simulations (Fig. 1).

Coarsening kinetics of emulsions in concentration gradients. The presence of a regulator gradient also affects the droplet kinetics [7]. There are a set of physical quantities relevant for the local kinetics of droplets, such as the position dependent supersaturation $\varepsilon(x) = c_\infty(x)/(c_{\text{out}}^{(0)}(x) - 1)$ and the equilibrium concentration $c_{\text{out}}^{(0)}(x)$, where $c_\infty(x)$ denotes the far field concentration of droplet material. These quantities determine the inhomogeneous ripening dynamics and can be used to develop a generic theory of droplet ripening in concentration gradients extending the classical laws of droplet growth derived by Lifschitz & Slyozov. The position dependence of these quantities drive the droplet kinetics leading to a position-dependent growth, drift of droplets and even deformations of their shape.

If droplets are far apart from each other, the growth rate of droplet $i = 1, \dots, N$ of radius R_i and at position x_i is:

$$\frac{dR_i}{dt} = \frac{D}{R_i} \frac{c_{\text{out}}^{(0)}(x_i)}{c_{\text{in}}^{(0)}} \left[\varepsilon(x_i) - \frac{\ell_\gamma}{R_i} \right], \quad (1a)$$

and the drift velocity of droplet i reads

$$\frac{dx_i}{dt} = \frac{D}{c_{\text{in}}^{(0)}} \left[3\partial_x c_\infty(x)|_{x_i} - \partial_x c_{\text{out}}^{(0)}(x)|_{x_i} \left(1 + \frac{\ell_\gamma}{R_i} \right) \right], \quad (1b)$$

where D is the diffusion constant and ℓ_γ the capillary length. For inter-droplet distances much larger than droplet size, droplets only interact via the far field concentration field $c_\infty(x, t)$. This field is governed by a diffusion equation including gain and loss terms associated with growth or shrinkage of drops.

We find that there are two novel possibilities of how droplet material is transported: Exchange of material between droplets at different positions along the concentration gradient due to a *position dependent droplet growth*, and *droplet drift* along the concentration gradient. Position dependent droplet growth implies

droplet growth and shrinkage with rates that vary along the gradient because the local equilibrium concentration $c_{\text{out}}^{(0)}(x)$ and the far field concentration $c_\infty(x)$ are position dependent. For a supersaturation $\varepsilon(x) = (c_\infty(x)/c_{\text{out}}^{(0)}(x) - 1) > \ell_\gamma/R$, a droplet located at position x grows, and shrinks in the opposite case. This position dependence implies a movement of the dissolution boundary $x_c(t)$ segregating all droplets toward one of the boundaries. Droplet drift results from an asymmetry of material flux at the interface parallel to the regulator gradient. We were able to calculate the movement of the dissolution boundary and the droplet drift for a single droplet and emulsions with many droplets.

By numerically solving the kinetic equations we have confirmed these calculations. The position-dependent equilibrium concentration and concentration field far away from the droplet indeed cause the drift of droplets along the gradient and dissolve all droplets everywhere except from a region close to one boundary of the system. Our numerical analysis also revealed that the droplet size distribution can dramatically narrow during the positioning dynamics which causes a transient arrest of droplet growth. After this arrest phase the positioned droplets are subject to a locally homogenous concentration environment and the system recovers the dynamics of classical Ostwald ripening.

Conclusion. The positioning of droplets occurs via a novel discontinuous phase transitions and the droplet kinetics can be understood as a position-dependent ripening process which segregates all droplets to one boundary of the system via position-dependent growth and droplet drift. Our theory is relevant to understand the spatial organisation of the biochemistry in living cells and for the development of novel applications in chemical engineering.

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2.20 How active stresses shape the mitotic spindle

DAVID ORIOLA, FRANZISKA DECKER, FRANK JÜLICHER AND JAN BRUGUÉS

The mitotic spindle is a self-organized complex machinery orchestrating chromosome segregation during cell division. The spindle is composed of an aligned array of microtubules - dynamic polymers that nucleate, grow and shrink - and energy transducing proteins such as molecular motors [1] that generate stresses and flows in the structure (see Fig. 1A). Several models have been proposed to understand the role of molecular motors in spindle self-organization; however, there is still no clear consensus on how the interactions between individual molecular components translate into the precise bipolar spindle-like shape of the structure. The spindle can be regarded as an active liquid crystal droplet with two $+1/2$ point defects at the spindle poles [4]. Given that microtubules in spindles are found in a highly ordered nematic phase, mitotic motors can generate active dipolar stresses [4]. In contrast to isotropic stresses which only modify the size, dipolar stresses can shape the structure and have no analogue in equilibrium systems. Despite active dipolar stresses have been measured in spindles, it is not known which motors are responsible for such stresses and how they shape the structure. Here we combine experiments and theory to understand how motor-generated stresses shape *Xenopus* egg extract spindles.

Dynein generates dipolar contractile stresses in spindles Dynein is a minus-ended directed molecular motor which clusters microtubule minus-ends and focus spindle poles. Given its contractile activity in egg extracts dynein is a good candidate for active stress generation in spindles. We wondered if a dynein-dependent contractile behaviour could be triggered in spindles by the creation of a large amount of microtubule minus-ends. In order to test our hypothesis, we ablated *Xenopus* egg extract spindles using a sequence of laser cuts to ensure the complete disconnection of a pole (see Fig. 1B). By ablating the structure, we created a large surface of newly born microtubule minus-ends. Immediately after the laser cuts, we observed a fast motion of the disconnected spindle pole towards the spindle body and at the same time, an advancing poleward front (see Fig. 1C,D yellow and cyan arrows, respectively). The combination of the two movements closed the wound after ~ 2 min. The poleward and rebinding speeds were found to be of the same order, $3.1 \pm 0.6 \mu\text{m}/\text{min}$ ($n = 7$, mean \pm SD) and $2.6 \pm 0.7 \mu\text{m}/\text{min}$ ($n = 7$, mean \pm SD), respectively. To test that dynein was indeed responsible for rebinding the disconnected pole, we fully inhibited the motor protein treating spindles with $8 \mu\text{M}$ p150-CC1.

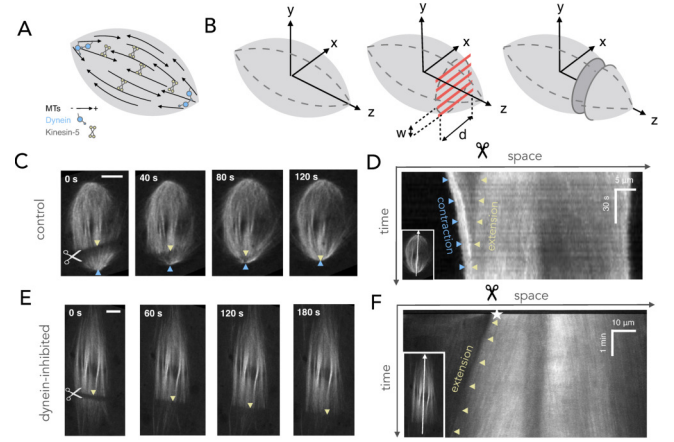


Figure 1: Laser ablation and spindle self-healing. A) Kinesin-5 and dynein generate stresses in the spindle. B) Laser ablation procedure. C,D) Spindle healing after laser ablation. E,F) Spindle healing after dynein inhibition.

In this case, disconnection of a pole did not result in any rebinding motion (see Fig. 1 E,F) and consequently the wound did not close. Instead, the poleward front generated by kinesin-5 (see Fig. 1A) displaced the disconnected pole until it eventually disassembled. The poleward front speed was not significantly altered respect to the control case ($2.6 \pm 0.6 \mu\text{m}/\text{min}$, $n = 5$, mean \pm SD).

An active liquid crystal theory explains spindle shape In order to understand how dipolar active stresses shape the structure, we formulated an active liquid droplet theory. We consider the spindle as a liquid crystal with orientational field p_i and density ρ . The bulk free energy F_b reads:

$$F_b = \int_V dV \left[\frac{K}{2} \partial_i p_i \partial_j p_j + \frac{A}{2} \left(\frac{\delta \rho}{\rho_0} \right)^2 \right] \quad (1)$$

where A is a compressibility coefficient, ρ is the number density of microtubules and ρ_0 a preferred density. We adopt the following plausible expression for the surface energy, commonly used in the study of liquid crystal droplets:

$$F_s = \int_S [\gamma + \tau (p_k n_k)^2] dS \quad (2)$$

where n_i is the normal vector to the interface, γ is the interfacial tension and τ is the anchoring strength. We neglect viscous stresses and only consider the total stress tensor in the system σ_{ij} as the sum of a passive nematic and an active contribution:

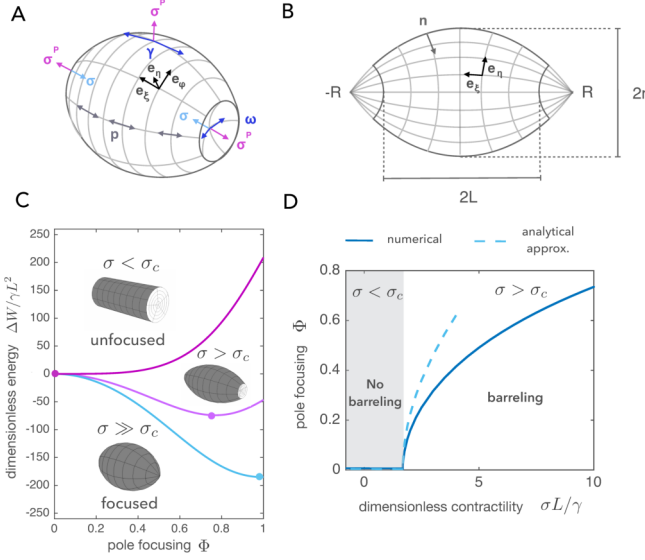


Figure 2: Barreling instability in spindles. A) Forces acting on the spindle surface. B) Spindle shape parametrization C) Barreling instability as a function of dynein contractility. D) Bifurcation diagram of the barreling transition.

$$\sigma_{ij}^p = -\Pi\delta_{ij} + h_i p_j - \frac{\partial f_b}{\partial(\partial_j p_k)} \partial_i p_k \quad (3)$$

$$\sigma_{ij}^a = \zeta \Delta \mu \left(p_i p_j - \frac{\delta_{ij}}{3} \right) \quad (4)$$

where $\Pi = \partial f_b / \partial \rho$ is the pressure, $h_i = -\delta f_b / \delta p_i$ is the molecular field, f_b is the integrand of Eq. 1 and the last term in Eq. 3 corresponds to the Ericksen stress. Force balance is imposed in the bulk ($\partial_j \sigma_{ij} = 0$) and the boundary condition on the surface implies $2H\Sigma = \sigma^p - \sigma$, where H is the mean curvature of the surface, $\sigma^p = n_i \sigma_{ij}^p n_j$, $\sigma = n_i \sigma_{ij}^a n_j$ and $\Sigma = \gamma + \tau(p_k n_k)^2$. To simplify the problem we parametrize the spindle using bispherical coordinates $X_i = X_i(\xi, \eta, \phi)$ and prescribe the orientational field as $p_i = \partial_\xi X_i / |\partial_\xi X_i|$ as depicted in Fig. 2A,B. By restricting the possible set of shapes (we only allow two dimensionless shape parameters: the aspect ratio $a = r/L$ and the pole focusing parameter $\Phi = L/R$), an equivalent problem can be formulated in terms of an effective work functional W taking into account the work generated by the active stresses on the spindle surface W_s . In this case, the shape can be obtained by minimizing a work function $W = F_b + F_s + W_s$ numerically. Close to the cylindrical configuration, i.e. $\Phi \ll 1$, the effective work function W of the spindle can be approximated to a quartic

form, where the pole focusing parameter Φ plays the role of the order parameter in Landau theory:

$$W(\Phi, a) = W_0(a) + W_2(a)\Phi^2 + W_4(a)\Phi^4 + \mathcal{O}(\Phi^6) \quad (5)$$

where the different coefficients can be explicitly obtained. In particular $W_2 \propto \sigma_c - \sigma$, where σ_c is the critical value for the transition to occur and σ is the magnitude of the contractile stress. The structure buckles axially or ‘barrels’ when the contractile stress exceeds a critical value σ_c and the cylindrical configuration ($\Phi = 0$) becomes unstable (Fig. 2C,D). In this case, the pole focusing parameter close to the bifurcation point follows $\Phi \sim \sqrt{\sigma/\sigma_c - 1}$ (see Fig. 2D, analytical curve). Otherwise, if $\sigma < \sigma_c$, poles are completely unfocused and the solution $\Phi = 0$ is stable (see Fig. 2D). To experimentally test our theory of spindle pole focusing, we studied spindle morphology by differentially inhibiting dynein. We titrated a dynein inhibitor (p150-CC1) in egg extracts after spindle assembly and analyzed the resulting morphologies using an LC-PolScope. The shapes were analyzed by fitting a tactoid to the retardance images, thus allowing to obtain the position of the virtual poles (R) and the spindle width (r). In Fig. 3A, the average values of the pole focusing parameter are plotted against the rescaled inhibitor concentration for different extract days. The analytical prediction for the rescaled bifurcation curve has no fitting parameters and quantitatively agrees to the averaged rescaled data. Finally, by comparing the shapes obtained exploring the parameter space and the experimental spindle shapes, we estimated the parameters in our model (see Fig. 3B). Overall, we conclude that a barreling-type instability successfully captures the process of pole focusing in spindles.

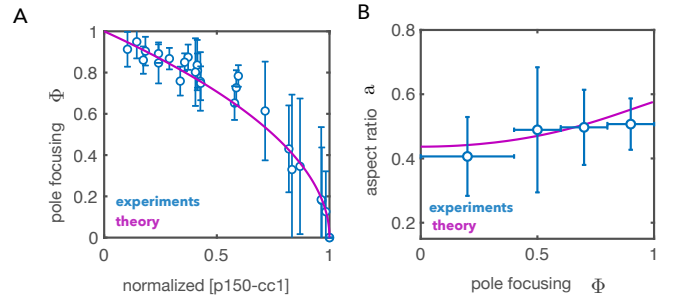


Figure 3: Dynein inhibitor titration and shape analysis. A) Experimental verification of a barreling instability. B) Shape space as a function of dynein activity.

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2.21 Autocatalytic microtubule nucleation determines the size and mass of *Xenopus laevis* egg extract spindles

FRANZISKA DECKER, DAVID ORIOLA, BENJAMIN DALTON, AND JAN BRUGUÉS

The mitotic spindle is a macromolecular machine responsible for segregating chromosomes during cell division. Its main building blocks, the microtubules, are short and turnover rapidly in comparison to the entire structure. Thus, microtubules have to be constantly created throughout the spindle, which is called nucleation. The mechanisms underlying the spatial regulation of microtubule nucleation and how they set spindle size, however, are still unclear [1]. This is partly because of the lack of methods to measure microtubule nucleation in spindles.

Here, we developed a new technique based on laser ablation to measure microtubule nucleation. As microtubules grow from the plus ends while minus ends remain stable [2], the location of minus ends functions as a marker for microtubule nucleation. To localize microtubule nucleation events, we measured the density of minus ends by analyzing synchronous waves of microtubule depolymerization from laser cuts similar to Ref. [3]. Briefly, cut microtubules rapidly depolymerize from the newly generated plus ends, while the new minus ends remain stable. The minus end density at the location of the cut can then be obtained from the decrease of the microtubule depolymerization wave, but as opposed to Ref. [3], our method resolves the minus end locations with a single laser cut. Using this technique, we measured the nucleation profile of a spindle structure in *Xenopus laevis* egg extract. This measurement showed that nucleation occurs throughout the entire structure and monotonically decreases from the chromosomes. In combination with biochemical experiments we showed that microtubules are nucleated via an autocatalytic process in close proximity to pre-existing microtubules and that the amount of active nucleators limits this autocatalytic growth [4].

To test whether a limited pool of active nucleators can quantitatively account for the size and microtubule nucleation in these structures, we developed a biophysical model of autocatalytic microtubule nucleation (see Fig. 1A). We define the microtubule bound and unbound populations of active nucleators as $n_b(x, t)$ and $n_u(x, t)$, respectively. When unbound, active nucleators can diffuse with diffusion coefficient D and become inactive with rate k_0 . Active nucleators can bind to microtubules with rate k_b and unbind with rate k_u . A bound nucleator can nucleate a microtubule from a pre-existing microtubule with rate k_{bra} . Since a daughter microtubule nucleates at a certain distance from the minus-end of the mother microtubule, there exists a flux of microtubule mass, which will advance with velocity v . The magnitude of the velocity v can be ob-

tained from the following argument: assuming that a nucleator can bind anywhere along a microtubule, since microtubule lengths are exponentially distributed with an average length ℓ , a nucleator will bind on average at a distance ℓ from the minus end of the mother microtubule.

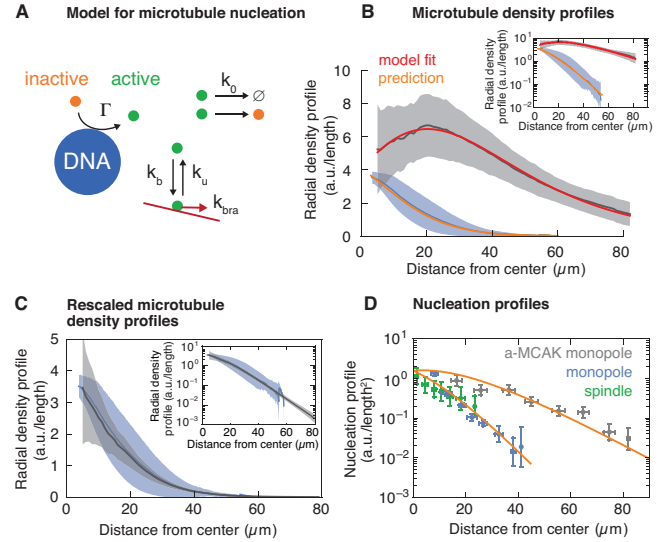


Figure 1: Model for microtubule-stimulated nucleation. (A) Inactive nucleators (orange circles) are activated around DNA at a constant rate Γ . As active nucleators diffuse (green circles), they can bind (rate k_b) and unbind (rate k_u) microtubules (red lines). Once bound, they can nucleate a new microtubule with a certain probability (rate k_{bra}). Active nucleators become inactive at a constant rate k_0 . (B) Radial microtubule density profiles measured from fluorescent images (mean \pm SD, $N_{monopoles} = 40$ (blue), $N_{a-MCAK} = 18$ (gray)) and corresponding model fit to the MCAK-inhibited and prediction to control monopoles. The ratio of the microtubule densities for control and MCAK-inhibited monopoles was determined using structures from the same extract reaction. (C) Parameter-free rescaling of the microtubule density profiles predicted by the model: $\rho_C = \rho_M \exp[(1/\ell_M - 1/\ell_C)x]$, where ρ_C , ℓ_C and ρ_M , ℓ_M are the density and length of microtubules for the control and MCAK-inhibited structures, respectively, and x is the distance from the center of the structure. In the graph, blue corresponds to the density profile of control monopoles and gray to the rescaled density profile of MCAK-inhibited monopoles. (D) Data and predictions (orange) for the nucleation profiles of control (blue) and MCAK-inhibited monopoles (gray) up to a global nucleation amplitude, and flux-corrected regular spindles (green) (mean \pm SD, $N_{control} = 117$, $N_{a-MCAK} = 74$, $N_{spindle} = 36$ cuts).

Finally, considering the average microtubule turnover rate is Θ , the velocity is $v = \ell\Theta$. We want to highlight there is a difference between v and the microtubule front velocity. The latter depends on k_{bra} and should be zero in the absence of autocatalytic nucleation. In a similar model of autocatalytic microtubule growth, the front velocity was explicitly calculated and depended

on the branching rate [5]. In our case, the steady state front velocity is zero, although v is different from zero. Finally, we denote the number density of microtubules as $\rho(x, t)$. Given the previous considerations, the dynamics of the system read:

$$\partial_t n_u = D\nabla^2 n_u - k_b \ell_b n_u \rho + k_u n_b - k_0 n_u \quad (1)$$

$$\partial_t n_b = k_b \ell_b n_u \rho - k_u n_b \quad (2)$$

$$\partial_t \rho = -\mathbf{v} \cdot \nabla \rho + k_{\text{bra}} n_b - \Theta \rho \quad (3)$$

where ℓ_b is a characteristic binding length scale for the active nucleators. Next, we consider a one-dimensional problem with the spatial coordinate x being the radial coordinate from the center of a monopolar spindle. A more involved two-dimensional description of the problem is found to lead to similar results. Unbound nucleators are assumed to be activated with constant rate Γ at the surface of chromatin in the center of the monopole ($x = 0$) (see Fig. 1A). This leads to a boundary condition for the flux of active nucleators at the chromosomes, which is expressed as $-D\partial_x n_u|_{x=0} = \Gamma$. At steady state, Eq. 2 leads to $n_b(x) = \ell_0 n_u(x) \rho(x)$, where $\ell_0 \equiv \ell_b k_b / k_u$. Using the last expression into Eq. 1 and the boundary condition at $x = 0$, at steady state we obtain:

$$n_u(x) = A e^{-x/\ell_u} \quad (4)$$

where $A = \frac{\Gamma}{\sqrt{Dk_0}}$ is the amplitude of the gradient, proportional to the rate of activation Γ at the chromosomes, and $\ell_u \equiv \sqrt{D/k_0}$ is the characteristic length scale of the gradient of unbound active nucleators. Finally, by using Eq. 3 we find the steady state distribution of microtubule minus ends:

$$\rho(x) = \lambda(x) e^{-x/\ell} \quad (5)$$

where $\lambda(x) = \rho(0) \exp[\alpha(1 - e^{-x/\ell_u})]$ is a lifetime-independent function, $\rho(0)$ is the density of minus ends at $x = 0$ and $\alpha \equiv \frac{\Gamma \ell_0 k_{\text{bra}}}{v k_0}$ is a dimensionless parameter. Since only bound nucleators can nucleate new microtubules, the nucleation process requires an initial source of microtubules acting as seeds for the autocatalytic growth. In our simplified model, this initial source corresponds to the boundary condition $\rho(0)$. The origin of these seed microtubules could be due to spontaneous microtubule nucleation in the cytoplasm, centrosomes, or RanGTP-mediated cytoplasmic nucleation in close proximity to chromosomes. However, our measurements on microtubule nucleation in control and MCAK-inhibited structures (MCAK is a depolymerizing motor), where the microtubule lifetime and length are increased threefold, show that microtubule-independent microtubule nucleation is not sufficient to explain spindle growth or the spatial dependence of microtubule nucleation, and

that microtubule independent nucleation can be accounted for as a boundary condition, suggesting that it is very localized in space.

There are two main length scales in the system: ℓ_u , which is dictated by the gradient of unbound active nucleators and does not depend on microtubule lifetime, and ℓ , which is the mean microtubule length. From our results, the inhibition of the motor protein MCAK affects the lifetime Θ and length ℓ , thus, not changing $\lambda(x)$. Therefore, the model predicts that if the control monopole profile is given by $\rho_C(x) = \lambda(x) e^{-x/\ell_C}$, the perturbed monopole profile reads $\rho_M(x) = \lambda(x) e^{-x/\ell_M}$. The ratio of the two profiles, which allows for a parameter-free rescaling of the microtubule density profiles (see Fig. 1C), follows:

$$\frac{\rho_C(x)}{\rho_M(x)} = \exp \left[x \left(\frac{1}{\ell_M} - \frac{1}{\ell_C} \right) \right]. \quad (6)$$

In Fig. 1B, the MCAK-inhibited microtubule profile is fitted to Eq. 5 with fitting parameters α and ℓ_u (notice that $\rho(0)$ only rescales the arbitrary amplitude), while the parameter ℓ_M is measured from laser ablation measurements in MCAK-inhibited monopoles. Conversely, the microtubule density profile for control monopoles is predicted by using Eq. 5 or 6 without the need of any fitting parameter, taking ℓ_C as the measured mean microtubule length from control monopoles. Finally, the fits on Fig. 1D for the microtubule nucleation profiles are done using the expression for $n_b(x)$ and adjusting the prefactor.

By combining our experiments and modeling, we showed that microtubules in large spindles are nucleated in an autocatalytic way and that a gradient of active nucleators produced at the DNA determines the size and microtubule mass of the entire structure. Since microtubules are dynamic polymers that grow and shrink very rapidly, our next aim is to investigate the relationship between autocatalytic nucleation, which depends on the total available substrate (i.e., the total mass of microtubules), and microtubule dynamics.

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2.22 A comparative genomics approach reveals insights into the importance of gene losses for mammalian adaptations

VIRAG SHARMA, NIKOLAI HECKER, DAVID JEBB, JULIANA ROSCITO, MICHAEL HILLER

An approach to accurately detect gene loss events

The loss (inactivation) of ancestral protein-coding genes is not only one of the most radical genomic changes, but can also reveal insights into genomic changes that are associated with phenotypic changes. To systematically address the role of gene loss for phenotypic evolution in mammals, we developed a genomics approach to accurately detect mutations that inactivate coding genes (stop codon mutations, splice site-disrupting mutations, frameshifting insertions and deletions, and deletions of entire exons or genes) [1]. To achieve a very high specificity, we had to overcome numerous challenges related to genome assembly and alignment issues and evolutionary gene structure changes. Key to achieving our final specificity of 99.7% was the development of the Hidden Markov Model-based method CESAR that takes splice site and reading frame information into account when aligning coding exons [2] [3]. CESAR is not only key to detect lost genes, but it is also a very accurate method to annotate conserved coding genes, as we have demonstrated by projecting human genes to 143 non-human vertebrate genomes [4].

Gene losses and mammalian adaptations We applied our gene loss detection approach to the genomes of 62 placental mammals. By analyzing this unprecedented dataset, we discovered numerous gene losses that provide mechanistic explanations for well-known examples of mammalian adaptations, such as life in water, extreme diving abilities or dietary specializations [1]. First, we analyzed genes that are specifically lost in cetaceans (whales and dolphins), which revealed a number of genes with hair- and epidermis-related functions (Figure 1A). This is interesting since the skin of cetaceans is well adapted to their aquatic environment by having a much thicker epidermis that enhances physical barrier properties and by lacking hair to reduce drag while swimming. Importantly, several of these genes recapitulate important aspects of the cetacean epidermis (thickness, hair loss) in mouse knockouts, suggesting that these gene losses could have contributed to the remodeling of the cetacean epidermis. Second, our gene loss catalogs revealed that the sperm whale is the only mammal known so far that lacks the enzyme to synthesize vitamin A, which can be explained by the squid-dominated diet that provides large amounts of vitamin A. We found that sperm whales have also lost the erythrocyte-specific AMPD3 gene (Figure 1B), which likely contributes to the exceptional diving ability in this species. Third, we dis-

covered that fruit bats lost genes that improve insulin secretion and insulin metabolism, which is likely an adaptation to their sugar-rich diet (Figure 1C). In summary, even though one would intuitively expect that gene loss is typically maladaptive, our results suggest that gene loss is an evolutionary mechanism for adaptation that may be more widespread than previously anticipated.

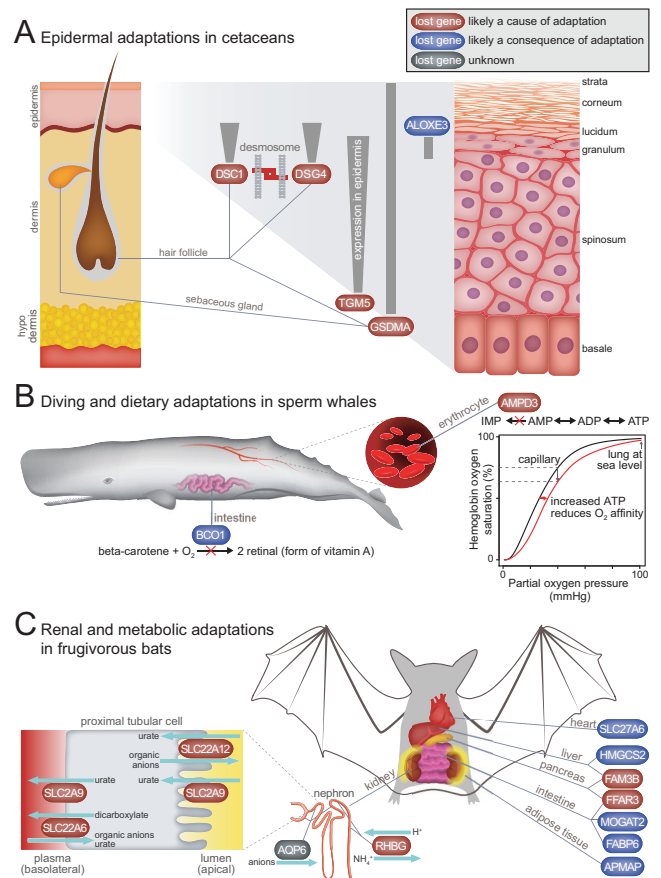


Figure 1: Gene loss as a consequence and likely cause of phenotypic adaptations. (A) Losses of hair- and epidermis-related genes in cetaceans are likely causally implicated in the remodeling of their skin. (B) The loss of the vitamin A synthesizing enzyme BCO1 in sperm whales is a consequence of their specialized diet that mainly consists of vitamin A-rich but beta-carotene poor squid. AMPD3 deaminates adenosine monophosphate (AMP) to inosine monophosphate (IMP) in erythrocytes. AMPD3 loss increases the level of ATP (an allosteric hemoglobin effector) and facilitates O₂ release, as illustrated by the O₂-emoglobin dissociation curve (wildtype, black; AMPD3 knockout, red). (C) Some gene losses in fruit bats (large and black flying foxes) are a consequence of their frugivorous diet. Other gene losses likely contributed to metabolic adaptations and their ability to efficiently excrete excess dietary water while preserving electrolytes.

Convergent gene losses Our systematic gene loss data also provides an opportunity to search for convergent gene losses that are linked to convergent phenotypes [1]. By adopting our Forward Genomics framework, we discovered that pangolins and armadillos, two mammals that possess body armor in the form of scales, have lost *DDB2*, a key gene required to repair DNA damage caused by UV light. This suggests that their body armor, which covers the entire sun-exposed, dorsal skin, protects sufficiently well from UV light-induced DNA damage that both lineages were permitted to lose this otherwise essential gene. Furthermore, we discovered that cetaceans and manatees have lost *MMP12*, a lung-expressed protease that is able to degrade insoluble elastin fibers. Both cetaceans and manatees exhibit a unique breathing adaptation called explosive exhalation that allows these fully-aquatic mammals to renew 90% of the air in a single breath. Since explosive exhalation requires extensive elastic tissue in the lung, the loss of the elastin-degrading *MMP12* likely contributed to the evolution of this breathing adaptation. Finally, we used this Forward Genomics strategy to discover gene losses that preferentially occurred in strict herbivorous or strict carnivorous mammals, which illuminated metabolic and physiological changes in these mammals [5].

Gene loss and the evolutionary history of traits Apart from linking phenotype to genotype, gene losses can also reveal important insights into evolutionary history. A prime example is the evolution of testicular descent, the developmental process that determines the final position of testes, which occurs in all placental mammals but is absent in several afrotherian species. Due to phylogenetic discrepancies at the root of placental mammals, it was unclear whether afrotherians lost testicular descent or whether other mammalian lineages independently gained descent. We discovered that afrotherians possess remnants of genes that are required for testicular descent [6]. These 'molecular vestiges' show that testicular descent was already present in the placental mammal ancestor and was subsequently lost in afrotherians. This resolves the controversially-discussed ancestry of this soft-tissue trait.

Another example is ketone body biosynthesis (ketogenesis), the metabolic process that makes energy stored in fatty acids available for the brain. It is assumed that ketogenesis was very important for brain size expansion in modern humans, as the brain of human newborns relies on ketone bodies as a major fuel. We found that *HMGCS2*, the key enzyme required for ketogenesis, is lost in three mammalian lineages, comprising dolphins and whales, elephants, and fruit bats [7].

Remarkably, several of these species have exceptionally large brains, and we could show that *HMGCS2* loss preceded brain size expansion in toothed whales and elephants (Figure 2). Thus, our work not only reveals unexpected flexibility in mammalian energy metabolism, but also shows that ketogenesis is not a universal precondition for the evolution of large mammalian brains.

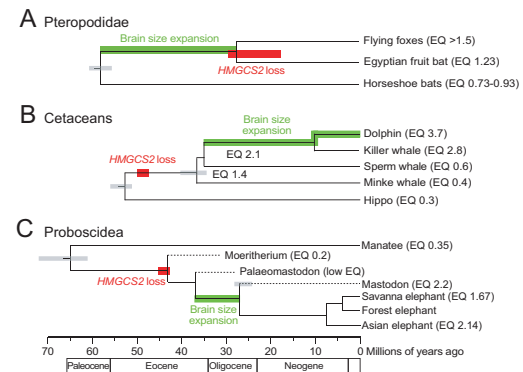


Figure 2: *HMGCS2* loss and brain size evolution. (A) In pteropodid bats, molecular dating estimates that the loss of *HMGCS2* likely happened after brain size expansion in this lineage. Brain size expansion is measured as an increase in the encephalization quotient (EQ > 1 indicates brains larger than expected for the respective body size). (B) Molecular dating estimates that *HMGCS2* loss happened early on the cetacean branch. Thus, brain size expansion in dolphins occurred after the loss of ketogenesis. (C) In the elephant lineage, *HMGCS2* loss happened between 45 and 42 Mya, suggesting that the loss of ketogenesis precedes brain size expansion.

Summary In summary, our work revealed that gene loss is an important evolutionary mechanism that cannot only be a consequence of adaptations, but may also contribute to adaptive evolution. As molecular vestiges, gene losses can reveal important insights into the evolution of traits. Our systematic gene loss catalogs not only provided numerous links between phenotypic and genomic changes in mammals, but also revealed that pleiotropic genes can get lost under special circumstances [8] [9]. Furthermore, our gene loss catalogs highlight numerous mammals that are natural knockouts for genes implicated in human disease.

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2.23 Phenotype loss is associated with widespread divergence of the gene regulatory landscape in evolution

JULIANA ROSCITO, BJOERN LANGER, KATRIN SAMEITH, MICHAEL HILLER

Background Phenotypic diversity is most easily observable as differences in morphology. Morphology is established during development and requires the patterning of the embryo, which is controlled by pleiotropic developmental genes. Expression of these genes must be tightly regulated in a spatio-temporal manner, which is achieved by cis-regulatory elements that can be located far away of the promoter. In contrast to the pleiotropic genes they control, an individual cis-regulatory element is often modular and controls gene expression only in specific tissues.

The loss of a complex phenotype is one extreme case of morphological evolution. Upon phenotype loss, we expect a different evolutionary trajectory for the genetic information underlying this phenotype. While developmental genes should be maintained due to selection on those gene functions that are not related to the lost phenotype, modular cis-regulatory elements required only for this trait are expected to evolve neutrally, resulting in sequence and functional divergence. Thus, evolutionary theory predicts that phenotype loss should lead to the divergence of cis-regulatory elements that were once necessary for the development of this phenotype.

Loss of limbs in snakes is associated with widespread divergence of limb regulatory elements To test this prediction, we first focused on the complete loss of limbs in snakes and investigated the fate of the limb-related cis-regulatory landscape in this lineage. To detect sequence divergence that is specific to snakes, it is necessary to compare snake genomes to genomes of fully limbed reptiles. Given the sparsity of reptile genomes, we sequenced the genome of the fully limbed tegu lizard. We combined Illumina short read, PacBio long read, and optical mapping data to generate a high-quality assembly with a scaffold N50 value of 55.4 Mb and a contig N50 value of 521 Kb, making it the most contiguous and complete reptile assembly so far [1].

Using the tegu genome as reference, we created a multiple genome alignment of a total of 29 genomes. To study the evolution of cis-regulatory elements, we focused on the 164,422 CNEs in this alignment, since CNEs often overlap cis-regulatory elements. For each CNE, we computed a per-species sequence divergence value by determining the percent of bases that are identical between the CNE sequence and the reconstructed sequence of the amniote ancestor. We identified 5,439 CNEs that are highly and specifically diverged in snakes [2].

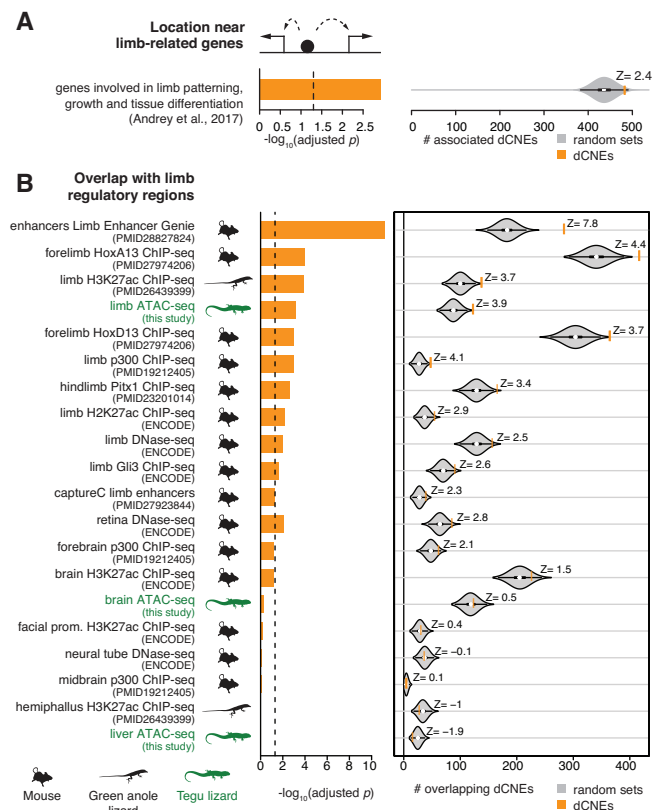


Figure 1: Characteristics of snake-diverged CNEs. (A) Snake-diverged CNEs are significantly associated with genes having limb-related functions. Left: Bars depict adjusted p-values derived by a one-sided Fishers exact test. Right: Observed (orange vertical bar) and expected number (grey violin plots, based on 10,000 random subsets sampled from all CNEs) of snake-diverged CNEs associated with genes in this set. The Z-score is indicated. (B) Snake-diverged CNEs significantly overlap regulatory elements active in embryonic limb tissue of tegu lizard, green anole lizard, and mouse. Orange bars correspond to limb regulatory datasets.

Using a computational enrichment analysis, we found that these 5,439 snake-diverged CNEs are significantly associated with limb-related genes (Figure 1A). To directly test if snake-diverged CNEs overlap cis-regulatory elements that are active during normal limb development, we obtained embryonic limb tissue of the tegu lizard and used ATAC-seq to identify regions of accessible chromatin. In comparison with the remaining non-diverged CNEs, we found a highly significant overlap between snake-diverged CNEs and limb-specific ATAC-seq peaks (Figure 1B). This is further corroborated by publicly available limb regulatory datasets. In contrast, we found no significant overlap with snake-diverged CNEs and ATAC-seq data from non-limb tissues (Figure 1B). By intersecting snake-diverged CNEs that overlap limb regu-

latory elements with the regulatory network that controls normal limb development, we found that most developmental genes are associated with such diverged limb enhancers. Together, this suggests that snake-specific divergence in many limb regulatory elements may have contributed to the loss of limbs in this lineage.

Associating transcription factor binding site (TFBS) divergence with phenotypic differences Since plain nucleotide divergence is suboptimal to capture differences in regulatory elements (Figure 2A,B), we developed two new approaches that are able to detect both the regulators (TFforge) and the regulatory elements (REforge) that are associated with a given phenotypic change [3] [4]. Both approaches rely on a common framework that uses ancestral sequence reconstruction and quantify differences in TFBS using Stubb [5] along every branch in the phylogeny (Figure 2C).

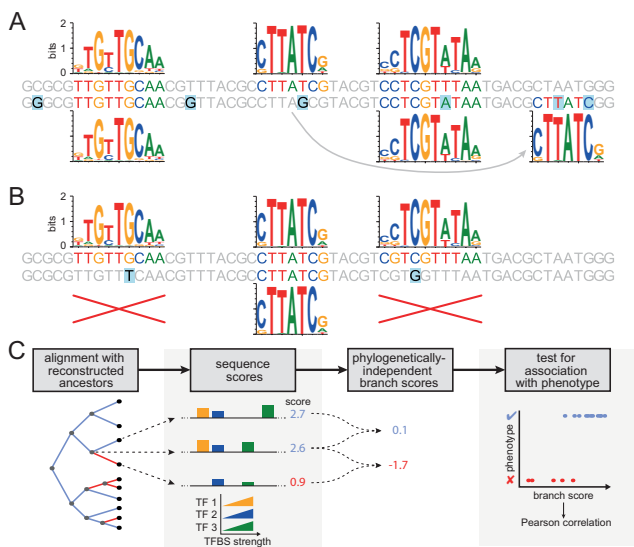


Figure 2: REforge incorporates knowledge about TFBS to associate divergence in cis-regulatory elements with phenotypic differences. (A) Illustration of multiple sequence changes (blue background) that largely preserve the TFBS ensemble of two sequences. The mutations are either located outside of binding sites, preserve the motif or result in TFBS turnover (grey arrow). (B) Illustration of just two sequence changes that destroy TFBS and thus are more likely to result in functional divergence. (C) Overview of REforge. For each node in the phylogenetic tree, REforge computes sequence scores that reflect the collective binding affinity of the given TF set. Branch scores, which are computed as the difference between the sequence scores, reflect TFBS changes. Finally, REforge tests if the branch scores of trait-loss branches (red) are lower than the branch scores of trait-preserving branches (blue).

We applied these approaches to detect CNEs that are associated with another complex phenotype, the degeneration of eyes in subterranean mammals. Of 351,279 CNEs, we detected preferential TFBS divergence in subterranean mammals for 3,711 (1.06%) CNEs. Using functional genomics data, we found that

these CNEs are significantly enriched in regulatory elements that are specifically active in mouse eye tissues (Figure 3). In contrast to REforge, the top-ranked 3,711 CNEs identified with standard Forward Genomics are not significantly enriched in eye-regulatory datasets (Figure 3), showing that REforge outperforms standard Forward Genomics and has a higher power to detect functional divergence in regulatory elements. Thus, our genome-wide screen detects widespread divergence of eye-regulatory elements and highlights regulatory regions that likely contributed to eye degeneration in subterranean mammals.

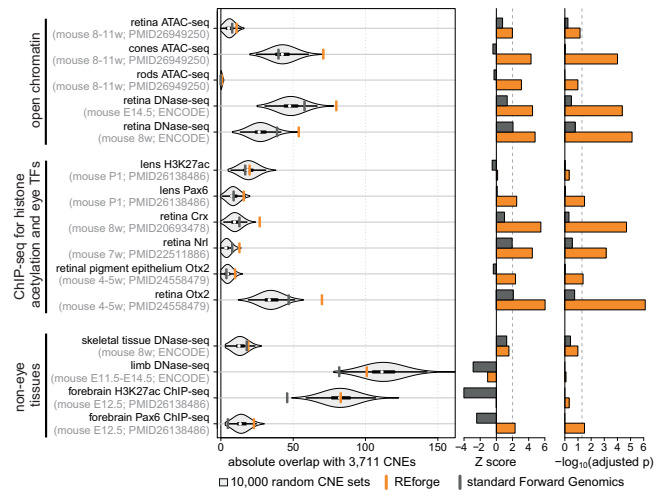


Figure 3: CNEs with TFBS diverged in subterranean mammals significantly overlap eye-related regulatory datasets. Left: Orange and grey vertical bars compare the observed overlap of the 3,711 top-ranked CNEs identified with REforge and standard Forward Genomics, respectively with functional genomics data. The expected overlap was determined by randomly sampling 3,711 CNEs from all CNEs and plotting the overlap of 10,000 such subsets as grey violin plots. Middle: Z-scores measure the number of standard deviations that the observed overlap is above the random expectation. Right: Adjusted p-values obtained with a one-sided Fishers exact test.

Summary Together, our genome-wide screens not only show that it is feasible to identify cis-regulatory elements whose divergence contributes to morphological change, but also reveal that genome-wide decay of the phenotype-specific cis-regulatory landscape is a hallmark of lost morphological traits. More generally, the combination of functional and comparative genomics has broad applicability to detect regulatory elements that are involved in many other morphological differences, and thus will help to uncover the genomic basis of nature's great morphological diversity.

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2.24 Extreme value analysis on a massive parallel scale

PHILIPP MÜLLER AND HOLGER KANTZ

Motivation It is well established that the Earth's climate is changing and that the global mean surface temperature is increasing. Most studies, data and model-based, focus on changes of temporal and spatial averages. It would be more than careless to not also investigate the evolution of the tails of distributions. After all, it is the extreme events, like massive rainfall, heat waves, or snow storms, causing the most harm to society. We therefore examine the temporal evolution of the extreme events in temperature and precipitation by a methodology, which is called Extreme Value Analysis (EVA), more precisely, we perform non-stationary EVA on large data sets to search for temporal and geographical patterns in extreme weather events [1].

Introduction to Extreme Value Theory In extreme value analysis (EVA) a time series X , which is assumed to be stationarity and short-range correlated, is compressed into a set of block maxima. These are the maximal values inside each block of N successive data points, obtained after a segmentation of the time series. In the limit of $N \rightarrow \infty$ and under appropriate normalization the distribution of the block maxima will converge to a member of a family of non-degenerated limit distributions.

These cumulative **generalized extreme value (GEV) distributions** contain three parameters,

$$G(z) = \exp \left\{ - \left[1 + \xi \left(\frac{z - \mu}{\sigma} \right) \right]^{-\frac{1}{\xi}} \right\}, \xi \neq 0 \quad (1)$$

called location μ , scale σ , and shape ξ . The latter one determines the sub-classes with the Fréchet distribution for $\xi > 0$, the Weibull distribution for $\xi < 0$, and the Gumbel distribution for $\xi = 0$.

Using the parameters of the GEV distribution we can make reliable estimates of the high quantiles of X and their fitting errors by calculating the **return levels** z_p

$$z_p = \mu - \frac{\sigma}{\xi} \left[1 - \{-\log(1-p)\}^{-\xi} \right], \xi \neq 0. \quad (2)$$

If the block length is one year, then the return level $z_{0.01}$, for example, $p = 0.01$, denotes the magnitude of an event, which occurs on average just once every 100 years. The parameters themselves are usually obtained using the well-established maximum likelihood (ML) approach [2, 3], which tries to minimize the negative

log-likelihood l ,

$$l(z; \mu, \sigma, \xi) = n \cdot \log \sigma + \sum_{i=1}^n \left[1 + \xi \left(\frac{z_i - \mu}{\sigma} \right) \right]^{-\frac{1}{\xi}} + \left(1 + \frac{1}{\xi} \right) \sum_{i=1}^n \log \left[1 + \xi \left(\frac{z_i - \mu}{\sigma} \right) \right], \quad (3)$$

with n being the number of block maxima and $\xi \neq 0$. For a gentle introduction into the extreme value theory and a treatment of its second flavor, the generalized Pareto distribution, please see [4].

Problems of the Estimation Routines Since Eq.(3) is nonlinear in the fit parameters, its optimization requires sophisticated algorithms. It turned out that all well-established specialized software packages, which are available, have some problems. Our goal is to perform a large scale analysis on 10^5 data sets representing grid points covering our globe. However, using available programs, about one fit in a hundred did fail. Some failures might be fixed by a manual choice of initial conditions, which is impossible in an automated analysis. The problem turned out to be indeed a conceptual one. The negative log-likelihoods of the GEV, Eq.(3) contain several logarithms and thus give rise to a region in parameter space inaccessible to the algorithm, in dependence of the values z_i . This itself would not spoil the optimization yet, but, unfortunately, the boundary to this forbidden region features a steep slope towards smaller values before hitting the undefined domain. This causes the algorithm to occasionally get trapped and to not reach the global minimum of the negative log-likelihood. Either this boundary effect or the initialization of a parameter combination inside the forbidden region, apart from unrelated bugs, caused the software packages to sometimes return numerical artifacts or throw an error.

Improving the Estimation To solve this numerical issues of the EVA, we introduced the nonlinear constrained optimization using the augmented Lagrangian method [5]. We provide an implementation of the fixed optimization routines via the software package **climex**, which was written in the statistical programming language R and published under GPL-3 license [6].

Application of the EVA Our scientific interest lies in the analysis of potential temporal changes of extreme weather events as they are claimed to occur in the context of climate change. We report here on EVA performed on the daily maximum temperature of the **ERA-Interim** reanalysis data set [7]. This data set is generated by assimilating all weather data from the

globe into a state-of-the-art weather model, over 39 years. This yields daily values of all relevant weather variables on 115680 grid points covering Earth.

To detect changes, the time series of annual maxima of each grid point was split into two overlapping time windows, 1979 till 2003 and 1993 till 2017. For each of the two sets of 25 maxima, we performed an ML fit of the GEV distribution. Due to the climate change a general shift of temperature towards higher values and thus more hot extremes is expected. Indeed, we found a general increase of the location parameters of the GEV distributions, which can be thought of as the mean event size. But the overall changes are far more complex and depend on the geographical location, as the location parameter is increasing almost exclusively on land and decreasing over large parts of the sea.

The change in the return levels, however, is even more complex and depends on the specific quantiles as well, which is quite unexpected. For, e.g., the 10 year return levels (see figure 1) a decrease was found in most parts of the globe. On the other hand, especially the Middle East, southern Europe, South America, East Asia, and the Arctic region feature a increase in the extremely hot temperatures.

ERA-Interim data are not true observations, but instead

state vectors of a weather model, which are tuned to be optimally compatible with the corresponding observations. In order to understand how this processing affects extreme values, we compared results obtained from ERA-Interim gridded data to those obtained from nearby station data within Germany. We found surprisingly weak correlations between the two data sets for the return levels and their changes.

Summary The change of the climate system is far from a simple shift towards higher temperatures or precipitation values. To access the fairly complex changes in the tails of the asymmetric temperature distribution, large sets of data are necessary, which can only be analyzed using an improved version of the commonly used ML fit of the GEV or GP distribution. With **climex** we designed an implementation, which seems to solve all problems.

Our analysis of huge data sets, which are supposed to represent climate change, shows clear limitations of the EVA approach, being reflected in counter-intuitive results. We suspect that the strength of EVA is commonly overestimated since in practice does have long range correlations, the block lengths are too short to be in the asymptotic regime, and the number of maxima is insufficient for accurate fits of the GEV parameters.

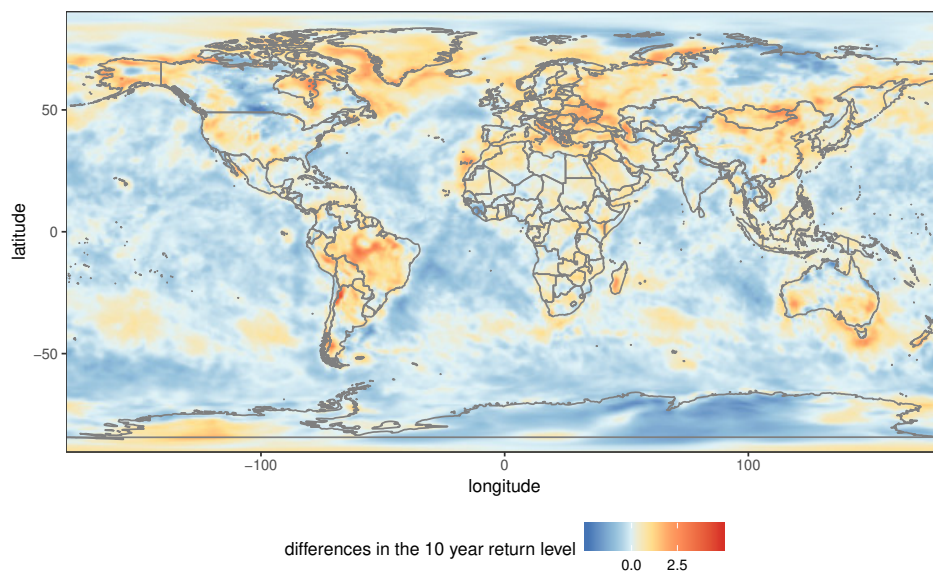


Figure 1: EVA of the ERA-Interim daily maximum temperatures in two overlapping time windows of 25 years. The 10 year return levels were calculated for each series and difference between the recent and former time window displayed to visualize their temporal evolution.

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2.25 Root causes of anomalous diffusion in a deterministic model

PHILIPP MEYER, KEVIN E. BASSLER AND HOLGER KANTZ

Anomalous diffusion Anomalous statistical behaviour, violating the law of large numbers and the central limit theorem, was observed in many real world systems. Several methods for its detection are in use, among them detrended fluctuation analysis DFA [4], developed in the nineties. These methods introduce different measures for anomalous statistics that are not necessarily equivalent. Previously, a framework for distinguishing root causes of anomalous behaviour has been introduced [5], which offers an intuitive way of understanding their features. Since well understood model systems are exclusively inherently stochastic processes with designed properties, it is astounding that a 1-dimensional deterministic map in dependence on some control parameter exhibits the full range of root causes for anomalous scaling, as we will show here.

Normal diffusion processes X_t exhibit scaling of its distribution at time t , $P(X_t)$ in time

$$P(X_t) = t^{-H} P^*(X_t/t^H), \quad (1)$$

where $H = 1/2$ is the so called Hurst exponent and P^* is the scaling function. If $H \neq 1/2$ the statistics of the process is called anomalous. There exist many stochastic processes, like fractional Brownian motion or continuous time random walks, that generate dynamics of the type described in Eq (1) with $H \neq 1/2$. However, it is till today unknown, how a real world system which is assumed to be deterministic without explicit time dependence can exhibit the same behaviour. One dynamical origin is intermittency as described by the Pomeau-Manneville (PM) map.

An aging deterministic system The PM map is a popular model for anomalous statistical behaviour. Despite being 1-dimensional on the interval $[-1,1]$, deterministic and without explicit time dependence, this map has been linked to intermittency and aging [6]. Its potential relevance for real systems was shown in [1], where we constructed a continuous time version of the system, that shares essential properties, as a nonlinear oscillator with periodic driving. The symmetric version of the map reads as follows

$$\delta_{t+1} = \begin{cases} -4\delta_t + 3 & \text{if } 0.5 < \delta_t \leq 1.0 \\ \delta_t \left(1 + |2\delta_t|^{z-1}\right) & \text{if } |\delta_t| \leq 0.5 \\ -4\delta_t - 3 & \text{if } -1 \leq \delta_t < -0.5 \end{cases}. \quad (2)$$

Summing up increments produced by this map for $z > 2$,

$$X_t = \sum_{s=0}^{t-1} \delta_s; \quad X_0 = 0, \quad (3)$$

leads to anomalous diffusion for the process X [2].

The reason is that the mean waiting time, i.e. the time the intermittent dynamics spends close to zero, is infinite for $z > 2$. So the probability for a trajectory to be close to zero, starting at a randomly chosen point, grows with time. Actually, the time dependence of the distribution of the variable δ can be made explicit by the following transformation,

$$|\delta| = \gamma ((z-1)t)^{\frac{1}{1-z}} / 2, \quad (4)$$

where γ then is a random variable with a stationary probability distribution [7] $P(\gamma) \propto 1/(1+\gamma^{z-1})$, shown in figure 1. The system can alternatively be described by an infinite invariant density [8]

$$P(|\delta_t|) \sim t^{\frac{2-z}{z-1}} P_{\text{inf}}(|\delta|) \quad (5)$$

for $|\delta_t|$ not close to zero. Here $P(|\delta_t|)$ is the physical density, which has to be normalizable. Therefore, it is truncated for small values of δ . For longer aging times t , the location of the cutoff of the density moves closer and closer towards zero. Thus, the infinite invariant density $P_{\text{inf}}(|\delta|) \propto |\delta|^{1-z}$ in the limit of large t has a well defined power law shape, but is not integrable.

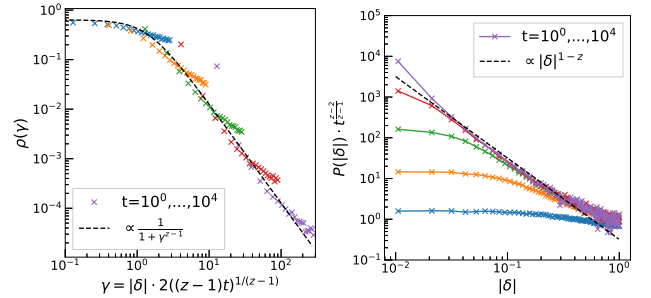


Figure 1: Left: Stationary distribution of the rescaled variable γ . Right: the convergence to the infinite density P_{inf} from Eq.(5).

Joseph, Noah and Moses effects The premises of the central limit theorem can be violated in three ways. There exist robust measures for all three effects [5]. The Joseph exponent J quantifies the increment correlations. If $J > 1/2$ the increments are positively long range correlated, as it is actually the case for fractional Brownian motion. J can be determined via R/S statistics or Detrended Fluctuation Analysis (DFA). The latent exponent L quantifies the effect of fat-tails in the increment distribution (Noah effect). When $L > 1/2$, the increment distribution has "fat tails", as it is the case for Levy flights. The Moses exponent M quantifies the effect of non-stationarity of the increment distributions. When $M > 1/2$ the increment distribution widens with time, and for $M < 1/2$ it shrinks with time, like, e.g., in

scaled Brownian motion. L and M can be calculated from the scaling of the ensemble average of the sum of the absolute value of δ and the ensemble average of the sum over δ^2

$$\begin{aligned} \left\langle \sum_{s=0}^{t-1} |\delta_s| \right\rangle &\sim t^{M+1/2}, \\ \left\langle \sum_{s=0}^{t-1} \delta_s^2 \right\rangle &\sim t^{2L+2M-1}. \end{aligned} \quad (6)$$

The relation of the exponents J , L and M with H is

$$H = J + L + M - 1. \quad (7)$$

If $H < 1/2$ the process is called sub-diffusive, and if $H > 1/2$ it is called super-diffusive.

Results For the PM map the left hand side of both equations (6) can be calculated using knowledge from infinite ergodic theory. The ensemble average of the absolute value $\langle |\delta| \rangle$ converges for $z < 3$ with respect to the infinite invariant density, whose time dependence is given in Eq. (5), as well as the ensemble average of the square $\langle \delta^2 \rangle$ for $z < 4$. For larger values of z in both equations rescaling according to Eq. (4) leads to an integrable distribution. So results for M and L are known analytically. Numerical calculations for both M and L along with J and H are shown in Fig. 2. H can be calculated analytically in the framework of stochastic renewal processes [2]. Comparing results from [3] and [2] we are able to identify the exponent J with the so called ensemble averaged time averaged mean squared displacement with is well known in the literature of anomalous diffusion

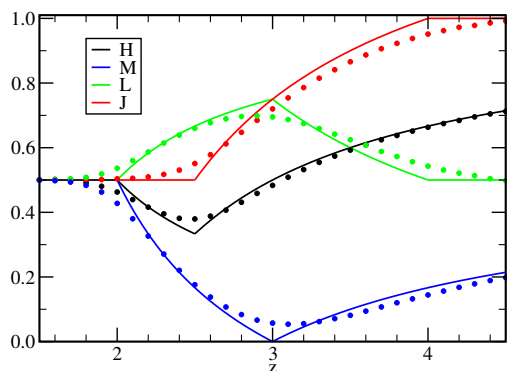


Figure 2: Theoretical and numerical results for all scaling exponents (L and M calculated replacing mean by median in Eq.(6)).

Figure 2 shows that theoretical solutions and numerical results align very well for long simulation times. For $z < 2$ diffusion is normal and nothing surprising happens. But for $z > 2$ there is a rich set of behaviors, subdiffusion as well as superdiffusion. How can this happen in a system whose increments are iterates

of a deterministic map from the interval $[-1, 1]$ onto itself? The Moses effect is probably the easiest to understand. For $2 < z$ the density is nonstationary and moves towards zero. However, since it has fat tails, the mean goes to zero more slowly than the density itself for $z < 3$. For larger values of z the distribution is steeper and the mean goes to zero with the same scaling as the distribution itself, hence the Moses effect is not as large any more. The Noah effect is a surprising feature since the increments are bounded. However the stationary rescaled distribution (4) has fat tails. For $z > 4$ the distribution still has power law tails but the power is small enough to have a finite variance. The Joseph effect in our system is also not trivial. The dynamics of two successive waiting periods can be considered independent. However, since the mean waiting time diverges, the correlation time still diverges for $z > 2.5$.

The Moses effect dominates for $2 < z < 2.5$, causing subdiffusion. For $z = 3$ it is balanced by the Noah effect and the Joseph effect. For larger values of z , the Joseph effect dominates, which yields superdiffusion.

Conclusion The Pomeau-Manneville map explains how anomalous statistical behaviour can occur in real world systems, which are deterministic, confined to a bounded phase space, and without explicit time dependence. We analyzed the root causes of anomalous diffusion for this 1-dimensional intermittent system. All three effects, long range correlations, non-stationarity, and fat tails in the probability distribution, are present in this model, in dependence of a control parameter.

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2.26 Wannier-Bloch approach to high harmonic generation in solids

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Introduction Recently, the techniques of attosecond science, traditionally applied to atoms and molecules in the gas phase, have been extended to the solid state. Emission of high-order harmonics from solids provides a new avenue in attosecond science. On the one hand, it allows to investigate fundamental processes of the non-linear response of electrons driven by a strong laser pulse in a periodic crystal lattice. On the other hand, it opens new paths toward efficient attosecond pulse generation, novel imaging of electronic wave functions, and enhancement of high-order harmonic generation (HHG) intensity. A key feature of HHG in a solid (as compared to the well-understood phenomena of HHG in an atomic gas) is the delocalization of the process, whereby an electron ionized from one site in the periodic lattice may recombine in any other (Fig. 1). The extent of this spatial delocalization, measured experimentally by ellipticity dependence [1-2], is believed to be important for attosecond pulse generation and imaging of the electronic wavefunction in solids.

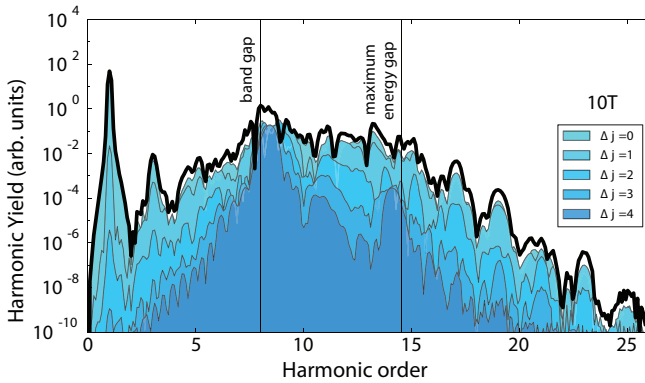


Figure 1: Schematic representation of the HHG in a periodic crystalline semiconductor via the Wannier-Bloch approach. Electron can be excited from the side j_0 in the valence band to the conduction band at the time t' . Then, the wavepacket (in blue) spreads in the conduction band and therefore may recombine with a different site in the valence band, $j_0 - 1, j_0 + 1, \dots$ at t . At the time of recombination, the excess energy is emitted as a high harmonics (violet oscillations) of the driving infrared field. On the right, the relative nearest-neighbor contributions to the HHG process for G-A orientation of ZnO.

Wannier-Bloch approach In collaboration with the group of Maciej Lewenstein at ICFO, we developed an analytic model, based on the localized Wannier wave functions in the valence band and delocalized Bloch functions in the conduction band [3]. This Wannier-Bloch approach assesses the contributions of individual lattice sites to the HHG process, and hence addresses

precisely the question of localization of harmonic emission in solids. Our mixed representation compares very well with the predictions of the Bloch-Bloch model, previously developed in Ref. [4], but provides additional information involving contributions of neighboring lattice sites to HHG (see Fig 1).

Results and Discussion We apply the Wannier-Bloch approach to investigate HHG in a ZnO crystal using mid-IR pulses for two different orientations, corresponding to wider and narrower valence and conduction bands, respectively. Interestingly, for narrower bands, the HHG process shows significant localization, similar to harmonic generation in atoms (see Fig. 1).

By using localized atomic sites in the valence band and delocalized functions in the conduction band, our model has the closest parallels to harmonic generation from atomic gas. As such, it allows one to access contributions of individual lattice sites, and hence assess the degree of localization of HHG in solids –something that has previously been inaccessible. In particular, we can describe a process in which an electron initially localized at the j' -th atom in the valence band has a certain probability to be excited to the conduction band, where it is accelerated to a high energy before recombining either to the parent atom, at j' -th site, or (with different probability) to any other j -th atom in the lattice.

Different displacements of the electron recombination atomic-sites, i.e. $\Delta j = |j - j'|$, give different contributions to the harmonic spectrum. This can be seen in Fig. 1. In particular, the main contribution was found to be given by $\Delta j = 0$, or electron recombining at the same atomic site it was excited from. Especially for the case of narrow bands in the band structure, lower Δj contribute by far the most to the harmonic spectrum, signifying substantial localization in the HHG process. On the other hand, we found enhanced contribution of high Δj in case of wider valence and conduction bands. This enhanced delocalization is likely due to small effective masses of electrons in a lattice, which corresponds to a large band width. In all cases, distant neighbor contributions were highest near the band-gap energy. This suggests that harmonic yield near the band gap energy should decline less (relative to other harmonics) with increasing ellipticity of laser light, since elliptical polarization tends to suppress local contributions.

Note that our results by means of the Wannier-Bloch approach employ a different framework than those presented by the Bloch-Bloch model in ref. [3]. While our model recreates the conventional atomic picture, the Bloch-Bloch model is based on the electron-hole

pair recombination. Thereby, it is clear that both approaches, while predicting similar total HHG spectra, provide different insights into the physics of the HHG process.

The present approach is particularly suitable to model HHG from nanostructures such as achieved in recent experiments. We expect that the effects of localization are crucial for such experiments, considering the plasmonic hot spots and the spatial variation of the electric field on a nanometer scale. Hence, a proper understanding of the degree of HHG localization in condensed matter experiments will be particularly relevant to nano-structures, where nanostructure geome-

try may even be designed to suppress or enhance far neighbor contributions. In addition to affecting HHG efficiency and attosecond pulse generation, suppressing delocalized contributions will also have a big impact on electronic wave function imaging, as recently pointed out in ref. [2].

Conclusion Our results suggest that it should be possible to control the localization of the HHG process by varying experimental parameters. Hence, by quantifying site specific contributions, our work paves the way to controlling HHG efficiency and imaging of the electronic wave function in a crystal lattice.

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2.27 Time delay and electron localization in a molecule

J. VOS, L. CATTANEO, S. PATCHKOVSKII, T. ZIMMERMANN, C. CIRELLI, M. LUCCHINI, A. KHEIFETS, A. S. LANDSMAN, U. KELLER

Introduction Attosecond metrology has characterized the dynamics of fundamental processes in quantum mechanics such as the photoelectric effect in atoms. Streaking experiments and RABBITT (Reconstruction of Attosecond Beating By Interference of Two-photon Transitions) have provided information on the timing of the photoionization process, known as Wigner time, defined as the energy derivative of the scattering phase of the electron wave packet (EWP) receding in the field of the ion. As the Wigner time delay, by its nature, is referenced to a freely propagating electron, it retrieves a photoionization time delay determined by the target-specific parameters of the scattering center. At present, most photoionization time delay experiments have been performed on atomic targets.

The experimental and theoretical study of molecular photoionization time delays, on the other hand, remains challenging due to the complexity of these targets. The congestion of electronic states accessible in the ionization process leads to many contributing channels of the same final energy, resulting in a multiplexed photoelectron (PE) spectrum. Additionally, molecules present a bond-length dependent spatial distribution of electron density in combination with a highly anisotropic potential landscape. Recently it has been shown that atomic photoionization time delays present an angular dependence and a more complex angular dependence is expected for molecules due to the lower degree of symmetry. This raises new questions about the angular dependence of the photoionization time delays in molecules and localization of the ionizing electron within the molecule (1).

Up to now, such questions concerning molecular targets remained unanswered due to the relative paucity of molecular photoionization time delay measurements. Extending attosecond metrology measurements to the molecular domain involves considerable experimental and theoretical challenges. Here we, in collaboration with the experimental group of Prof. Keller at ETH Zurich, showed that molecular attosecond measurements provide access not only to the orientation- and energy-dependent photoionization time delays, but also to the mean position of the ionization within the molecular potential of the diatomic carbon monoxide (CO) molecule. We thereby give a complete description of the molecular photoionization dynamics (2).

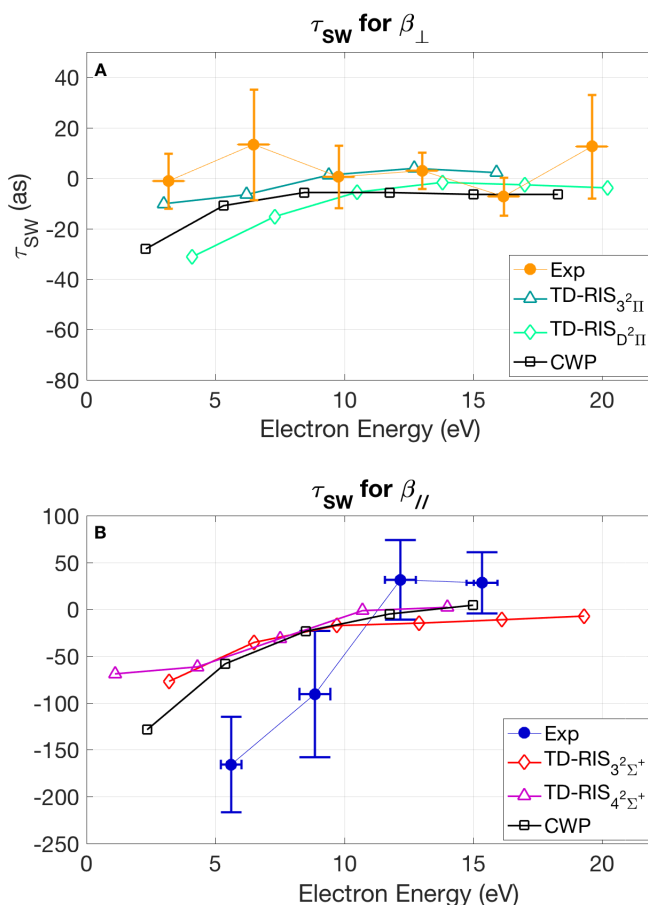


Figure 1: (A) Stereo Wigner time delay for molecules oriented perpendicular with respect to the laser field. (B) For parallel orientation, a highly negative stereo Wigner time delay is measured at low electron energies. A direct comparison between experiment and theory based on the Classical Wigner Propagation (CWP) method (squares) is possible as the stereo Wigner time delays are shown integrated over all contributing states. In contrast, state-resolved stereo Wigner time delays computed using the Time-Dependent Resolution in Ionic States (TD-RIS) are shown for dominant isolated states (diamonds and triangles).

Wigner time delay A quantity unique to molecular ionization processes, namely the stereo Wigner time delay (SWTD) presents a varying photoionization time delay depending on the location within the molecular frame from which the EWP escapes (3). Photoionization of the inner valence states of the CO molecule has been extensively studied in the past. In contrast to the isoelectronic, homonuclear N_2 molecule, the CO molecule is expected to show a stereo Wigner time delay caused by the asymmetry of the molecular nuclear constituents. This symmetry-breaking gives access to a complementary observable in addition to the traditional Wigner time delay, commonly extracted from

attosecond pump-probe experiments. Although the Wigner time gives access to electron photoionization delays specific to the molecular potential landscape, the self-referenced stereo Wigner time delay can be used to follow intramolecular photoionization dynamics on an attosecond timescale.

Results and Discussion To understand the highly varying SWTD for parallel orientation, we used two complementary, independent theoretical models. The first model, developed by S. Patchkovskii, is the Time Dependent Resolution in Ionic States (TD-RIS) method. It describes the ionization dynamics initiated by the XUV pulse in a fully quantum mechanical manner including the dynamics of electrons in the ion core. TD-RIS simulations do not account for the dynamics in the IR probe field and nuclear motion. The second model, the Classical Wigner Propagation (CWP) method is based on the approximate, classical propagation of the Wigner function of the photoelectron, including the IR-field (4). Combining the CWP method with the quantum nonadiabatic dissociation dynamics, we compute the contributions of specific states to each RABBITT sideband and thereby the photoionization time delays, which are directly comparable to the experimental results.

In the perpendicular orientation, both TD-RIS and CWP methods predict small SWTDs as is expected for symmetry reasons. Both theories compare well to the experimental values, which are close to zero within the error margin. To obtain further insight into the highly negative SWTDs measured in parallel orientation, we calculated the Wigner functions of the dipole matrix element of the Dyson orbitals for each ionization channel (see Figure 2), which we refer to as the source function. This source function provides a coordinate and momentum representation of the electron wave packet at the instance of birth. From Fig. 2 it is clear that a large (small) asymmetry of the source function translates into a large (small) SWTD. Because the source function is symmetric with respect to the sign of the initial photoelectron momentum, the time difference can originate from either an asymmetry in the initial localization or an asymmetry in the molecular potential experienced by the departing electron. The comparison between the SWTDs and the dipole moments of the

corresponding ionic states suggests that the asymmetry of the molecular potential is not a decisive contributor. The asymmetry of the source function with respect to position, on the other hand, correlates very well with the computed delays and seems to be the main factor determining the SWTD.

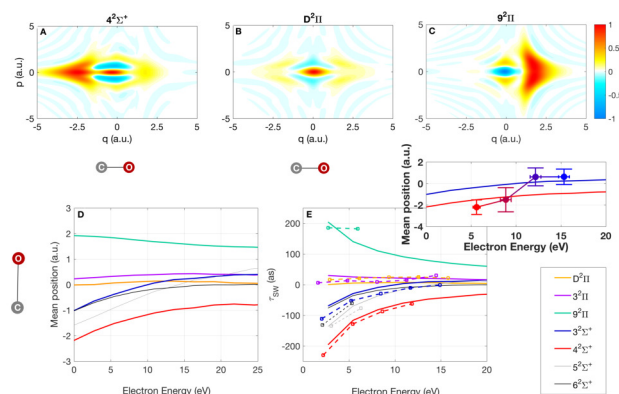


Figure 2: Stereo Wigner time delay and electron localization. (A-C) Coordinate and momentum representation of the escaping electron at the instance of birth (provided by the source function) for three representative electronic states. (D) and (E) show relationship between electron mean position at the instance of ionization and the Stereo Wigner time delay.

Conclusion To conclude, we find that electron localization at the time of ionization can be inferred from the stereo-Wigner time delay measurements. We show that the experimentally extracted mean position of the excited electron wave packet starts to the left of the carbon atom and quickly moves right towards the oxygen atom with increasing energy of the absorbed photon. The SWTD thereby serves as an additional source of information for molecular photoionization dynamics next to the commonly extracted Wigner time delay. In particular, in CO, the SWTD measurements allow for a straightforward extraction of the relative mean position of the ionizing electron at the moment of ionization as a function of electron energy. Therefore, measurements of the stereo Wigner time delay could complete the description of the photoelectric effect in molecules by adding sub-angstrom spatial-resolution to the existing attosecond temporal-resolution.

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2.28 Anyons in fractal dimensions

BIPLAB PAL, WEI WANG, ANNE E. B. NIELSEN

Introduction Elementary particles are all either bosons or fermions. Nevertheless, quasiparticles that appear in systems built out of interacting elementary particles can under certain conditions behave as anyons, i.e. as particles that are neither bosons, nor fermions. This observation is intriguing from a fundamental science point of view, and the properties of anyons also open up new possibilities for quantum technology. It is known that anyons can appear in two-dimensional systems, and they have been realized experimentally in the context of the fractional quantum Hall effect. They can also appear in one-dimensional systems, e.g. in the Haldane-Shastry model. Here, we demonstrate that anyons can exist in dimensions between one and two.

Fractals Structures with dimensions between one and two appear in nature in the form of fractals. Here we consider the Sierpinski Gasket (dimension $\log(3)/\log(2) \approx 1.585$) shown in figure 1, which is obtained by repeatedly making three copies of the triangle, scaling them, and stacking them into a new triangle. In practice, there is a limit to how many repetitions there can be, since the biggest and smallest length scales in our systems are limited. We are therefore interested in the physics happening at length scales that are large compared to the lattice spacing, and small compared to the complete fractal.

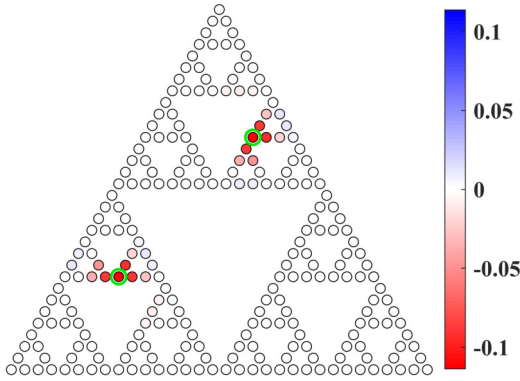


Figure 1: Two anyons in a Laughlin-like state with $q = 2$ on a fractal lattice. The lattice points are shown with circles, and the color of the i th lattice site shows $\langle \hat{n}_i \rangle_Q - \langle \hat{n}_i \rangle_0$ computed from Monte Carlo simulations. The centers w_k of the anyons are on the lattice sites marked by green rings. The number of particles is 30 for the state without anyons and 29 for the state with anyons.

Construction The fractional quantum Hall effect has been obtained in the boundary layer between two semiconductors, and the setup involves a strong magnetic field in the direction perpendicular to the plane. It is

therefore natural to consider a configuration, where the flux does not penetrate the full two-dimensional plane, but only the regions covered by the fractal. Specifically, we take the total flux through each lattice site in figure 1 to be $-\eta$.

Laughlin-like state The physics of the fractional quantum Hall effect is captured by families of trial states, such as the Laughlin states. To build a Laughlin-like state for the fractal lattice with $1/q$ particles per flux unit, we associate a vertex operator $V_{n_j}(z_j) = : e^{i(qn_j - \eta)\phi(z_j)/\sqrt{q}} :$ to each of the N lattice sites. Here $n_j \in \{0, 1\}$ is the number of particles on the j th site, and $\phi(z_j)$ is the field of a free, massless, chiral boson evaluated at the position z_j of the j th site written as a complex number. Correspondingly, we associate a vertex operator $W(w_k) = : e^{i\phi(w_k)/\sqrt{q}} :$ to each of the Q anyons at the positions w_k . We then construct [1] the Laughlin-like state $|\psi\rangle_Q \propto \sum_{n_1, \dots, n_N} \langle 0 | \prod_k W(w_k) \prod_j V_{n_j}(z_j) | 0 \rangle | n_1, \dots, n_N \rangle$, which evaluates to

$$|\psi\rangle_Q = \mathcal{C}^{-1} \sum_{n_1, \dots, n_N} \delta_n \prod_j e^{i\phi_j n_j} \prod_{i,j} (w_i - z_j)^{n_j} \times \prod_{i < j} (z_i - z_j)^{qn_i n_j - n_i \eta - n_j \eta} | n_1, \dots, n_N \rangle, \quad (1)$$

where \mathcal{C} is a real normalization constant, δ_n is unity if the number of particles is $\sum_j n_j = (N\eta - Q)/q$ and zero otherwise, and $\phi_j \in \mathbb{R}$ are unspecified single particle phase factors.

Quasiparticle properties For the two-dimensional case, we already know that (1) describes a Laughlin state with Q anyons [2]. The question is, whether the same is true for the fractal. Figure 1 shows $\langle \hat{n}_i \rangle_Q - \langle \hat{n}_i \rangle_0$, i.e. how much the presence of the anyons disturbs the average number of particles on each site. The disturbance is seen to be local, and the anyons are hence screened as in the normal Laughlin states. By summing over a small region around the anyons, one can see that there is on average 0.5 particle missing in each of the regions. This shows that the anyons have charge $1/2$ as expected for the Laughlin state with $q = 2$. When the anyons are screened and have charge $1/q$, one can use (1) to analytically compute the phase factor acquired by the wavefunction when one anyon is moved around another one [2], which is topologically equivalent to two exchanges. Subtracting the Aharonov-Bohm phase, the result is $e^{2\pi i/q}$. This confirms that the wavefunction indeed describes Laughlin type anyons.

We have checked that the size of the anyons is roughly independent of the number of repetitions, as long as

we scale the fractal such that the number of particles per area remains the same and the typical distance between particles is large compared to the lattice spacing and small compared to the total fractal.

Exact parent Hamiltonian So far we have shown that anyons can exist on fractals, but we would also like to know a Hamiltonian, which has (1) as its ground state. One can show [2] that $\Lambda_i|\psi\rangle_Q = 0$ as long as $\eta - Q/N < 1 + q/N$, where

$$\Lambda_i = \sum_{j(\neq i)} \frac{1}{z_i - z_j} [T_j^{-1} \hat{d}_j - T_i^{-1} \hat{d}_i (q \hat{n}_j - 1)], \quad (2)$$

$$T_k = e^{i\phi_k} e^{-i\pi(k-1)} \prod_i (w_i - z_k) \prod_j (z_j - z_k)^{1-\eta}, \quad (3)$$

\hat{d}_j is the particle annihilation operator on site j , and $\hat{n}_j = \hat{d}_j^\dagger \hat{d}_j$. It follows that $|\psi\rangle_Q$ is a ground state of the 3-body Hamiltonian $H = \sum_i \Lambda_i^\dagger \Lambda_i$, and we find numerically that the ground state is unique when the number of particles is fixed.

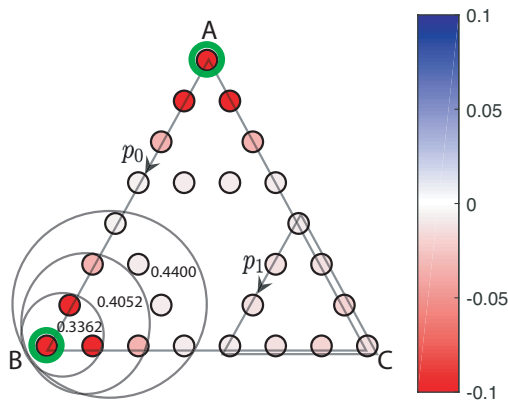


Figure 2: Anyons in the ground state of the fractal lattice flux Hamiltonian. The centers of the anyons are placed at the sites marked by green rings, and the color of the i th lattice site shows the difference between $\langle \hat{n}_i \rangle$ for the state with 4 particles and two trapping potentials and $\langle \hat{n}_i \rangle$ for the state with 5 particles and no trapping potentials. The numbers inside the large circles give how many particles are missing inside the circle compared to the case without anyons.

Fractal lattice flux Hamiltonian Instead of constructing a Laughlin-like state, one could use the idea of fluxes arranged in a fractal pattern to construct a Hamiltonian. The particles can hop between neighboring sites, and the phase factors of the hopping terms are the Aharonov-Bohm phases that a charged particle

would pick up for the given magnetic flux configuration when moving between the sites. An infinite on-site interaction imposes the constraint that there is at most one particle on each site. This Hamiltonian is better suited for implementation in ultracold atoms in optical lattices [3] than the one above.

Since we use exact diagonalization, we restrict our computations to the lattice with 27 sites in figure 2. We trap quasiparticles on the sites A and B by increasing the potential on these sites [4]. For the case of 4 particles, the anyons are almost separated. When summing over the 9 sites closest to an anyon, there is 0.44 particle missing, which is close to the expected value 0.5 for perfectly separated anyons. This is a first hint that the quasiparticles are indeed Laughlin anyons.

We now exchange the anyons twice by moving one anyon from B to C , one anyon from A to B , one anyon from C to A , and the same a second time. Anyons are moved by slowly decreasing the potential at one site and simultaneously increasing it on the neighboring site [4]. The acquired phase factor is $e^{2\pi i \cdot 0.35}$. We cannot subtract the Aharonov-Bohm phase directly, since the lattice is too small to compute it. We can only compute the Aharonov-Bohm phase for one anyon moving around the smaller path p_1 , while the other is fixed at A . Considering the system with 4 particles and only 1 anyon (and hence also a slightly different total flux), we estimate the ratio between the phase for the path p_0 and the phase for the path p_1 to be 4.25. Assuming that the same number applies for the case with 4 particles and two anyons, we get that the phase factor for the double exchange after subtracting the Aharonov-Bohm phase is $e^{2\pi i \cdot 0.40}$. If we exchange two quasiparticles with charge 0.44 twice, we would expect the phase factor to be $e^{2\pi i \cdot 0.39}$. This also suggests that the quasiparticles are indeed anyons, although a larger lattice would be needed to make an accurate test.

Conclusion and outlook We have shown by construction that it is possible to obtain fractional quantum Hall physics and anyons in systems with dimensions between 1 and 2. The fractal lattices differ from the two-dimensional systems in many ways, and it would be interesting to further investigate the consequences of these differences for the properties of the systems. We have also proposed a simpler fractal lattice flux Hamiltonian and provided first evidence that it realizes the sought states. As a next step, it would be interesting to propose an explicit scheme for implementing the physics in ultracold atoms in optical lattices.

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2.29 Quasielectrons in lattice fractional quantum Hall models

S. MANNA, J. WILDEBOER, I. GLASSER, I. D. RODRIGUEZ, A. E. B. NIELSEN

Introduction The fractional quantum Hall effect is one of the many fascinating phenomena that can appear in strongly correlated quantum many-body systems. The quasiparticles in the systems are neither bosons, nor fermions, but anyons. The effect was originally discovered in solid state materials, but at present there is also much interest in finding fractional quantum Hall physics in lattice systems. This is, in part, due to the aim of realizing the effect in ultracold atoms in optical lattices, which would open up new possibilities for detailed experimental investigations of the effect. Another motivation is that in lattices, one can replace the physical magnetic field with a much stronger artificial magnetic field. This gives the hope that it might be possible to realize the fractional quantum Hall effect at room temperature [1]. Finally, the presence of the lattice creates new features that are interesting to study by themselves.

The discovery of analytical trial wavefunctions, such as the Laughlin [2] and Moore-Read states [3], was a key element in developing the theoretical understanding of the fractional quantum Hall effect. It has turned out that Laughlin and Moore-Read states can be expressed as correlation functions in a conformal field theory [3], and the same construction can also be used to construct wavefunctions containing positively charged anyons (quasiholes). In experiments, one can create quasiholes by increasing the magnetic field slightly, and quasielectrons (negatively charged anyons) are correspondingly realized by decreasing the magnetic field slightly. Nevertheless, it has turned out to be much more challenging to construct trial wavefunctions containing quasielectrons theoretically. The problem is that a singularity appears in the wavefunction if one tries directly to construct the quasielectron as the inverse of a quasihole. Different types of quasielectron states have been proposed to overcome this problem (see e.g. [4, 5]). The states are, however, relatively complicated, and this makes it difficult to numerically investigate the properties of quasielectrons.

Here we show that the same problem does not appear in fractional quantum Hall states defined on lattices. This means that on lattices, the complexity of describing quasielectrons is the same as the complexity of describing quasiholes. We construct trial states for Laughlin and Moore-Read quasielectrons, and this allows us to study the size, shape, charge, and braiding properties of quasielectrons in great detail for relatively large system sizes. We also derive few-body Hamiltonians, which have the considered states as their exact ground states. Finally, we show that our results for the ana-

lytical wavefunctions are relevant for fractional Chern insulator models.

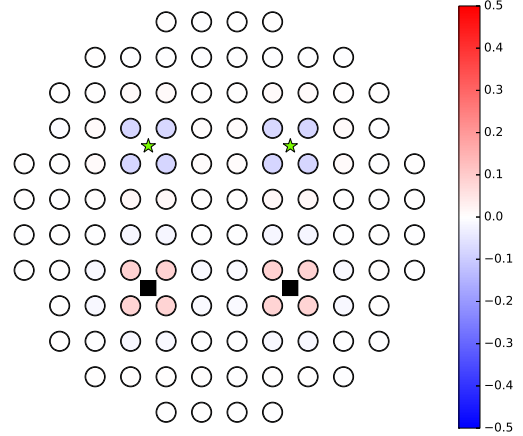


Figure 1: Two quasiholes (the centers are at the green stars) and two quasielectrons (the centers are at the black squares) in a Moore-Read state on a lattice. The color of the lattice sites shows $\langle \hat{n}_i \rangle_{\vec{p}} - \langle \hat{n}_i \rangle_{\vec{0}}$.

Quasielectron wavefunctions We will here discuss the Laughlin case [6] (the explicit form of the Moore-Read quasielectron states can be found in [7]). We start from a lattice consisting of N lattice sites at the positions z_j in the complex plane. On the j th lattice site there are $n_j \in \{0, 1\}$ particles. We have shown previously [8] that the state

$$|\psi\rangle_{\vec{p}} = \mathcal{C}^{-1} \sum_{n_1, \dots, n_N} \delta_n \prod_j e^{i\phi_j n_j} \prod_{i,j} (w_i - z_j)^{p_i n_j} \times \prod_{i < j} (z_i - z_j)^{q n_i n_j - n_i \eta - n_j \eta} |n_1, \dots, n_N\rangle \quad (1)$$

describes a Laughlin-like state on the lattice with $q \in \mathbb{N}$ fluxes per particle and Q quasiholes at the positions w_j . Here, \mathcal{C} is a real normalization constant, δ_n is unity if the number of particles is $\sum_j n_j = (N\eta - \sum_i p_i)/q$ and zero otherwise, $e^{i\phi_j n_j}$ (with $\phi_j \in \mathbb{R}$) are unspecified single particle phase factors, and η is a parameter that determines the lattice filling. In the following, we scale the lattice such that the area per lattice site is $2\pi\eta$, which corresponds to setting the magnetic length to unity. Finally $\vec{p} \equiv (p_1, p_2, \dots, p_Q)$ is a vector of positive integers p_k . Our claim is that if we choose some of the p_k to be negative integers, then (1) describes a state with quasielectrons at those positions.

Charge and braiding properties To confirm the claim, we need to show that the quasielectrons have the correct charge and braiding properties. As an

example, figure 1 shows quasiholes and quasielectrons in a Moore-Read state. This plot confirms that the quasielectrons are screened and have the correct charge $-1/4$. We also find that the Laughlin quasielectrons are screened and have the correct charge. Using these observations, it can be shown analytically [6] that the Laughlin quasielectrons have the correct braiding properties. For the Moore-Read states, we have confirmed the correct braiding properties using numerical computations (see [7] for details).

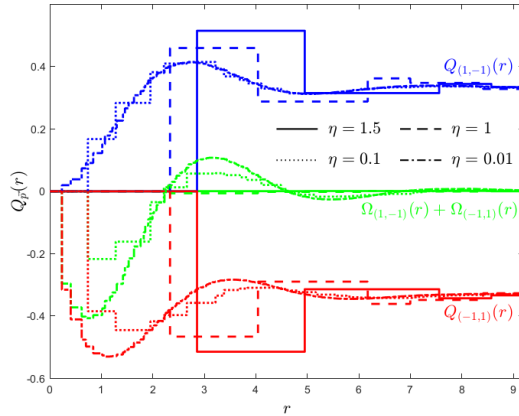


Figure 2: Excess charge (2) of a quasihole (blue curves) and a quasielectron (red curves) in a $q = 3$ Laughlin state on a kagome lattice, and the sum of the two (green curves). The lattice filling factor is $\eta/3$ (hence the curve for $\eta = 1.5$ is for a half filled lattice, while $\eta = 0.01$ has very low lattice filling and is close to the continuum).

Shape of the quasielectrons Figure 2 compares the shapes of quasiholes and quasielectrons for a $q = 3$ Laughlin state. The plot shows the excess charge

$$Q_{\vec{p}}(r) = - \sum_{\{i | |z_i - w_1| \leq r\}} (\langle \hat{n}_i \rangle_{\vec{p}} - \langle \hat{n}_i \rangle_{\vec{0}}) \quad (2)$$

within a circle of radius r centered at the center of the anyon. The excess charge approaches $\pm 1/3$ for large r . For a lattice filling of $1/2$, there is a perfect symmetry between the shapes of the quasiholes and the quasielectrons. When we approach the continuum by increasing the number of lattice sites, while keeping the number of particles fixed, the quasielectron continues to have the right charge and braiding properties, but the shape is no longer the same as for the quasihole.

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Parent Hamiltonians In addition to being able to construct the quasielectron wavefunctions, we would like to know Hamiltonians for which these states are ground states. Utilizing the analytical form of the states (1), it can be shown [6] that $\Lambda_i |\psi\rangle_{\vec{p}} = 0$, provided $\eta - \sum_i p_i/N < 1 + q/N$. Here,

$$\Lambda_i = \sum_{j(\neq i)} \frac{1}{z_i - z_j} [T_j^{-1} \hat{d}_j - T_i^{-1} \hat{d}_i (q \hat{n}_j - 1)], \quad (3)$$

$$T_k = e^{i\phi_k} e^{-i\pi(k-1)} \prod_i (w_i - z_k)^{p_i} \prod_j (z_j - z_k)^{1-\eta}, \quad (4)$$

\hat{d}_j is the particle annihilation operator on site j , and $\hat{n}_j = \hat{d}_j^\dagger \hat{d}_j$. It follows that (1) is a ground state of the 3-body Hamiltonian $H = \sum_i \Lambda_i^\dagger \Lambda_i$, and a numerical check shows that the ground state is unique, when the number of particles is fixed. Parent Hamiltonians for the Moore-Read quasielectron states are given in [7].

Comparison to fractional Chern insulator models

Fractional Chern insulators are another route to obtain fractional quantum Hall physics in lattices. For fractional Chern insulators, the ground states are normally not known analytically, and therefore only small system sizes can be considered. One may ask if there is a connection between the analytical states investigated above and fractional Chern insulators. We find that there is an overlap of 0.99 between the ground state of the model in [9] and the analytical Laughlin state on a 6×6 lattice with 3 particles, 1 quasihole, and 1 quasielectron. For the analytical Moore-Read states, the computed shape of the quasielectrons is similar to the shape of quasielectrons in the Kapit-Mueller model [10].

Conclusion We have found a simple way to construct analytical fractional quantum Hall quasielectron wavefunctions on lattices. The simplicity of the states has allowed us to make detailed investigations of the properties of the quasielectrons. We have derived exact parent Hamiltonians of the states and shown that the states are relevant for Chern insulator models. The insight obtained in this work may also lead to a way to remove the singularity in the continuum states.

2.30 Correlation and topology in 2D layered delafossites

SOTA KITAMURA, ROBERT-JAN SLAGER, ANDY MACKENZIE, RODERICH MOESSNER AND TAKASHI OKA

Replica spectrum in PdCrO₂ and the Kondo lattice model [2] PdCrO₂ is a member of the broad class of layered triangular lattice materials whose layer stacking sequence (see Fig. 1A) is that of the delafossite structural family ABO₂ [1].

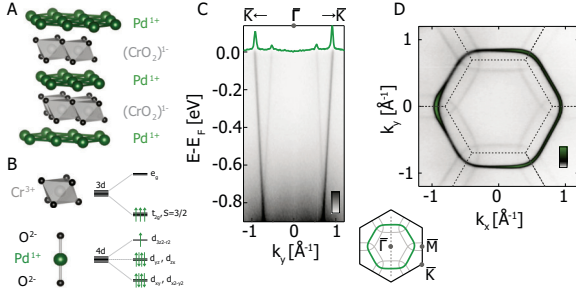


Figure 1: **Low-energy electronic structure of PdCrO₂** [2] (A) The layered crystal structure of PdCrO₂. (B) Pd layers are metallic, while the CrO₂ layers are Mott insulating and antiferromagnetically ordered below $T_N=37.5\text{K}$. (C) Dispersion measured by ARPES along the Γ -K direction (dashed line on the schematic of the crystallographic Brillouin zone) showing steep Pd-derived metallic bands, as well as replicas of these bands, apparently back-folded across the magnetic Brillouin zone boundary (dashed lines in D). The observed reconstructed spectral weight is approximately energy independent over nearly 1 eV, remaining clearly visible at the Fermi level, as evident in the momentum distribution curve (green line in C), and the measured Fermi surface.

PdCrO₂ is a high conductivity metal featuring broad conduction bands whose character is dominantly that of the A site cation Pd with the B-site Cr³⁺ cation in the Mott insulating configuration. PdCrO₂ can be considered as an atomic layer-by-layer superlattice of a nearly-free electron metal and a Mott insulator. An ARPES measurement revealed replicas of the metallic ‘main band’ shown in Fig. 1 C and D. Given the antiferromagnetic order of the Mott layer, this was at first sight, considered unremarkable. A simple ‘band folding’ picture due to the magnetic order does give replica bands. This standard picture, however, cannot explain the experimental observations. The spectral weight of the replicas observable by ARPES should fall off rapidly away from the new zone boundaries. Experimentally, however, the replicas are clearly observed all the way from the magnetic zone boundary to the Fermi level (Fig. 1C, D), an energy range approximately two orders of magnitude larger than the hybridisation gap scale of 10meV. Over the same energy range the simple ‘band folding’ model predicts a 100-fold decrease in spectral weight (dashed line in Fig. 2A), which would render the backfolded bands invisible to ARPES. In contrast, the measured intensity of the

reconstructed weight (I_{RW}) changes by less than a factor of 2 (points in Fig. 2A).

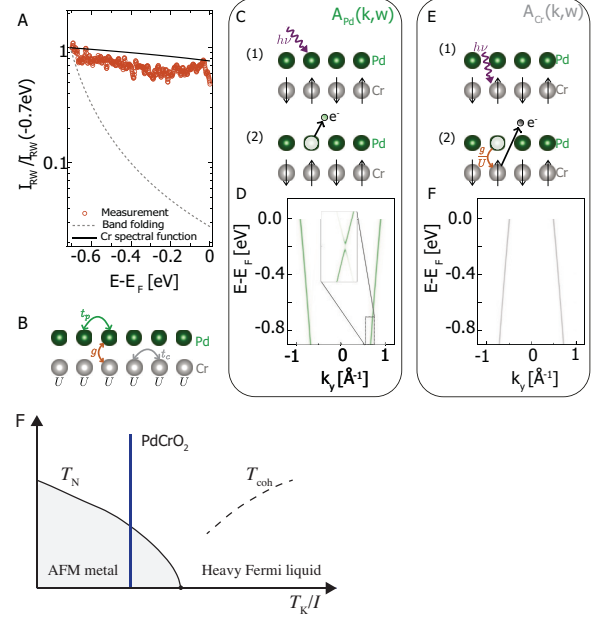


Figure 2: **Intertwined spin and charge response** [2] (A) Fits to the dispersion shown in Fig. 1C, showing that the reconstructed weight (I_{RW}) varies only weakly with binding energy. (B) The starting point of the theory is a Hamiltonian which includes hopping within (t_p , t_c) and between (g) the layers, as well as the on-site Coulomb repulsion on the Cr sites (U). (C) Schematic illustration of photoemission of Pd electrons. (D) The corresponding spectral function is equivalent to that predicted by the ‘band folding’ model. (E) Photoemission of a Cr electron can proceed via a virtual process involving tunnelling of the Cr hole to the Pd layer. (F) This results in a spectral function that is a convolution of the Pd spectrum and the spin correlation function of the Mott layer, thus appearing as a copy of the Pd spectral function shifted by the wavevector of the AF order, in agreement with the experiment (Fig. 1C). (F) Doniach’s phase diagram of the Kondo lattice (I : Heisenberg and RKKY interaction, T_K : Kondo temperature), reproduced from Ref. [3], with PdCrO₂’s approximate position marked.

In order to explain the origin of the replica bands, we performed a strong coupling expansion starting from a multi-layer Hubbard model capturing the layered metal-Mott structure (Fig. 2 B). The resulting low energy effective model is given by the Kondo lattice (+Heisenberg) model

$$H_{\text{eff}} = -t_p \sum_{ij\sigma} p_{i\sigma}^\dagger p_{j\sigma} + \frac{4t_c^2}{U} \sum_{ij} \vec{S}_i \cdot \vec{S}_j + \frac{4}{U} \sum_{ijk\sigma\sigma'} g_{ij} g_{kj} p_{i\sigma}^\dagger (\vec{S}_j \cdot \vec{\sigma}_{\sigma\sigma'}) p_{k\sigma'}, \quad (1)$$

where p denotes the metallic Pd electron and \vec{S}_i represents the localized spin on the Cr atoms. The ARPES spectrum predicted from this model in the magnetic phase for the metallic Pd-electrons are shown in Fig. 2 C and roughly coincides with that derived from the 'band folding' model. However, the spectrum of the Mott insulating Cr-electrons shows a distinctive feature: It become "spin-charge intertwined". That is, photo emission of Pd-electrons triggers a two step process Fig. 2 E (1)-(2); The hole created at the Cr site by the laser irradiation is quickly refilled by the Pd electron. This leaves a charge excitation (hole) in the metallic Pd layer and a spin excitation (magnon) in the Mott insulating Cr layer. The ARPES spectrum can be theoretically expressed as a convolution of the charge and spin dynamical correlation function.

The Kondo lattice model Eq.(1) is a well studied model in the field of strongly correlated electrons [3]. We believe that PdCrO₂ is an idealistic realization of this model, where the material sits in the Heisenberg or RKKY dominant regime of the general Doniach's phase diagram as shown in Fig. 2 F. It is currently unclear if the non-trivial heavy fermion behaviors that is captured by the Kondo lattice model can be observed in this material. The effect of the long range RKKY interaction mediated by the metallic Pd electrons which induces the three dimensional spin coupling is also an important problem to be studied in the future.

Spin Hall effect in PtCoO₂ and topology [4]

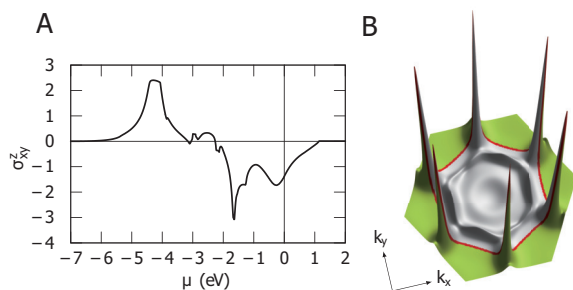


Figure 3: **Spin Hall effect.** (A) Spin Hall conductivity of PtCoO₂ per layer (in unit of the quantized value $e/2\pi$), as a function of chemical potential μ . (B) Momentum-resolved spin Hall conductivity of the band forming the Fermi surface. Red curve represent the Fermi surface.

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PtCoO₂ is another member of the delafossite family which is renowned for the lowest room temperature resistivity among all oxides, close to that of the top two materials Ag and Cu. In this material, the CoO₂ layer is a band insulator, in contrast to a CrO₂ layer which would be a Mott insulator. We theoretically predict a strong intrinsic spin Hall effect (Fig.3). This originates from six strongly-tilted Dirac cones that we find in the electronic structure near the Fermi surface, where a gap is opened by large spin-orbit coupling.

This is underpinned by rich topological properties; in particular, the phenomenology of a mirror Chern metal is realized not exactly, but very accurately, on account of an *approximate* crystalline symmetry. We expect that such 'vicinity topology' to be a feature of relevance well beyond this material. For example, a helical edge state with a small gap opening shows up in the spectrum (Fig. 4). In addition, our Wilson loop analysis indicates further elaborate features such as fragile topology.

Conclusion Our finds highlight the delafossite family to be promising materials to study the interplay between strong correlation, possible heavy fermion physics, magnetism and also topology.

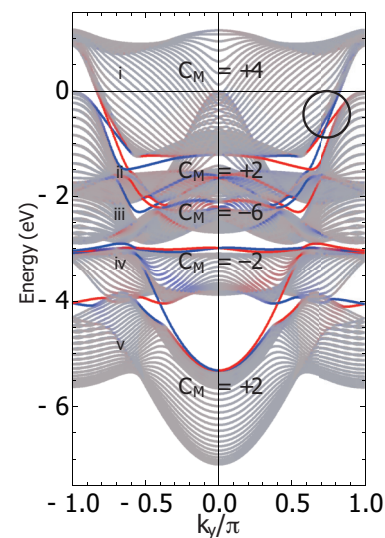


Figure 4: **Topological structure and helical edge state.** Band structure in a slab geometry where the bulk states are denoted by gray dots, and edge states by red and blue dots.

2.31 Floquet engineering of quantum materials

SOTA KITAMURA AND TAKASHI OKA

Floquet engineering How fast and drastically can we change properties of materials, and what would be the most efficient way to do this? One powerful tool is the concept of *Floquet engineering*, i.e., the control of quantum systems using time-periodic external fields. Theoretically, continuous irradiation of a laser can be modeled by a time periodic perturbation and the Hamiltonian $H(t)$ describing the irradiated system inherits the time periodicity

$$H(t + T) = H(t), \quad (1)$$

where the periodicity $T = 2\pi/\Omega$ is related to the photon energy or driving frequency Ω (we set $\hbar = 1$). During the past decades, with the help of the Floquet theo-

rem, the understanding of periodically driven systems has advanced considerably. It is possible to dynamically induce interesting exotic quantum states by carefully selecting the driving laser that matches the target material. While Floquet engineering is now applied in several fields of solid state physics (Fig. 1), most notably in band topology engineering, here we focus on its application in Mott insulators. Namely, by applying laser to an Mott insulator, it is possible to control its spin state [2] and if the field is stronger, a field induced insulator-to-metal transition takes place realizing exotic quantum properties [3].

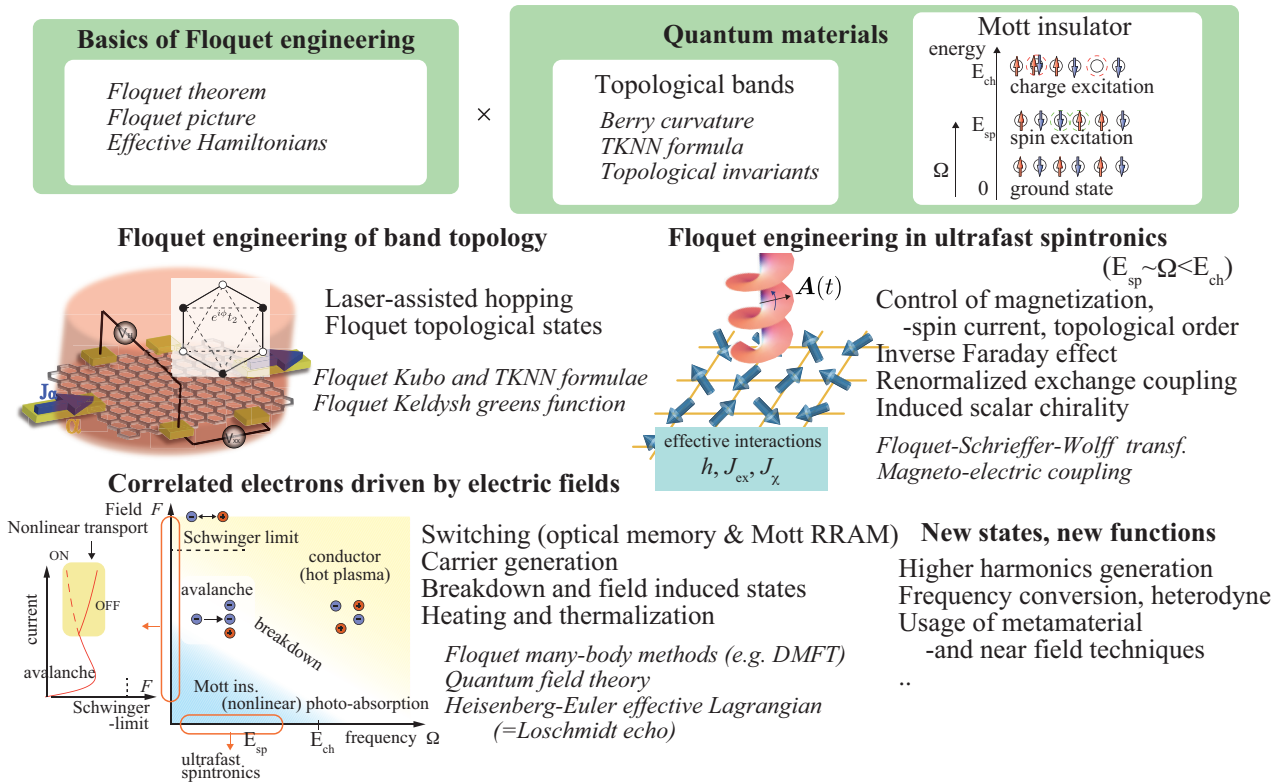


Figure 1: **Floquet engineering in quantum materials** [1] Various processes take place when an intense laser or electric field is applied to quantum materials with exotic properties such as topological bands, Dirac and Weyl semimetals and strong correlation.

Control and detection of spin chirality using laser [2]

Spintronics is a new branch of electronics where the spin degrees of freedom are used to carry and store information via spin currents and magnetization. In ultrafast spintronics, a laser is used to control spins and magnetism on the time scales of pico-seconds or

faster. An intriguing possibility is to induce an emergent interaction term that is absent in a static model by irradiating with a laser. This can be achieved by applying a field which breaks some symmetry of the original system. For instance, time-reversal symmetry is broken when circularly-polarized laser irradiation is applied. If we perform a Floquet-strong-coupling ex-

pansion to fourth-order in the Hubbard model at half-filling (Fig.2 A), the emergent term is the scalar spin chirality term $\chi_{ijk} = \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$, the lowest order term that breaks time reversal symmetry but preserves the SU(2) rotational symmetry. A classical spin configuration with a nonzero scalar chirality is shown in Fig.2 B for illustration. Upon irradiation, an effective scalar chirality term $\delta H_{\text{eff}} = \sum_{ijk} J_{\chi,ijk} \chi_{ijk}$ emerges [2]. This opens the intriguing possibility of Floquet engineering exotic quantum phases such as a chiral spin liquid phase. The light-induced interaction also has a potential application as a new probe: For the above example, the circularly-polarized laser acts as a conjugate field to the scalar spin chirality for general Mott insulators, in analogy with the magnetic field being conjugate to the spin. Namely, the coupling constant for the scalar chirality is reduced to be

$$J_{\chi,ijk} \sim \frac{2\mathcal{A}_{ijk}|t_{ij}|^2|t_{jk}|^2\Omega(7U^2 - 3\Omega^2)}{U^2(U^2 - \Omega^2)^3} i(\mathbf{E}^* \times \mathbf{E})_z, \quad (2)$$

in the leading order of the field amplitude, where \mathcal{A}_{ijk} is the area enclosed by sites i, j, k . The interaction term describes the modulation of the dielectric function proportional to the scalar chirality, when it is seen as a term in the Hamiltonian of the electromagnetic field. From Eq.(2), the modulation is obtained as an imaginary off-diagonal part leading to circular dichroism [2]

$$\begin{aligned} \epsilon_{xy}(\omega) & \\ &= i \sum_{ijk} \frac{4|t_{ij}|^2|t_{jk}|^2\omega(7U^2 - 3\omega^2)}{U^2(U^2 - \omega^2)^3} \mathcal{A}_{ijk} \langle (\hat{S}_i \hat{S}_j) \cdot \hat{S}_k \rangle. \end{aligned} \quad (3)$$

In other words, one can read out the presence of the scalar chirality via the circular dichroism. Fig.1 C shows the difference of the dielectric function between circularly polarized light with a different chirality.

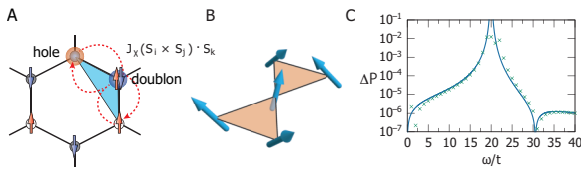


Figure 2: (A) Laser assisted virtual hopping process leading to the scalar spin chirality term. (B) Classical configuration of spins with nonzero scalar chirality, $(\hat{S}_i \times \hat{S}_j) \cdot \hat{S}_k$. (C) Circular dichroism: Difference of the induced electric polarization between left and right circularly-polarized lasers, as a function of the photon energy. Crosses are numerical results for a three-site Hubbard cluster, and the solid curve is obtained from Eq.(3).

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Current induced Mott semimetal [3] Mott insulators can host a surprisingly diverse set of quantum phenomena when their frozen electrons are perturbed by various stimuli. Superconductivity, metal-insulator transition, and colossal magnetoresistance induced by element substitution, pressure are prominent examples. In an experiment done in Maeno's group at Kyoto university, it was reported that strong diamagnetism in the Mott insulator calcium ruthenate (Ca_2RuO_4) is induced by dc electric current (Fig. 3 (A)). The application of a current density of merely 1 ampere per centimeter squared induces diamagnetism stronger than that any other non-superconducting materials. This change is coincident with changes in the transport properties as the system becomes semimetallic. Starting from the multi-orbital Hubbard model, we have developed a theory to explain the semimetallic state [3]. As the Mott gap close due to the current application, the upper and lower Hubbard bands shifts closer to the Fermi energy, forming bands reminiscent of those in indirect semiconductors. A state coined as a "Mott semimetal" is realized (Fig. 3 B) when the gap close, and when we calculate the diamagnetic response of this state, we found out that it becomes very large due to the lightness of the quasi-particles (Fig. 3 C).

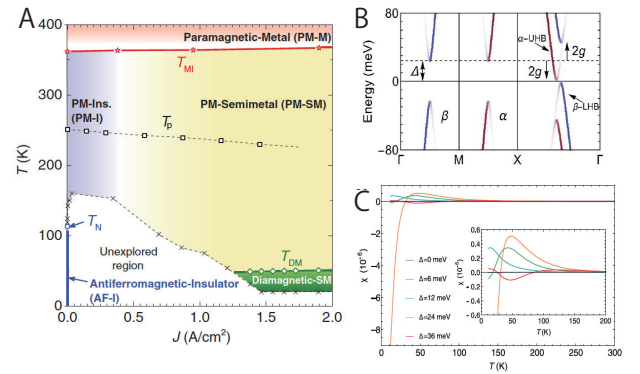


Figure 3: **Current induced Mott semimetal [1]** (A) Phase diagram of current induced states in Mott insulator Ca_2RuO_4 . (B) Single body spectrum of the proposed Mott semimetallic state. The bands consist of the coherent part of the upper and lower Hubbard bands. (C) Calculated diamagnetic response.

Conclusion These findings suggest that laser fields and dc current may be efficient means to control the magnetic and many-body properties of materials in the vicinity of a Mott transition.

2.32 Many-body systems of strongly interacting photons

JOHANNES LANG, DARRICK CHANG, FRANCESCO PIAZZA

Introduction. The possibility to implement interactions between photons in the quantum regime is recently attracting a lot of interest [1]. One reason is technological, as photon-photon interactions are essential for quantum information processing and would allow to build quantum networks exploiting the ability of photons to efficiently carry information over long distances. From a more fundamental, many-body perspective, an ensemble of strongly interacting photons shows crucial differences from any condensed-matter counterpart and is therefore likely to show novel collective phenomena which have no analog in conventional materials. The first such difference is that the photon number is never conserved so that repumping is needed to compensate losses and reach a driven-dissipative steady state, the latter thus generically being far away from thermal equilibrium. Furthermore, photons do not interact in vacuum and need a material to mediate their mutual interactions. The electromagnetic (EM) modes hybridize with the material giving rise to polaritonic excitations. Here we concentrate on materials made of uncharged but polarizable atoms, where the polaritons (and therefore the photons) inherit their interactions from the latter. This implies a second important feature, namely that the interaction between two photons is a higher order process, requiring the intermediate excitation of the atomic dipoles. The theoretical description of such a strongly-interacting, driven-dissipative system of photons in the many-body regime constitutes a challenging task. In particular, the large interaction cross sections prevent a perturbative treatment, the driven-dissipative nature does not allow to exploit fluctuation-dissipation relations and prevents for instance the application of Monte Carlo methods, while the long-range interactions additionally hinder an efficient employment of tensor network methods, even in one spatial dimension.

Non-equilibrium diagrammatic approach. We developed a non-equilibrium field-theoretical approach based on a systematic diagrammatic expansion for strongly interacting photons in optically dense atomic media. It is applicable when the characteristic photon-propagation range L_P is much larger than the inter-atomic spacing a and where the density of atomic excitations is low enough to neglect saturation effects. In the highly polarizable medium the photons experience nonlinearities through the interactions they inherit from the atoms. If the atom-atom interaction range L_E is also large compared to a , we show that the subclass of diagrams describing scattering processes with momentum transfer between photons is

suppressed by a factor a/L_E . The whole set of diagrams contributing to the photon Green's function (GF) up to order $1/L_P(1/L_E)$ is shown in Fig. 1 (for further detail we refer to [2]). We are then able to perform a self-consistent resummation of a specific (Hartree-like) diagram subclass and obtain quantitative results in the highly non-perturbative regime of large single-atom cooperativity. Here we find important, conceptually new collective phenomena emerging due to the dissipative nature of the interactions, which even give rise to novel phase transitions, as we discuss below.

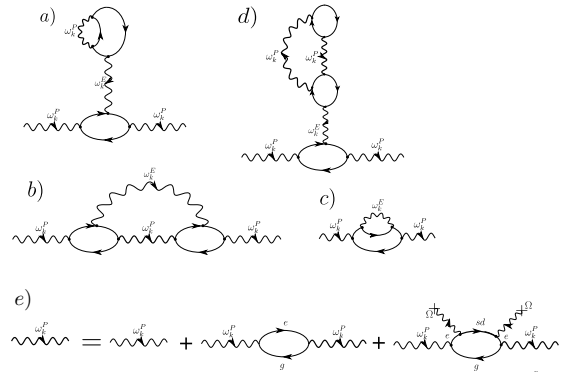


Figure 1: Feynman diagrams contributing to the photon Green's function (GF) up to order $1/L_P(1/L_E)$. Wiggled lines labelled by ω^P indicate the GF of the photon propagating through the atomic medium, while wiggled lines labelled by ω^E indicate the GF of the exchange particle mediating the interactions between the atoms. The atomic GFs (solid lines) are shown for the specific setup shown in Fig.2.

Application to atomic arrays near waveguides. We consider a periodic array of four-level atoms at fixed positions, as illustrated in Fig. 2. In such a configuration the propagating photons with dispersion $\omega_P(k)$, that are near-resonant with the $|g\rangle - |e\rangle$ transition, hybridize with atomic excitations to $|s\rangle$ which can lead to Electromagnetically-Induced Transparency (EIT) [3]. The latter happens through destructive interference between the $|g\rangle \rightarrow |e\rangle$ and $|g\rangle \rightarrow |e\rangle \rightarrow |s\rangle \rightarrow |e\rangle$ excitation pathways, which suppresses population of $|e\rangle$ and the associated spontaneous emission, leading to the photons propagating within a narrow frequency and momentum window. Diagrammatically, EIT is introduced by the interference between the last two diagrams of Fig.1e). The so called dark-state polaritons associated with this otherwise linear optical effect can be made to interact strongly by coupling $|s\rangle$ to a second excited state $|d\rangle$, via a second control field and via a separate photonic band with dispersion relation $\omega_E(k)$ and polarization orthogonal to the P -band. The interaction of the atoms with laser and guided photons is described

by the Hamiltonian

$$\hat{H}_{\text{int}} = \sum_z \left[\Omega e^{-i\omega_L^{(1)}t} \hat{a}_e^\dagger(z) \hat{a}_s(z) + \Omega_s e^{-i\omega_L^{(2)}t} \hat{a}_d^\dagger(z) \hat{a}_s(z) + \sum_{j=P,E} \int_k g_j \hat{a}_j(k) e^{ikz} u_k^j(z) \hat{a}_{\text{exc}(j)}^\dagger(z) \hat{a}_{\text{gs}(j)}(z) + h.c. \right]$$

with the notation $\text{gs}(P/E) = g/s$, $\text{exc}(P/E) = e/d$, and where \sum_z runs over the sites of the atomic lattice and $u_k^{P/E}(z)$ represents the periodic part of the Bloch functions of either polarization at quasi-momentum k . The incoherent dynamics is described by

$$\left(\sum_{j=e,d,z} \gamma_j \mathcal{D}[\hat{a}_j(z)] + L \int_k (\kappa_s \mathcal{P}[\hat{a}_P(k)] + \sum_{j=P,E} \kappa_j \mathcal{D}[\hat{a}_j(k)]) \right) \hat{\rho}$$

with the dissipator $\mathcal{D}[\hat{L}]\hat{\rho} = -(\{\hat{L}^\dagger \hat{L}, \hat{\rho}\} - 2\hat{L} \hat{\rho} \hat{L}^\dagger)/2$ describing the spontaneous decay of the excited atomic states plus the photon losses out of the guided modes, and the pump $\mathcal{P}[\hat{L}]\hat{\rho} = -(\{\hat{L} \hat{L}^\dagger + \hat{L}^\dagger \hat{L}, \hat{\rho}\} - 2\hat{L}^\dagger \hat{\rho} \hat{L} - 2\hat{L} \hat{\rho} \hat{L}^\dagger)/2$ homogeneously injecting P-photons into the waveguide.

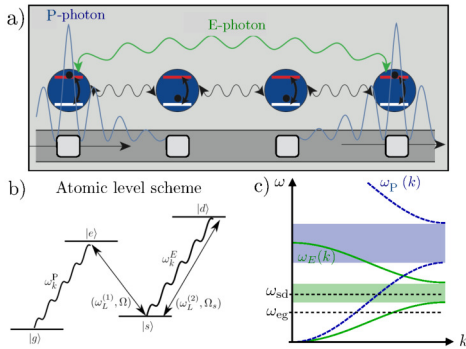


Figure 2: Setup considered for the application of the diagrammatic approach given in Fig.1.

Interaction-induced transparency. The steady-state phase diagram as a function of the P-photon pump κ_s and $s-d$ drive Ω_s is shown in Fig. 3a). We find two possible steady-state phases: i) an “opaque” phase characterized by a small atomic excitation density n_s and ii) a “transparent” phase exhibiting instead a much larger n_s . Those two phases are separated by a first order phase transition that includes a bistable region and terminates in a bi-critical point where the transition is continuous.

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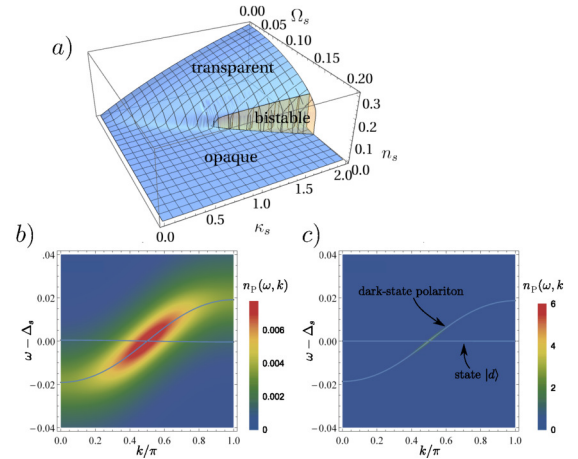


Figure 3: a) Steady-state phase diagram of the system. The distribution of the propagating-photon density is shown in the opaque b) and transparent c) phase.

More insight into the properties of the opaque and transparent phases are obtained by examining the frequency- and momentum-resolved occupation $n_P(\omega, k)$ shown in Fig. 3b),c). In the opaque phase (panel b)), the dark-state-polariton branch is essentially empty i.e. no sign of the EIT window is left. The latter is destroyed by coupling the metastable state $|s\rangle$ to the excited state $|d\rangle$, introducing an additional decay channel inherited by the dark-state polariton.

In the transparent phase (panel c)) on the other hand the intensity is concentrated within a very sharp region around a specific wavenumber k_{EIT} of the dark-state polariton branch. This means that in the phase transition the system has reconstructed the transparency window. We named this effect Interaction-Induced Transparency (IIT), as the transparency window is reconstructed via destructive interference, this time between the four different excitation pathways involving the state $|d\rangle$ and corresponding to four different diagrams of the class shown in Fig.1a) (see [4]). Other than in the non-interacting EIT, the interfering pathways here involve the E-photons i.e. interactions between polaritons, which renders IIT intrinsically nonlinear. In the lossy system this implies that IIT takes place through a first-order phase transition showing bistability. In the context of nonlinear quantum optics, IIT constitutes a novel, genuine quantum many-body effect. From the more fundamental perspective of many-body physics, the IIT phenomenon is a non-equilibrium phase transition in the driven-dissipative steady state which has no analogue so far in condensed matter, as it stems from the dissipative and retarded nature of the interactions between polaritons.

2.33 A novel, hybrid, topological quasi-particle in quantum light-matter systems

KIERAN FRASER, FRANCESCO PIAZZA

Introduction. Hybrid systems involving photons and neutral atomic gases have emerged as ideal platforms for nonlinear quantum optics [1], characterized by effective interactions between photons even at very low light intensities. In such systems the low-lying excitations are polaritons, which emerge as long-lived quasi-particles. In the usual scenario polaritons are a linear superposition of non-interacting photonic and atomic excitations, while the optical nonlinearities of the system are generated by the interactions between polaritons inherited from the atoms. In [2] we recently showed that a different situation can arise, where a new type of long-lived hybrid quasi-particle emerges. As we discuss below, this new quasi-particle is not simply a superposition of non-interacting atomic and photonic degrees of freedom, but rather an effect of the optical nonlinearities themselves. It is a composite made of an atom trapped inside optical soliton forming a topological defect in an emergent crystalline structure.

Setup and model. We considered a degenerate Fermi gas of N transversally-pumped neutral atoms interacting with the multimode radiation field of an optical waveguide in the configuration of Fig. 1. The internal atomic transition between the ground state manifold to the excited electronic state is driven by a pump laser of Rabi frequency Ω and frequency ω_L , and coupled with rate g_k with the waveguide's electromagnetic-field modes. The latter we separate into a series of running guided modes denoted by $\eta_k = e^{ikx}$. We work in the regime of large atomic detuning $\delta_A = \omega_L - \omega_A$ where the population of the excited state is negligible and spontaneous emission is suppressed, so that the excited atomic state can be adiabatically eliminated. Using the rotating-wave and dipole approximations the Hamiltonian in the frame rotating at the pump frequency reads $\hat{H} = \hat{H}_0 + \hat{H}_{int}$, with the free part $\hat{H}_0 = -\sum_k \delta_k \hat{a}_k^\dagger \hat{a}_k + \sum_{\sigma=\{\uparrow,\downarrow\}} \int dx \hat{\psi}_\sigma^\dagger(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2}\right) \hat{\psi}_\sigma(x)$, and the light-matter interaction being

$$\hat{H}_{int} = \sum_{\sigma=\{\uparrow,\downarrow\}} \int dx \hat{\psi}_\sigma^\dagger(x) \sum_k \frac{\lambda_k}{\sqrt{N}} \left(\eta_k^*(x) \hat{a}_k^\dagger + \text{h.c.} \right) \hat{\psi}_\sigma(x) \quad (1)$$

The spin degree of freedom for the fermions indexed by σ can be introduced using hyperfine levels within ground-state manifold. We assumed an external trapping potential which restricts the atomic motion to along the waveguide axis, x . We approximate the dispersion of the guided modes to be quadratic so that $\omega_k = \omega_0 + wk^2$. The detuning of the pump from the waveguide field mode of wavenumber k is denoted $\delta_k = \omega_L - \omega_k$. Since the dipole coupling g scales like

$1/\sqrt{L}$ with L the length of the waveguide, we define the coupling $\lambda_k = \Omega g_k \sqrt{N} / \Delta_A$ which is intensive in the thermodynamic limit $N, L \rightarrow \infty, N/L = n = \text{const.}$ The ground-state fermionic annihilation operator is labelled $\hat{\psi}$ and satisfies the relation $\{\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}')$. The bosonic annihilation operator for a photon in the waveguide mode k satisfies the relation $[\hat{a}_k, \hat{a}_{k'}^\dagger] = \delta_{k,k'}$.

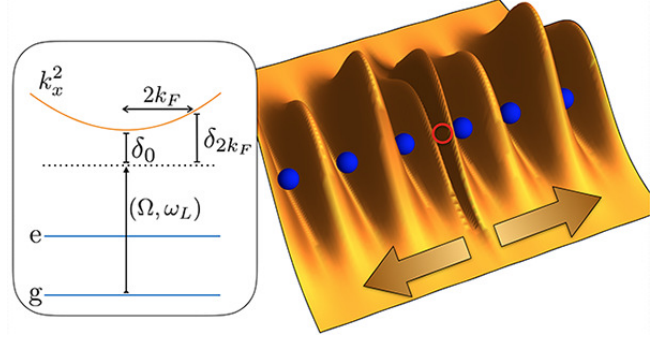


Figure 1: Pictorial representation of the system. A (quasi-) one-dimensional cloud of fermionic atoms (blue spheres) is transversally driven by a coherent laser and is coupled to a set of guided modes. The corresponding light intensity (including the homogeneous background) is shown as a dark-yellow surface with a transverse exponential damping indicating the guided nature of waveguide modes (arrows indicate the propagation direction of the guided modes). The situation shown corresponds to the presence of a light-matter defect at the center where an optical soliton traps an excess particle (red circle). The optical soliton connects two spatially ordered regions with different dimerization. The inset shows the atom internal level structure (spacings not to scale) together with the dispersion of the guided electromagnetic modes. The laser frequency is ω_L , its Rabi-frequency is denoted by Ω , and k_F is the Fermi momentum of the atomic cloud.

Low-energy theory. In order to compute the phase-diagram and low-lying excitations we derive an effective, low-energy theory for our system formulated within a path-integral formalism. We refer to [2] for further detail. We consider atomic degrees of freedom only in the vicinity of the Fermi surface, thereby linearizing the dispersion around $\pm k_F$. Correspondingly, the electromagnetic field has to be restricted to momentum components around $Q = \pm 2k_F$, i.e. those modes responsible for Umklapp scattering. With these restrictions the effective low-energy action becomes $S = S_a + S_{ph} + S_{a/ph}$, where:

$$\begin{aligned} S_a &= \int dx \int d\tau \sum_{\sigma=\uparrow,\downarrow} \Psi_\sigma^\dagger (\partial_\tau - iv_F \partial_x \sigma_3) \Psi_\sigma; \\ S_{ph} &= \int dx \int d\tau \Delta^* \left(\frac{\sqrt{n}}{2\lambda} \partial_\tau + \tilde{\delta}_{2k_F} \right) \Delta; \\ S_{a/ph} &= \int dx \int d\tau \sum_{\sigma=\uparrow,\downarrow} \Psi_\sigma^\dagger \sigma_1 \text{diag}(\Delta^*, \Delta) \Psi_\sigma \end{aligned} \quad (2)$$

are the atomic, photonic and interaction elements of the action, respectively and we have introduced the spinor $\Psi(x) = (u(x), v(x))^T$ with $u(v)$ denoting a fermionic right(left) mover: $u_k(v_k) = \psi_{k+k_F}(\psi_{k-k_F})$. These are coupled by the electromagnetic field components $\Delta_q = a_{2k_F+q}$. At low energy we have assumed $\lambda_k \simeq \lambda$ and rescaled $(2\lambda/\sqrt{n})\Delta \rightarrow \Delta$ such that this field has units of energy. Correspondingly $\tilde{\delta}_{2k_F} = -n\delta_{2k_F}/2\lambda^2$. The action is invariant under the $U(1)$ transformation $\Delta \rightarrow \Delta \exp(i\chi)$, $u \rightarrow u \exp(i\chi/2)$, $v \rightarrow v \exp(-i\chi/2)$. Note indeed that this phase contributes to the electromagnetic field $a(x)$ through the term $\cos(2k_F x + \chi)$, so that choosing χ fixes the position of the minima of the optical potential i.e. breaks the spatial translation invariance of the theory. Moreover, the low-energy theory possesses an additional \mathbf{Z}_2 symmetry corresponding to the invariance under a particle-hole transformation: $\Psi \rightarrow \Psi^\dagger$ combined with a π -phase shift of the electromagnetic field: $\Delta \rightarrow -\Delta$. The low-energy theory in Eq. (2) we obtain for our light-matter system turns out to be the same as the continuum limit of the SSH model [3] for electrons coupled to lattice vibrations. We will be interested in the mean-field solutions given by the saddle-point of the action (2), which satisfy a set of Bogoliubov-deGennes (BdG) equations for the fields u, v, Δ : $\epsilon_\ell \Psi_\ell = [-iv_F \sigma_3 \frac{\partial}{\partial x} + \sigma_1 \text{diag}(\Delta^*, \Delta)] \Psi_\ell$ and $\tilde{\delta}_{2k_F} \Delta = -\sum'_\ell u_\ell v_\ell^*$, where we restricted to zero temperature. The index ℓ labels the atomic eigenstates $\Psi_\ell^T(x) = (u_\ell(x), v_\ell(x))$ and the primed sum runs over the occupied states. These BdG equations are well studied in the context of the SSH-model. We are thus able to use the solutions obtained there.

Crystalline insulator. The spatially homogeneous phase corresponds to $\Delta = 0$, so that the left and right movers are free particles, decoupled from each other. The presence of a sharp Fermi surface in 1D coupled to a continuum of electromagnetic modes renders the spatially homogeneous system unstable towards density modulations with wavenumber $Q = 2k_F$. Indeed, above a critical light-matter coupling given by $\lambda_c^2 \simeq -\frac{\delta_{2k_F}}{2\nu_{k_F}} \frac{n}{\ln(\frac{E_F}{T})}$ the solution of BdG equations shows a finite $\Delta(x) = \Delta_0$. The field Δ thus plays the role of the order parameter for the crystallization, as the transition breaks the $U(1)$ translation-symmetry by fixing the phase χ . Here we can choose it such that Δ_0 is real. The additional \mathbf{Z}_2 symmetry of the action is simultaneously broken by choosing the sign of Δ_0 . We note that the critical coupling for crystallization vanishes logarithmically at zero temperature in 1D due to resonant Umklapp scattering between $\pm k_F$. An anal-

ogous kind of instability was described by Peierls for electrons coupled to lattice vibrations [4]. The crystalline system now has a spatial periodicity π/k_F and is a band insulator where the lower of the two bands: $\epsilon_{k,\sigma} = \pm \sqrt{(v_F k)^2 + \Delta_0^2}$ is filled (we set the zero of energy at the Fermi energy, $\mu = 0$).

Emergent quasi-particles. Let us now consider the crystalline insulating phase with a filled lower band and study the low-lying excitations. Naturally, there are particle-hole excitations at the energy cost of $2\Delta_0$ which leave the optical field unchanged. However, our system additionally features hybrid excitations with even lower energy involving a distortion of the optical field. Those are found as solutions of the BdG equations whose form is available analytically. The solitonic distortion of the lattice takes the following form (reinstating dimensional units)

$$\Delta(x, T) = \pm i \Delta_0(T) \tanh\left(\frac{\lambda \Delta_0(T)}{\sqrt{n} \hbar v_F} x\right), \quad (3)$$

where $\Delta_0(T)$ is the constant value of the order parameter in the non-distorted lattice i.e. the amplitude of the $2k_F$ component of the electromagnetic field. The soliton solution (3) (see Fig. 1 for the corresponding total light intensity profile) connects a negative(positive) order parameter at $x \rightarrow -\infty$ with a positive(negative) order parameter at $x \rightarrow +\infty$, that is, it matches two differently dimerized configurations in either one of the two possible ways. Therefore, we can assign to each solitonic defect a \mathbf{Z}_2 topological number. The presence of the solitonic distortion of the lattice creates a single-particle bound state (with spin degeneracy equal to two) which is occupied by a single fermion. The bound state lies in the middle of the gap between the valence and conduction band. Those bands consists of delocalized states similar to the ones we have in absence of the defect. The size of the optical soliton at zero temperature is given by $l_{s0} \sim \frac{2}{3k_F} \exp\left(\frac{2\delta_{2k_F}^2}{g^2 \Omega^2 \nu_{k_F}}\right) = \frac{2}{3k_F} \frac{E_F}{T_c}$. It is interesting to note that we are dealing with an optical soliton whose overall size is set by a scale belonging to the quantum degenerate atoms, namely the inverse Fermi momentum. Differently from their counterparts in the electron-phonon context, the size of the light-matter defects in our case can be easily tuned by optical parameters, like the detunings or the laser strength.

Outlook. Future directions involve the study of the topological-defect dynamics and mutual interactions, as well as understanding the role played quantum fluctuations and photon-dissipation.

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2.34 The shear sound of two-dimensional Fermi liquids

JUN YONG KHOO AND INTI SODEMANN

Introduction. Classical liquids have only longitudinal sound waves, in contrast to classical solids which also have transverse sound. We demonstrate here that Fermi liquids can differ dramatically from classical liquids by developing a sharp transverse sound mode outside of the particle-hole continuum for sufficiently strong interactions. This shear sound mode is unaltered by the presence of Coulomb interactions and might be present in a variety of strongly interacting metals, in particular two-dimensional metals in which the quasiparticle mass is renormalised to be about twice the bare mass. Here, we study this mode within the bosonization description of Landau Fermi liquids by solving for the entire spectrum of coherent and incoherent excitations of a Fermi liquid with non-zero F_0 and F_1 Landau parameters. This is accomplished by mapping the kinetic equation into a 1D non-hermitian tight binding model. We also discuss potential routes to realize this mode in experiments.

Bosonization of Fermi Surface. Higher dimensional bosonization is essentially a second quantized field theoretic version of Landau Fermi liquid theory. We will describe a short path between the bosonization and conventional Fermi liquid theory which highlights this intimate connection. In particular, the harmonic nature of the bosonized theory leads to an equivalence between classical and quantum equations of motion for collective modes, analogous to how the Ehrenfest theorem relates the dynamics of classical and quantum Harmonic oscillators [1–4].

The long-wavelength and low-energy description of most phases of matter involves a finite number of continuum fields. However, Landau Fermi liquids depart radically from this, in that they have an *infinite* number of slow degrees of freedom which parametrize the shape of the Fermi surface [2]. The state of a Landau Fermi liquid can be parametrized by the Fermi radius at any point in space \mathbf{x} , $p_{\mathbf{x},\theta}^F = p_F^0 + u_{\mathbf{x},\theta}$, where θ is the angle on the Fermi surface. In bosonization the Fermi radius becomes a quantum mechanical operator whose algebra is given by [2–6]:

$$[\hat{u}_{\mathbf{x},\theta}, \hat{u}_{\mathbf{x}',\theta'}] = \frac{(2\pi)^2}{ip_F} \delta(\theta - \theta') \partial_n \delta(\mathbf{x} - \mathbf{x}') + O(\hat{u}), \quad (1)$$

where $\partial_n = \hat{\mathbf{p}}_\theta \cdot \partial_{\mathbf{x}}$ is the derivative along the normal $\hat{\mathbf{p}}_\theta$ of the Fermi surface. The Hamiltonian governing the dynamics of the Fermi surface can be written as:

$$\hat{H} = \int d^2\mathbf{x} \hat{u}_{\mathbf{x},\theta}^\dagger h_{\theta,\theta'} \hat{u}_{\mathbf{x},\theta'}, \quad (2)$$

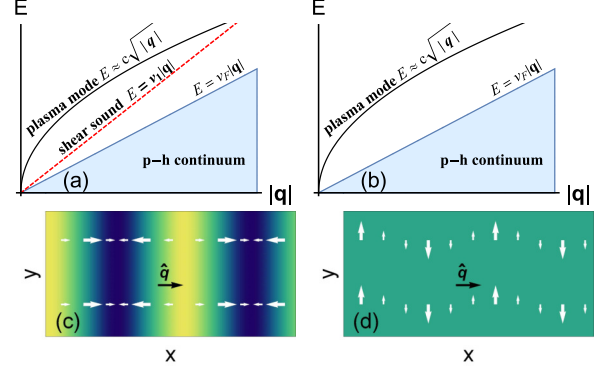


Figure 1: Particle-hole (p-h) continuum and the collective modes of the Fermi liquid in 2D (a) with and (b) without shear sound (red, dashed line). In neutral Fermi liquids, the zero sound (plasma modes in metal) will have a linear dependence instead of the square root dependence shown here. (c) Zero and (d) shear sound with wavevector \mathbf{q} parallel to the x -axis. The color scale represents the density and the arrows the current fluctuations.

where $h(\theta, \theta') = v_F p_F (2\pi \delta(\theta' - \theta) + F(\theta' - \theta)) / 2(2\pi)^3$. $F(\theta' - \theta)$ is the Landau function characterizing the interactions between quasiparticles. To exploit translational invariance we introduce the Fourier modes of the Fermi surface deformations $\hat{u}_{\mathbf{q},\theta} \equiv \int d^2\mathbf{x} \hat{u}_{\mathbf{x},\theta} e^{-i\mathbf{q}\cdot\mathbf{x}}$. The equation of motion following from Eqs. (1) and (2) for these operators is: $i\partial_t \hat{u}_{\mathbf{q},\theta} = [\hat{u}_{\mathbf{q},\theta}, \hat{H}] = K_{\theta,\theta'} \hat{u}_{\mathbf{q},\theta'}$, where:

$$K(\theta, \theta') = v_F \mathbf{q} \cdot \hat{\mathbf{p}}_\theta \left(\delta(\theta - \theta') + \frac{1}{2\pi} F(\theta - \theta') \right). \quad (3)$$

The equation above can be recognized to be an operator version of the classic Landau's linearized kinetic equation [7, 8]. We emphasize that $\hat{u}_{\mathbf{q},\theta}$ do not satisfy canonical bosonic commutation relations and that the kinetic matrix, $K_{\theta,\theta'}$, is non-Hermitian. We now state a mapping between the classical solutions of Landau's kinetic equation and their quantum counterpart. For each *classical* eigenfunction of the kinetic equation, $\psi_{\lambda,\mathbf{q},\theta}$, there is a *quantum* eigenmode, $\hat{\psi}_{\lambda,\mathbf{q}}$, given by: $\hat{\psi}_{\lambda,\mathbf{q}} = \psi_{\lambda,\mathbf{q},\theta}^\dagger T_{\theta,\theta'}^{-1} \hat{u}_{\mathbf{q},\theta'}$, where $K_{\theta,\theta'} \psi_{\lambda,\mathbf{q},\theta'} = E_\lambda \psi_{\lambda,\mathbf{q},\theta}$ and $i\partial_t \hat{\psi}_{\lambda,\mathbf{q}} = E_\lambda \hat{\psi}_{\lambda,\mathbf{q}}$. By choosing a suitable normalization for the classical solutions, $\psi_{\lambda,\mathbf{q},\theta}^\dagger T_{\theta,\theta'}^{-1} \psi_{\lambda',\mathbf{q},\theta'} = \text{sgn}(E_\lambda) \delta_{\lambda,\lambda'}$, we arrive at canonical bosonic eigenmodes describing the fluctuations of the shape of the Fermi surface: $[\hat{\psi}_{\lambda,\mathbf{q}}, \hat{\psi}_{\lambda',\mathbf{q}'}^\dagger] = (2\pi)^2 \delta(\mathbf{q} - \mathbf{q}') \text{sgn}(E_\lambda) \delta_{\lambda,\lambda'}$, where the sign of the eigenvalue E_λ dictates which one of the pair $\hat{\psi}_{\lambda,\mathbf{q}}, \hat{\psi}_{\lambda',\mathbf{q}'}^\dagger$ is the raising and which one is lowering operators. These

eigenmodes describe both collective oscillations such as the zero sound and also the continuum of particle-hole excitations. Any two-body operator can be represented as a linear combination of these modes and in particular: $\hat{u}_{\mathbf{q},\theta} = \sum_{\lambda} \text{sgn}(E_{\lambda}) \hat{\psi}_{\lambda,\mathbf{q}} \psi_{\lambda,\mathbf{q},\theta}$.

Mapping to a chain. We assume rotational symmetry and choose $\mathbf{q} = q\hat{x}$. We measure the angle along the Fermi surface, θ , from this axis. Additionally, we assume a mirror symmetry $F(\theta) = F(-\theta)$, $K_{\theta,\theta'} = K_{-\theta,-\theta'}$, which decouples the even and odd parity eigenmodes, which we label with a superscript $\sigma = \pm$ denoting: $\psi_{\lambda,\mathbf{q},\theta}^{\sigma} = \sigma \psi_{\lambda,\mathbf{q},-\theta}^{\sigma}$. There is also a time-reversal symmetry $K_{\theta,\theta'}^* = K_{\theta,\theta'}$ which implies that the eigenfunctions can be taken to be purely real. The kinetic equation also has a particle-hole-like symmetry which follows from an inversion in momentum space: $K_{\theta+\pi,\theta'+\pi} = -K_{\theta,\theta'}$. Therefore the eigenfunctions, $\psi_{\lambda,\mathbf{q},\theta}^{\sigma}$, come in pairs with opposite eigenvalues. Namely, if $\psi_{\lambda,\mathbf{q},\theta}^{\sigma}$ is an eigenfunction with eigenvalue E_{λ}^{σ} , then $\psi_{\lambda,\mathbf{q},\theta+\pi}^{\sigma}$ is an eigenfunction with eigenvalue $-E_{\lambda}^{\sigma}$. For fixed \mathbf{q} these two solutions describe physically distinct modes. We decompose into angular momentum channels, $F(\theta) = F_0 + \sum_{l=1}^{\infty} 2F_l \cos(l\theta)$, $\psi_{\lambda,\theta}^{\pm} = \psi_{\lambda,0}^{\pm} + \sum_{l=1}^{\infty} 2\psi_{\lambda,l}^{\pm} \cos(l\theta)$, $\psi_{\lambda,\theta}^{-} = \sum_{l=1}^{\infty} 2\psi_{\lambda,l}^{-} \sin(l\theta)$. With this the kinetic equation takes the form of a non-Hermitian tight-binding model in which the sites are the angular momentum channels:

$$E_{\lambda}^{\sigma} \psi_{\lambda,l+1}^{\sigma} = t_l \psi_{\lambda,l}^{\sigma} + t_{l+2} \psi_{\lambda,l+2}^{\sigma}, \quad (4)$$

where $t_l = v_F q(1 + F_l)/2$. We see that the Landau parameters play the role of bond-disorder in the effective tight binding model. A similar structure has been found in recent studies of collective modes for spin orbit coupled systems [9].

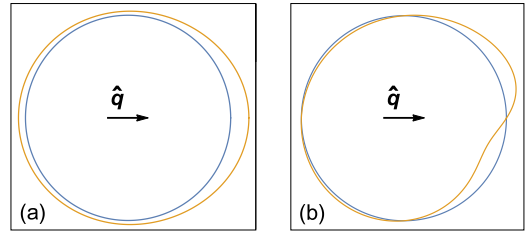


Figure 2

Shear sound. We consider a model which has non-vanishing $\{F_0, F_1\}$ Landau parameters. We solve the tight-binding model from the previous section. A shear sound mode can be found in the odd sector and the dispersion is found to be:

$$\frac{E_1}{v_F q} = \frac{1 + F_1}{2\sqrt{F_1}}, \quad F_1 > 1, \quad (5)$$

The shape of the Fermi surface deformations associated with shear and zero sound modes are illustrated in FIG. 2. This extra collective mode features transverse current fluctuations with no density oscillations in analogy with the shear sound of elastic media. The Landau parameter F_1 controls the ratio of the quasiparticle mass to the transport mass: $m^*/m = 1 + F_1$. Therefore, we expect that in systems where interactions have rendered $m^* \gtrsim 2m$ ($F_1 > 1$) the shear sound will emerge out of the particle-hole continuum as a sharp excitation, provided that the higher angular momentum Landau parameters ($l \geq 2$) remain small.

We suspect that such relatively moderate renormalization should be accessible in a variety of two-dimensional LFLs, such as ^3He films on graphite where m^* diverges on approaching a Mott transition [10, 11], quasi-2D metals near criticality such as the Iron based superconductors which have a diverging m^* [12, 13], and two-dimensional transition metal dichalcogenides [14–16].

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2.35 Floquet engineering of optical solenoids and quantized charge pumping along tailored paths in two-dimensional Chern insulators

F. NUR ÜNAL, BOTAO WANG, ANDRÉ ECKARDT

Introduction The adiabatic creation of quasi-particle/hole excitations in a quantum Hall state by inserting a magnetic flux quantum through an infinitely thin solenoid is a famous *gedanken* experiment in solid state physics [1]. In a recent paper, we presented the first proposal for the experimental creation of such local solenoid-type magnetic fluxes in an optical-lattice system [2]. The realization of local solenoid-type fields can open a novel route towards the creation and manipulation of elementary excitations of topological states of matter, a prerequisite also for robust topological quantum information processing. Moreover, we found that such a tool can also be used for controlled adiabatic charge pumping along tailored paths in two dimensions which offers, for example, a means for coherent population of chiral edge modes.

Our scheme builds on two recent experimental milestones in optical lattices: the creation of artificial magnetic fields in optical lattices on the one hand and the ability of single-site addressing in quantum gas microscopes on the other. It is based on Floquet engineering, i.e. on the control of the system using strong time-periodic driving [3]. In order to show its feasibility, we simulate the full time evolution of the periodically driven system.

Scheme Let us start with the realization of a homogeneous magnetic flux via photon-assisted tunneling in a 2D optical square lattice [3]. We consider non-interacting particles under a time-periodic driving of period $T = 2\pi/\omega$. The Hamiltonian can be written as

$$\hat{H}(t) = - \sum_{\langle \ell, \ell' \rangle} J_{\ell\ell'} e^{i\theta_{\ell\ell'}(t)} \hat{a}_{\ell'}^\dagger \hat{a}_\ell, \quad (1)$$

where \hat{a}_ℓ (\hat{a}_ℓ^\dagger) is the annihilation (creation) operator for a particle on site ℓ and $J_{\ell\ell'}$ the parameter for tunneling between nearest-neighboring sites ℓ and ℓ' . The on-site potential $w_\ell(t) = w_\ell^{\text{dr}}(t) + \nu_\ell \hbar \omega$ induces the time-dependent Peierls phases $\theta_{\ell\ell'}(t) = \int_{t_0}^t dt' w_{\ell\ell'}(t')/\hbar$ for integer ν . For sinusoidal driving, the relative modulation between two neighboring sites $w_{\ell\ell'}(t) = w_{\ell'}(t) - w_\ell(t)$ takes the form of

$$w_{\ell\ell'}(t) = K_{\ell\ell'} \cos(\omega t - \varphi_{\ell\ell'}) + (\nu_{\ell'} - \nu_\ell) \hbar \omega, \quad (2)$$

where $K_{\ell\ell'} > 0$ and $\varphi_{\ell\ell'}$, represent the driving strength and phase. In the high-frequency regime ($\hbar\omega \gg J_{\ell\ell'}$), the time-dependent Hamiltonian (1) can be approximated by its cycle average $\hat{H}^{\text{eff}} = \frac{1}{T} \int_0^T dt \hat{H}(t) =$

$-\sum_{\langle \ell, \ell' \rangle} J_{\ell\ell'}^{\text{eff}} \hat{a}_{\ell'}^\dagger \hat{a}_\ell$. The artificial magnetic flux ϕ piercing a lattice plaquette is given by the sum of the Peierls phases $\theta_{\ell\ell'} = \arg(J_{\ell\ell'}^{\text{eff}})$ picked up when moving around this plaquette. The Harper-Hofstadter model with homogeneous $\phi = \pi/2$ flux per plaquette has been successfully engineered experimentally [4] by implementing this sinusoidal drive in a square optical lattice with staggered potential offsets ν_ℓ along one direction.

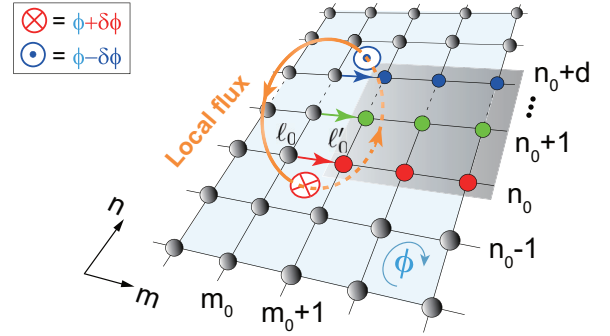


Figure 1: Realization of solenoid-type local plaquette fluxes. The bonds labeled by colored arrows acquire an additional Peierls phase $\delta\phi$ due to the modification of the driving potentials in shaded area, resulting in additional $\pm\delta\phi$ flux in plaquettes labeled by \otimes, \odot on top of the homogeneous background flux ϕ .

To engineer additional solenoid-type fluxes piercing two lattice plaquettes on top of this uniform flux ϕ , we consider additional driving potentials $K_\ell \sin(\omega t - \varphi_\ell)$ induced by digital mirror devices [5] in the shaded sub-region of Fig. 1. Within the rows along x -direction labeled by the same color, identical driving is imposed on every site. Thus, the tunneling processes within these rows remain unaffected. However, for tunneling on the link connected by an unmodified site and a modified one, the relative modulation [Eq. (2)] is changed. We choose the additional driving so that the strength of tunneling remains the same, while the tunneling phase obtains a shift $\delta\phi$. The values of $\delta\phi$ can be varied continuously from 0 to 2π by simultaneously tuning both the strength K_{ℓ_0} and the phase φ_{ℓ_0} of the additional driving [cf. Fig. 1]. For the other rows in the shadowed area, the same strategy is applied and the same $\delta\phi$ is implemented on each of the modified links [labeled by arrows in Fig. 1]. This results in solenoid-type local fluxes $\phi \pm \delta\phi$ for the plaquettes denoted by \otimes, \odot in Fig. 1, while the other plaquettes remain to have the uniform background flux ϕ . Ideally, the engineered system is captured by a modified Harper-Hofstadter model with a homogeneous tunneling amplitude J . For $\phi = \pi/2$, the system possess four bands with the

lowest band characterized by the topologically non-trivial Chern number $C = 1$. We shall fill it completely with noninteracting spinless fermions to form a Chern insulator.

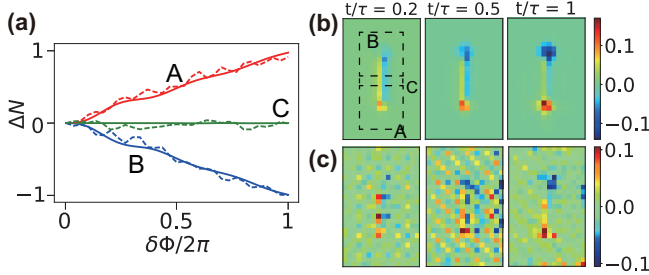


Figure 2: (a) The particle number difference $\Delta N_i = N_i(t) - N_i(0)$ in regions $i = A, B, C$ [defined in (b)] as a function of $\delta\phi(t)$ linearly ramped from 0 to 2π within the time $\tau = 10\hbar/J$, for $K/\hbar\omega = 0.35$. The solid and dashed lines are obtained by simulating the time evolution with the ideal Hamiltonian and the full time dependent Hamiltonian (1). (b,c) Respective changes in spatial densities.

Creating quasiparticles and quasiholes For $C = 1$, we expect that locally a quasiparticle (quasihole) of “charge” +1 (-1) can be created adiabatically by linearly increasing $\delta\phi$ from 0 to 2π within a proper ramping time τ , i.e. $\delta\phi(t) = (2\pi/\tau)t$. We consider a 16×25 square lattice with the two modified plaquettes separated by 10 lattice constants and track the particle number differences $\Delta N_i(t) = N_i(t) - N_i(t=0)$ at time t in three regions $i = A, B, C$. A (B) is a square-shaped region of size 10×10 , centered at the plaquette with additional flux $\delta\phi$ ($-\delta\phi$), and C is the area between A and B [see Fig. 2(b)]. We numerically calculate the spatial density distribution by solving the time-dependent Schrödinger equation.

The values ΔN_i near ± 1 at $\delta\phi = 2\pi$ suggest the creation of a quasiparticle (quasihole) around the plaquette where the additional flux $\delta\phi$ ($-\delta\phi$) was inserted. The snapshots of the evolution of the spatial density distributions are plotted in Fig. 2(b) for the ideal time-independent Hamiltonian with local flux. In Fig. 2(c), we not only consider the full time-dependent Hamiltonian (1), but also start from the adiabatic preparation of the initial Chern insulator state by ramping up the background flux. While this simulation of the full time

evolution reveals imperfections in the post ramp density, we can see from the dashed line in Fig. 2(a) that overall transport of charge remains quantized.

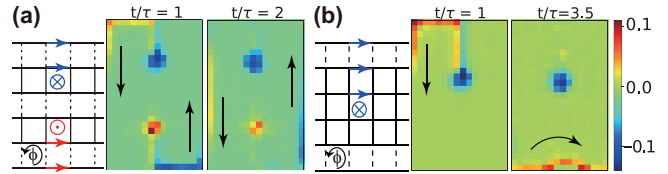


Figure 3: (a) Local flux configuration as in Fig. 1(a), but for a different final gauge, with corresponding spatial density distributions. (b) Additional flux in a single plaquette with robust chiral edge transport against an impurity potential of $10J$ at the lower edge. The results are obtained from time evolution governed by the ideal Hamiltonian with $\delta\phi(t) = 2\pi\tau/t$ for $t < \tau$ and $\delta\phi(t) = 2\pi$ for $t > \tau$, where $\tau = 10\hbar/J$.

Controlled charge pumping Fig. 2(b) shows that a quantum of charge is transported along the path defined by the sequence of bonds with the additional Peierls phase $\delta\phi$. As shown in Fig. 3(a), by adding phases $\delta\phi$ on the bonds starting from the target plaquettes to the edge instead of between them, a different particle transport is induced. Apart from the previous bulk excitations, a quasiparticle and a quasihole appear at the edges. Again quanta of charge are transported along the path defined by the modified Peierls phases. Thus, the final gauge used to implement the local flux dictates the path along which a quantum of charge is pumped. This effect is related to the artificial electric fields $\propto \dot{\theta}_{\ell\ell}$ that are present during the ramp. This mechanism can be a useful tool, e.g., to populate and probe robust chiral edge modes as visualized in Fig. 3(b).

Conclusion We proposed a scheme for the coherent manipulation of quasiparticle and hole excitations in 2D Chern insulators. It is based on coherent spatio-temporal driving via tailored light-shift potentials. In a subsequent paper, we showed that it can be employed also to create, manipulate and probe the fractionally charged anyonic excitations of fractional Chern insulators [6]. Thus, our scheme might provide a step towards building a toolkit for robust topological quantum information processing in quantum gas microscopes.

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2.36 Resonance eigenfunction hypothesis for chaotic systems

KONSTANTIN CLAUSS, ARND BÄCKER, AND ROLAND KETZMERICK

Introduction Eigenvalue spectra and the structure of eigenfunctions are the key to understanding any quantum system. Universal properties are usually expected for quantum systems with chaotic classical dynamics. For closed systems the statistics of eigenvalues follows random matrix theory, and the structure of eigenfunctions is described by the semiclassical eigenfunction hypothesis. It states that eigenfunctions are concentrated on those regions explored by typical classical orbits. If the dynamics is ergodic, this is proven by the quantum ergodicity theorem, showing that almost all eigenfunctions converge to the uniform distribution on the energy shell in phase space.

Experimentally one often deals with chaotic scattering systems, which appear for example in nuclear reactions, microwave resonators, and optical microcavities. Thus the counterparts of the fundamental results of closed systems are desired for scattering systems. In particular, the fractal Weyl law relates the growth rate of the number of long-lived resonances to the fractal dimension of the chaotic saddle of the classical dynamics. For the structure of chaotic resonance eigenfunctions many aspects have been understood for billiards, optical microcavities, and maps, but a complete understanding was still missing. Recently, we proposed a resonance eigenfunction hypothesis for fully chaotic systems with escape [1], see Fig. 1, which we will review here.

Chaotic systems with escape For simplicity, we consider a time-periodically kicked system with escape from a phase-space region Ω , as shown in Fig. 2(c). Classically, for chaotic dynamics of a map with escape almost all points on phase-space Γ will be mapped into the opening Ω eventually and thus escape. Only a set of measure zero does not leave the system under forward and backward iteration. This invariant set usually is a fractal and is called the *chaotic saddle* Γ_s , see Fig. 2(a). Its unstable manifold consists of points approaching Γ_s under the inverse map and is therefore called the *backward-trapped set* Γ_b , see Fig. 2(b). Generic initial phase-space distributions asymptotically converge to the uniform distribution on Γ_b , the so-called *natural measure* μ_{nat} , with corresponding decay rate γ_{nat} [2].

Quantum mechanically, the support of resonance eigenfunctions is given by the backward trapped set Γ_b [3,4]. Furthermore, long-lived eigenfunctions with decay rates $\gamma \approx \gamma_{\text{nat}}$ are distributed as the natural measure μ_{nat} on phase space, see Fig. 1, which corresponds to the steady-state distribution in the context of optical microcavities. For arbitrary γ the integrated weight on Ω and on each of its preimages $M^{-i}(\Omega)$ depends on γ [4], which is generalized by so-called conditionally

invariant measures [2]. There are simple conditionally invariant measures proportional to μ_{nat} on Ω , which describe classically the weight of eigenfunctions on either side of a partial barrier [5]. However, there occurs an additional localization of resonance eigenfunctions within the opening Ω [1], which is not explained by these measures. We find a classical description for this effect, which relies on the finite phase-space resolution h of the chaotic saddle Γ_s .

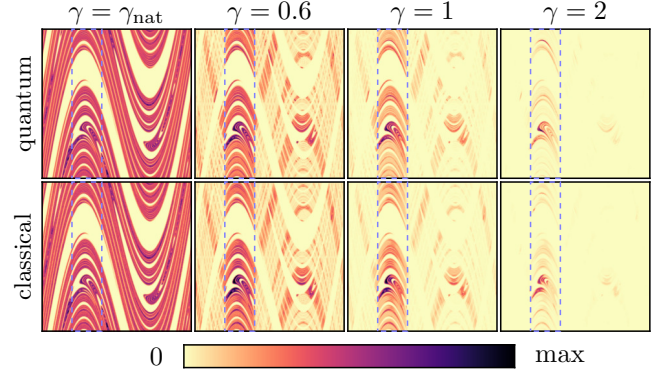


Figure 1: Average Husimi distribution of resonance eigenfunctions (top) compared to constructed classical measures μ_{γ}^h (bottom) with decay rates $\gamma \in \{\gamma_{\text{nat}} \approx 0.23, 0.6, 1, 2\}$ for $h = 1/16000$. Chaotic standard map with $\kappa = 10$ on phase space $\Gamma = [0, 1] \times [0, 1]$ with opening $\Omega = [0.2, 0.4] \times [0, 1]$ (blue dashed line). Colormap with fixed maximum for each γ and h . Prominent localization for increasing γ and overall quantum-classical agreement.

Resonance eigenfunction hypothesis We postulate that in chaotic systems with escape through an opening the average phase-space distribution of resonance eigenfunctions with decay rate γ for effective Planck's constant h is described by a measure that (i) is conditionally invariant with decay rate γ and (ii) is uniformly distributed on sets with the same temporal distance to the h -resolved chaotic saddle.

Combining both properties yields a measure

$$\mu_{\gamma}^h(A) = \frac{1}{\mathcal{N}} \int_A e^{t_h(x) \cdot (\gamma - \gamma_{\text{nat}})} d\mu_{\text{nat}}(x), \quad (1)$$

for all $A \subset \Gamma$ with normalization constant \mathcal{N} . Here the temporal *saddle distance* $t_h(x) \in \mathbb{R}$ fulfills $t_h(M^{-1}(x)) = t_h(x) - 1$ for almost all $x \in \Gamma_b$, i.e. each backward iteration of the map M on Γ_b reduces the saddle distance by one. An important implication of Eq. (1) is that μ_{γ}^h is enhanced with increasing $\gamma > \gamma_{\text{nat}}$ in those regions of Γ_b having the largest saddle distance due to the exponential factor. These regions must be in the opening Ω , which is easily shown by contradiction. Thus the hypothesis leads to a classical prediction for the localization of resonance eigenfunctions in chaotic systems.

For any decay rate γ there are infinitely many different conditionally invariant measures [2]. Property (ii) selects a specific class of these measures which are uniformly distributed on subsets of Γ_b . Uniform distribution with respect to Γ_b (the support of conditionally invariant measures) is equivalent to proportionality to the natural measure, explaining the appearance of μ_{nat} in Eq. (1). In analogy to quantum ergodicity for closed systems it is reasonable to consider for resonance eigenfunctions a uniform distribution on Γ_s , as classically this is an invariant set with chaotic dynamics. The quantum mechanical uncertainty relation, however, implies a finite phase-space resolution \hbar replacing Γ_s by a quantum resolved saddle Γ_s^h . It is desirable to combine the assumption of uniformity on the saddle, the finite quantum resolution, and conditional invariance. This is achieved by introducing a temporal distance $t_h(x)$ to the quantum resolved saddle Γ_s^h for all $x \in \Gamma_b$ and assuming uniformity on all sets with the same temporal distance. The resulting measures μ_γ^h , Eq. (1), are indeed conditionally invariant as can be easily shown.

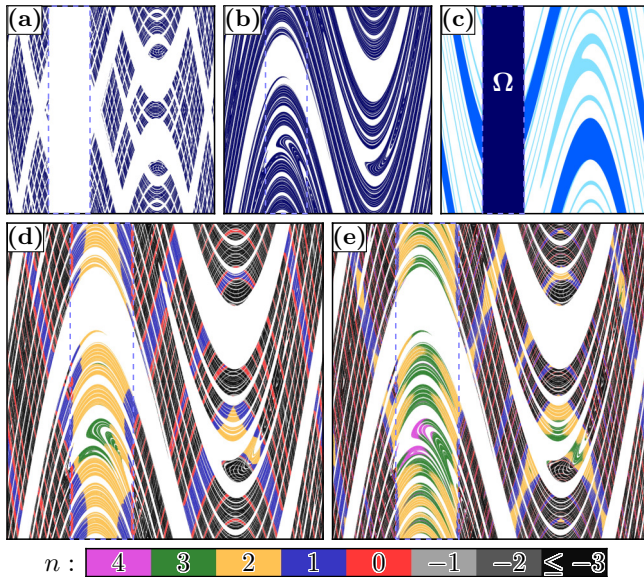


Figure 2: Classical sets for standard map as in Fig. 1. (a) Chaotic saddle Γ_s , (b) backward trapped set Γ_b , (c) opening Ω and preimages $M^{-1}(\Omega)$, $M^{-2}(\Omega)$ (from dark to light), (d, e) partition of the backward trapped set Γ_b with colored sets \mathcal{E}_n^h with integer saddle distance $n \leq m_h$ for (d) $h = 1/1000$ with $m_h = 3$ and (e) $h = 1/16000$ with $m_h = 4$. Regions with $n \leq 0$ are within the h -resolved saddle.

For the saddle distance $t_h(x)$ a convenient and simple implementation is to consider Γ_s^h as a symmetric surrounding of Γ_s , $\Gamma_s^h = \{x \in \Gamma : d(x, \Gamma_s) \leq \sqrt{\hbar/2}\}$, with Euclidean distance d smaller than the width of coherent states. Then an *integer saddle distance* $n \in \mathbb{Z}$ is defined for $x \in \Gamma_b$ as the number of backward steps to enter the h -resolved saddle, $t_h(x) = n \Leftrightarrow M^{-n}(x) \in \Gamma_s^h$, with $M^{-i}(x) \notin \Gamma_s^h$ for all $i < n$. For points inside of Γ_s^h this leads to $n \leq 0$. Defining $\mathcal{E}_n^h := \{x \in \Gamma_b : t_h(x) = n\}$ as the sets with integer saddle distance n we obtain a partition of Γ_b with $\mathcal{E}_n^h = M^n \mathcal{E}_0^h$, see Fig. 2(d) and

(e). Note that the maximum m_h increases with h . According to Eq. (1) in each of these regions the measures are proportional to the natural measure, $\mu_\gamma^h(A \cap \mathcal{E}_n^h) = 1/\mathcal{N} e^{n(\gamma - \gamma_{\text{nat}})} \mu_{\text{nat}}(A \cap \mathcal{E}_n^h)$.

Comparison In Fig. 1 we show the average phase-space distributions $\langle \mathcal{H} \rangle_\gamma$ for $\gamma \in \{\gamma_{\text{nat}}, 0.6, 1, 2\}$ and $h = 1/16000$. Here $\mathcal{H}(q, p)$ is the Husimi distribution, i.e. the expectation value of the projector on a coherent state $|q, p\rangle$. The classical analogue is obtained by a convolution of the constructed measures μ_γ^h with a Gaussian of the same width as the coherent state, i.e. with standard deviation $\sqrt{\hbar/2}$. This allows for quantum-classical comparison on the phase space. Overall we observe very good agreement concerning the support of the distributions, their weight on the opening Ω , and their localization within Ω .

The Husimi distributions show the following features: First, they are supported by the smoothed backward trapped set. Secondly, one observes that their density on the opening Ω is larger than on its surrounding. The other stripes with larger density (than their surrounding) fall on the preimages $M^{-1}(\Omega)$ and $M^{-2}(\Omega)$, shown in Fig. 2(c). Thirdly and most importantly, the Husimi distributions within Ω are not uniform on Γ_b , but show localization, which is stronger for larger γ .

The same three observations hold for the constructed measures μ_γ^h , where they directly follow from properties (i) and (ii). The first two observations are implied by conditional invariance. Note that the integrated weight on Ω increases with γ as $\mu_\gamma^h(\Omega) = 1 - e^{-\gamma}$. It also implies for the k -th preimage of the opening $\mu_\gamma^h(M^{-k}(\Omega)) = e^{-k\gamma} \mu_\gamma^h(\Omega)$, which agrees with the quantum mechanical analysis [4]. For the third observation we explicitly need the saddle distance in our classical construction, which follows from property (ii). Those parts of Ω with maximal saddle distance m_h , see Fig. 2(d) and (e), show the largest enhancement due to the exponential factor in Eq. (1). Consequently, regions with smaller saddle distance are less enhanced.

Conclusion The presented hypothesis gives a classical explanation for the localization hypothesis gives a classical explanation for the localization of resonance eigenfunctions, as well as a description of their entire phase-space distribution on scales of order h . Improvements of the resulting measures are possible by more elaborate definitions of Γ_s^h and $t_h(x)$. A future challenge is the application to optical microcavities, which requires a generalization to partial transmission and reflection.

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2.37 Transition from asynchronous to oscillatory dynamics in balanced spiking networks

MATTEO DI VOLO AND ALESSANDRO TORCINI

The dynamics of neurons in the mammalian brain is characterized by irregular firing due to the balance between excitation and inhibition. The balanced state is typically associated to asynchronous dynamics, however this is not the only regime observable during spontaneous cortical activity. As a matter of fact, oscillations at different frequencies are typically observed in neural recordings at the global scale (e.g. EEG, LFP), thus indicating the emergence of collective dynamics. We have shown that the balanced microscopic activity can sustain collective oscillations (COs) in sparse neural networks even in the absence of synaptic or delay time scales [1].

Introduction Cortical neurons fire quite irregularly and with low firing rates, despite being subject to a continuous bombardment from thousands of excitatory and inhibitory neurons. This apparent paradox can be solved by introducing the concept of balanced network, where excitation and inhibition balance each other and the neurons are kept near their firing threshold. In this regime spikes, representing the elementary units of information in the brain, are elicited by stochastic fluctuations in the net input current yielding an irregular microscopic activity.

In neural network models balance can emerge spontaneously in coupled excitatory and inhibitory populations thanks to the dynamical adjustment of their firing rates [2, 3]. The usually observed dynamics is an asynchronous state characterized by irregular neural firing joined to stationary firing rates [2], this state has been experimentally observed both in vivo and in vitro [4]. However, during spontaneous cortical oscillations excitation and inhibition wax and wane together, suggesting that balancing is crucial for the occurrence of these oscillations with inhibition representing the essential component for the emergence of the synchronous activity [5].

The emergence of COs in inhibitory networks has been widely investigated in networks of spiking leaky integrate-and-fire (LIF) neurons. In particular, it has been demonstrated that COs emerge from asynchronous states via Hopf bifurcations in presence of an additional time scale, beyond the one associated to the membrane potential evolution [3, 6]. As the frequency of the COs is related to this additional time scale this mechanism induces fast (>30 Hz) oscillations and it remains unclear which other mechanisms could be invoked to justify the broad range of COs' frequencies observed experimentally [7].

We have found a novel mechanism for the emergence of COs in balanced spiking inhibitory networks in ab-

sence of any synaptic or delay time scale. In particular, we show that COs arise from an asynchronous state by increasing the in-degree and that COs can survive only in presence of irregular spiking dynamics due to the dynamical balance. The origin of COs can be explained by developing a mean-field formulation for the dynamics of Quadratic Integrate-and-Fire (QIF) neurons in sparse balanced networks. A stability analysis of the mean-field model reveals that the asymptotic macroscopic solution is a stable focus and determines the frequency of the associated relaxation oscillations. The agreement of this relaxation frequency with the COs' one measured in the spiking network suggests that the irregular microscopic firings of the neurons is able to sustain COs corresponding to the relaxation dynamics towards the macroscopic focus.

Model and indicators We consider a balanced network of N pulse-coupled QIF inhibitory neurons, whose membrane potential evolves as

$$\tau_m \dot{v}_i = v_i^2 + I - 2\tau_m g \sum_{j \in \text{pre}(i)} \varepsilon_{ij} \delta(t - t_j), \quad (1)$$

where I is the external DC current, g is the inhibitory synaptic coupling, $\tau_m = 20$ ms is the membrane time constant and instantaneous synapses are considered. The neurons are randomly connected, with in-degrees k_i distributed according to a Lorentzian PDF peaked at K and with a half-width half-maximum (HWHM) Δ_K . The elements of the adjacency matrix ε_{ij} are one (zero) if the neuron j is connected (or not) to neuron i . The DC current and the coupling are rescaled with the median in-degree as $I = \sqrt{K} I_0$ and $g = g_0 / \sqrt{K}$, as usually done in order to achieve a self-sustained balanced state for sufficiently large in-degrees [2]. Furthermore, we assume $\Delta_K = \Delta_0 \sqrt{K}$.

In order to characterize the network dynamics we measure the mean membrane potential $V(t) = \sum_{i=1}^N v_i(t) / N$, the instantaneous firing rate $R(t)$ (i.e. the number of spikes emitted per unit of time) and the population averaged coefficient of variation CV measuring the fluctuations in the neuron inter-spike intervals. Furthermore, the level of coherence in the neural activity can be quantified in terms of the indicator $\rho \equiv \sqrt{\sigma_V^2 / (\sum_{i=1}^N \sigma_i^2 / N)}$, where σ_V is the standard deviation of the mean membrane potential, $\sigma_i^2 = \langle V_i^2 \rangle - \langle V_i \rangle^2$ and $\langle \cdot \rangle$ denotes a time average. A coherent macroscopic activity is associated to a finite value of ρ (perfect synchrony corresponds to $\rho = 1$), while an asynchronous dynamics to a vanishingly small, $\rho \approx \mathcal{O}(1/\sqrt{N})$.

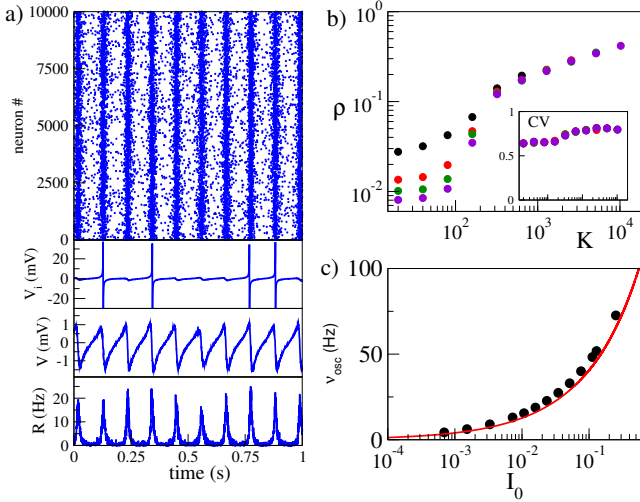


Figure 1: a) From top to bottom: the raster plot and the corresponding time traces for the membrane potential $v_i(t)$ of a representative neuron, for $V(t)$ and $R(t)$. b) Order parameter ρ versus K , the inset reports the corresponding CVs. The data refer to various system sizes: $N = 2000$ (black), 5000 (red), $10,000$ (green) and $20,000$ (violet). c) ν_{osc} versus I_0 . The red solid line refers to ν_{th} . The parameter values are $N = 10000$, $K = 1000$, $g_0 = 1$, $(\Delta_0, I_0) = (0.3, 0.015)$ in (a), $(\Delta_0, I_0) = (0.1, 0.006)$ in (b) and $\Delta_0 = 0.3$ in (c).

Results. As shown in Fig. 1 (a), we can observe collective firings occurring at almost constant frequency ν_{osc} . Despite the almost regular macroscopic oscillations in the firing rate $R(t)$ and in the mean membrane potential $V(t)$, the microscopic dynamics of the neurons $v_i(t)$ is definitely irregular, as expected for asynchronous balanced networks. Asynchronous dynamics is observable also for our model for sufficiently sparse networks (small K), indeed a clear transition is observable from an asynchronous state to COs for K larger than a critical value K_c . In Fig. 1 (b), we report the coherence indicator ρ as a function of K for various system sizes from $N = 2,000$ to $N = 20,000$. In particular, ρ vanishes as $N^{-1/2}$ for $K < K_c$, while it stays finite above the transition thus indicating the presence of collective motion. In the present case, in both of the observed dynamical regimes the microscopic dynamics remains quite irregular for all the considered K and system size N , as testified by the fact that $CV \simeq 0.8$ (as shown in the inset of Fig. 1 (b)).

The relevance of the microscopic fluctuations for the existence of the COs in this system can be appreciated by considering a value of the in-degree $K > K_c$ in order to observe COs and then by increasing the external current I_0 or the parameter Δ_0 controlling the structural heterogeneity. In both cases we observe that for large I_0 (Δ_0) the microscopic dynamics is now imbalanced with few neurons firing regularly with high rates and the majority of neurons suppressed by this high activity. This induces a vanishing of the microscopic fluctuations, due to the balanced irregular spiking activity,

and as a consequence also COs disappear.

Effective Mean-Field Model. In order to understand the origin of these macroscopic oscillations we consider an exact macroscopic model recently derived in [8] for fully coupled networks of pulse-coupled QIF with synaptic couplings randomly distributed. Such formulation can be applied to sparse networks, like (1), indeed the quenched disorder in the connectivity can be rephrased in terms of a random synaptic coupling. Namely, each neuron i is subject to an average inhibitory synaptic current of amplitude $g_0 k_i R / (\sqrt{K})$ proportional to its in-degree k_i . Therefore we can consider the neurons as fully coupled, but with random values of the coupling distributed as a Lorentzian of median $\bar{g} = -g_0 \sqrt{K}$ and HWHM $\Gamma = g_0 \Delta_0$. The mean-field dynamics of the network can be expressed in terms of only two collective variables (namely, V and R), as follows

$$\tau_m \dot{R} = R(2V + \frac{g_0 \Delta_0}{\pi}) \quad (2)$$

$$\tau_m \dot{V} = V^2 + \sqrt{K}(I_0 - \tau_m g_0 R) - (\pi R \tau_m)^2 \quad (3)$$

The stationary solutions (\bar{V}, \bar{R}) of Eqs. (2,3) are always stable foci characterized by two complex conjugates eigenvalues with imaginary part Λ_I . Therefore the relaxation frequency towards the stable fixed point is given by $\nu_{th} = \Lambda_I / 2\pi$. This represents a good approximation of the frequency ν_{osc} of the sustained COs observed in the QIF network over a wide range of values ranging from ultra-slow rhythms to high γ band oscillations, as shown in Fig. 1 (c).

Conclusions. We have shown that in balanced spiking networks with instantaneous synapses COs can be triggered over a broad range of frequencies by microscopic irregular fluctuations. Furthermore, for balanced excitatory-inhibitory populations we have revealed the existence of COs characterized by two distinct frequencies, whose emergence is due, also in this case, to the excitation of a mean-field focus induced by fluctuation-driven microscopic dynamics [1].

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2.38 Complex-systems approaches to text analysis

MARTIN GERLACH & EDUARDO G. ALTMANN

Introduction. The development of many scientific fields in the XXI century has been driven by the availability of large databases of human activities. Many of these datasets are in form of written text and a major challenge is how to extract useful information from large collections of documents (e.g., from social media). While many of the recent developments in this field come from Computer Science (e.g., machine learning techniques), ideas from Statistical Physics and Complex Systems play an important role in these problems, being found at the foundation of these methods or providing alternative methods to this rapid evolving field.

One important idea coming from Statistical Physics is that different datasets show universal statistical properties. For instance, Fig. 2 shows the word-frequency distribution in three large collections of English texts: from 1850, 1900, and 1950. We see that the distribution itself remains essentially the same, a heavy-tailed Zipf distribution

$$p(r) \propto r^{-\gamma}, \quad (1)$$

where p is the frequency of the r -th most frequent word and $\gamma \gtrsim 1$. Changes are seen in the frequency p (or rank) of specific words, e.g., *ship* lost and *genetic* won popularity. Heavy-tailed and broad distributions of symbol-frequencies such as Eq. (1) are typical in critical phenomena and complex systems.

Underlying different methods and applications is the idea of quantifying the similarity between different documents based solely on the text they contain. In the example above, based on the frequency of words in the texts of each year we would like to quantify how fast the language is changing over time. The slow decay observed in a broad range of frequencies implies that there is no typical frequency for words and therefore relevant changes can occur in different ranges of the p -spectrum. Below we report two approaches to the fundamental question of identifying the similarity between documents, both deeply rooted in Complex Systems Theory. In the first case [1–3], we start by noting that quantifying the similarity of symbolic sequences is a classical problem in information theory and we consider the effect of generalized entropies in this task. In the second case [4], we consider the relationship between documents based on word co-occurrence to construct a network between documents. This was then used to establish a formal relationship between the problems of community detection in complex networks and of finding topic in documents (one of the most popular machine-learning approaches in natural language processing).

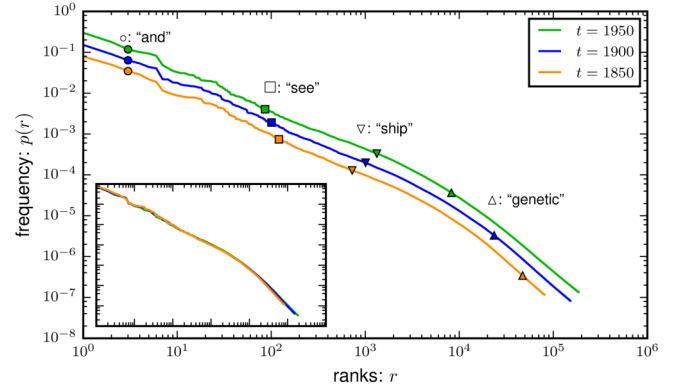


Figure 1: The English vocabulary in different years. Rank-frequency distribution $p(r)$ of individual years t for $t = 1850, 1900,$ and 1950 of the Google-ngram database, multiplied by a factor of 1, 2, and 4, respectively, for better visual comparison. The inset shows the original un-transformed data (same axis), highlighting that the rank-frequency distributions are almost indistinguishable. Individual words (e.g. “and”, “see”, “ship”, “genetic”) show changes in rank and frequency (symbols), where words with larger ranks (i.e. smaller frequencies) show larger change. Reproduced from Ref. [1]

Document Similarity. Consider the probability distribution $\mathbf{p} = (p_1, p_2, \dots, p_S)$ of a random variable over a discrete, countable set of symbols $i = 1, \dots, S$. In information theory, the natural quantification of the difference between \mathbf{p} and \mathbf{q} is the Jensen-Shannon divergence (JSD)

$$D(\mathbf{p}, \mathbf{q}) = H\left(\frac{\mathbf{p} + \mathbf{q}}{2}\right) - \frac{1}{2}H(\mathbf{p}) - \frac{1}{2}H(\mathbf{q}), \quad (2)$$

where H is the Shannon entropy $H(\mathbf{p}) = -\sum_i p_i \log p_i$. We consider the generalization of JSD in which H is replaced by the generalized entropy of order α

$$H_\alpha(\mathbf{p}) = \frac{1}{1 - \alpha} \left(\sum_i p_i^\alpha - 1 \right), \quad (3)$$

yielding a spectrum of divergence measures D_α parameterized by α , introduced by Burbea and Rao in 1982.

The first question we address [1,2] is what are the properties of H_α and D_α when estimations are done in textual data. In particular, what is the effect of Zipf’s law (1)? The large range of different frequencies at which word appears typically makes estimators to be dominated either by the few very frequent words or by the large number of low frequency words. Varying α we obtain that different word frequencies dominates the estimations so that changing α magnifies differences in the vocabulary at different scales of the (heavy-tailed) frequency spectrum, thus providing different information on the vocabulary change. We then analytically computed the accuracy (bias) and precision (variance) of estimations of D_α based on finite-size texts of size N and find that in heavy-tailed distributions the

convergence often scales as $1/N^\beta$ with $\beta < 1$, much slower than expected from the (usual) central limit Theorem for short-tailed distributions.

Having clarified the statistical properties of our estimators, we applied them to different problems of interest. Using a collection of millions of books scanned by Google, we obtained [1] a detailed quantification of how the (vocabulary of the) English language has changed over the last centuries (e.g., with $\alpha = 1$ we obtain $\approx 5\%$ of change per century). Using a collection of millions of scientific papers made available by ISI-Web of Knowledge, we obtained [2, 3] a new characterization of the relationship and temporal evolution of scientific disciplines. In particular, in Fig. 2 we show the evolution of the distance between Physics and different scientific disciplines in the last decades. While different trends can be observed (e.g., the increasingly central role of computer science), overall the distance between disciplines is neither increasing nor decreasing, suggesting that tendencies towards specialization and unification of disciplines have been in balance.

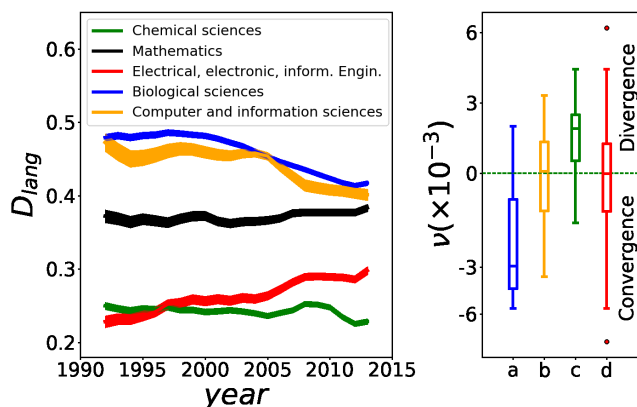


Figure 2: Evolution of the similarity between disciplines in the last three decades. Left panel: distance $D_{\alpha=2}(i, j)$ between papers in Physical Sciences (i) and other five selected disciplines (j , three-year moving averages). Right panel: total variation ν of the distance for pairs of disciplines with histories longer than 12 years. Each boxplot corresponds to the distribution of ν for pairs of disciplines where we fixed one of the disciplines: (a) Computer and Information Sciences, (b) Chemical sciences, (c) Psychology and (d) all pairs of disciplines. Reproduced from [3].

Network approach to Topic Modeling. Our second approach to analyze collections of written documents is to revisit the popular machine-learning field of topic models. Our key observation, summarized in Fig. 3, is that the document-word representation used in topic-modeling (and many other document-classification

methods) is equivalent to a bi-partite multigraph network. Building on this analogy we show how topics of documents can be inferred using state-of-the-art methods of community detection in networks (more specifically, we use Stochastic Block Models). We find [3] that our approach leads to improved results because it overcomes important theoretical limitations of the usual topic model methods (e.g., the so-called Latent Dirichlet Allocation method), which are typically based on the simplifying assumption of Dirichlet priors.

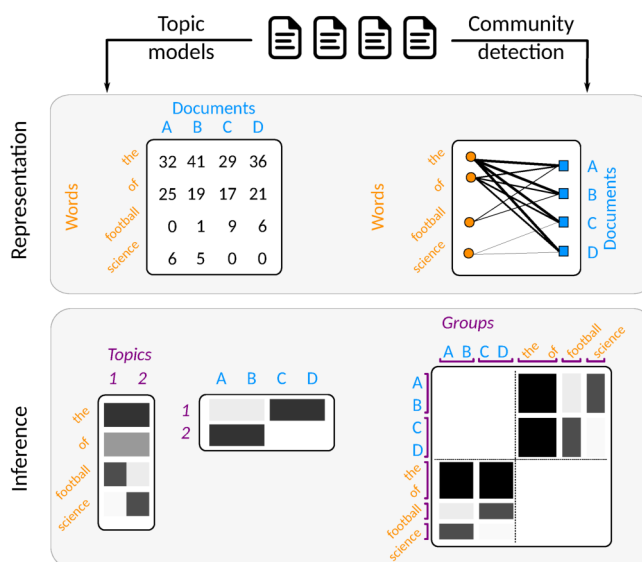


Figure 3: Two approaches to extract information from collections of texts. Topic models represent the texts as a document-word matrix (how often each word appears in each document) which is then written as a product of two matrices of smaller dimensions with the help of the latent variable topic. Our approach represents texts as a network and infers communities in this network. The nodes consists of documents and words and the strength of the edge between them is given by the number of occurrences of the word in the document, yielding a bipartite multigraph that is equivalent to the word-document matrix used in topic models. Reproduced from Ref. [3]

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Chapter 3

Details and Data

3.1 PhD Training

The training of PhD students is one of the central tasks of the **mpipks**. It is realized through a large PhD program, our leading role in the IMPRS *Many Particle Systems in Structured Environments* (see next section) and our participation in the IMPRS *Cell, Developmental and Systems Biology* which is coordinated by the Max Planck Institute of Molecular Cell Biology and Genetics.

Prospective PhD students have several options of contacting scientific advisors at the **mpipks**: 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 2016, a total of 72 PhD students were working at the **mpipks**, including 35 students from abroad (also counting those who finished or started their studies during that year). The respective numbers for 2017 were 85 PhD students working at the **mpipks**, including 50 from abroad, and in 2018 we had 84 PhD students (53 from abroad). We counted 8 successful final PhD exams for the year 2016, 8 for the year 2017, and 14 for the year 2018.

In addition to the scientific training by their supervisor, PhD students at the **mpipks** 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 **mpipks** (p. 187). Presentation skills can be practiced in regular group seminars or through active participation in the events of the Workshop and Seminar Program. The institute organizes 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. 188). Students from foreign countries receive financial and logistic support for joining German language courses.

The majority of the PhD students at the **mpipks** receive their degree from the TU Dresden (p. 190). 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

For a history, participating organizations and supervisors, see p.14.

PhD students – There are currently 48 students enrolled in the graduate school. As befits an international research school, the breakdown of the student body by country of origin shows a large spread: there are 4 students from America (Chile, Colombia and two from Mexico), 5 from India, 1 Iranian, 2 from Taiwan and 1 from China. The rest are from across Europe (Austria 1, Croatia 1, Czech Republic 9, Germany 12, Greece 1, Hungary 1, Italy 2, The Netherlands 1, Poland 5, Portugal 1, Ukraine 1). Nine of the

students are women. The distribution across partner institutions is TUD 12, MPI PKS 21, IOCB 4, UCT 5, UW 1, ILTSR 4, CPfS 1.

Annual Events – The IMPRS organizes annual events for the students of the graduate school. Since the foundation of the IMPRS at **mpipks** there has been a late summer retreat at a location around the time-independent centre of mass of the participating institutions. The retreat is a three day meeting intended to encourage interactions especially between students working in different aspects of the school's research activities. The retreat is framed around student talks and discussion sessions and is a key component in introducing new PhD students to the scientific landscape of the IMPRS, for them to benefit from the insights of students at more advanced stages of their PhD and for all students to follow the advancing research of their peers. For some retreats, partners of the school are invited to introduce themselves and to give colloquium style talks on their research topics. The 2017 retreat took place at the Ringhotel Nicolai in Lohmen in Swiss Saxony and the 2018 retreat was at the Hotel Horal Orea in Špindlerův Mlýn in the Czech Republic.

The 2016 summer school took place during the period July 11th to 14th at the Institute of Low Temperature and Structure Research in Wrocław with a series of lectures on Floquet physics. The 2018 summer school was at Villa Lanna in central Prague from the 27th to the 29th of August with lectures on a diverse range of topics including machine learning for many-body physics, frontiers in molecular dynamics, open quantum systems and non-Hermitian quantum mechanics.

In place of a summer school in 2017, four International Max Planck Research Schools joined forces to organize a spring workshop at **mpipks** bringing together the PhD students of the schools for a series of talks from school partners, external invited speakers and students focussing on the shared goals of understanding quantum matter and developing quantum technologies. The joint initiative involved the IMPRS for condensed matter science in Stuttgart, for chemistry and physics of quantum materials in Dresden, for quantum science and technology in Garching and the IMPRS MPSSE.

Other Events – The day-to-day operation of the IMPRS is structured around events that offer a forum for the students to meet and discuss. The IMPRS seminar is a research talk from one of the IMPRS students preceded by a colloquium style talk from an external invited speaker whose role it is to place the student speaker's research in context. The external speakers are proposed by the advisors and students from the participating groups and every student member of the IMPRS gives such a seminar during their doctoral years.

The lecture program of the IMPRS is framed around the courses offered by the Technische Universität Dresden during the winter (October - February) and summer (April - July) semesters. The lectures are given by professors at the university and by other members of the various partner institutions including **mpipks**. Of the courses offered by the university, the IMPRS selects English language lectures in topics related to the research focus of the school. Students of the IMPRS are required to complete a certain number of courses monitored by a credit point system.

In addition to the seminar and lecture program, the IMPRS organizes career seminars in which alumni of the institute are invited back to share their experiences of work and life beyond academia. Our focus in organizing these talks has been on sectors of industry where a background in theoretical physics may be attractive to employers. These include areas of software engineering and industrial research in machine learning and data science. These talks have proven very popular and are often one of the main ways for students to hear firsthand accounts of career possibilities where their unique skills and interests may be an asset to the company.

In autumn of 2018, we launched a scientific presentation series on classic results in many-body physics. The motivation for these journal club style blackboard talks is to familiarize students with results that are important and generally known by senior researchers but which might not be covered in typical graduate lectures. The presentations are given by the students themselves and the topics are selected by students and their advisors together with the school coordinator. The talks are technical but pitched at an audience of beginning graduate students so that all members of the IMPRS can follow.

The daily running of the graduate school - contacting students, administration around the applications, advertising, event organization and the maintenance of the webpage - is carried out by the coordination office at **mpipks**.

3.3 Workshop and Visitors Program

The Visitors Program of the **mpipks** hosts guest scientists for a period of up to two years. Excellent working conditions are offered to highly qualified, mostly young, scientists. In close collaboration with the other service departments of the **mpipks**, 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, obtaining a visa, etc.

A Mentoring Program 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 "Machine Learning for Quantum Many-body Physics", June 25 - 29, 2018

During the past three years, the numbers of guest scientists including predocs with contracts for at least three months hosted by the **mpipks** were 225, 241 and 245 (in 2016, 2017 and 2018, respectively).

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 actively participate in the Workshop and Seminar Program (see p. 140).

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 June 2015 and December of 2018, we had six PKS Fellows working at the **mpipks**: *Dr. Robert Johne* (until November 2015), *Dr. Alexander Croy* (until July 2016), *Dr. Edgar Roldan* (until March 2018), *Dr. Andre Cardoso Barato* (until July 2018), *Dr. Felix Mackenroth* (since September 2016) and *Dr. Falko Pientka* (since September 2018).

To strengthen the transfer of knowledge and experience at the **mpipks**, 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 academic year at the **mpipks** and can nominate a young guest scientist for the Visitors Program. Between 2016 and 2018, our institute had the honor to host four Gutwiller Fellows: *Prof. E. J. Heller* (Harvard University), *Prof. C. H. Greene* (Purdue University), *Prof. R. Golestanian* (University of Oxford) and *Prof. W. Krauth* (École Normale Supérieure, Paris).

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 timely topic from the field of the physics of complex systems. From June 2015 until December 2018, we enjoyed vivid activities of four Advanced Study Groups: In the second half of 2015, we hosted the groups *Semiclassical Methods*:

Insight and Practice in 'Many' Dimensions under its convenor Prof. E. J. Heller and *Statistical Physics and Anomalous Dynamics of Foraging* initiated by Dr. R. Klages. The group *From Microscopic to Collective Dynamics in Neural Circuits*, coordinated by Prof. A. Torcini was conducted in 2016 and 2017, and the group *Forecasting with Lyapunov Vectors* headed by Prof. M. W. Beims began its activities at **mpipks** in November 2018 (see reports on p. 50).

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 **mpipks** research groups and other institutes. Their number reached 299 during the year 2016, 289 during the year 2017, and 329 during the year 2018.

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 outside of academia, mainly in sectors such as applied research, informatics, finance, or consulting.

3.3.1 Institute's Fellows

3.3.1.1 Gutzwiller-Fellows

Gutzwiller Fellowship 2017

(Prof. Chris H. Greene)

My stay from January 4, 2017 until June 5, 2017 was extremely dynamic, stimulating, and productive. Much of my scientific progress was a continuation of collaborative work with Panos Giannakeas, who also stayed at the MPI-PKS during this same period. We worked together mostly on universal aspects of the 3-body problem with short-range interactions, the so-called heavy-heavy-light Efimov physics problem. The progress of our collaboration was rapid, and we began preparing our first major article to submit on this topic before the end of my stay in Dresden. This article was later finalized, and it appeared in the following journal article, early in 2018: *Ultracold Heteronuclear Three-Body Systems: How Diabaticity Limits the Universality of Recombination into Shallow Dimers*, *Physical Review Letters* **120**, 023401 (2018). Our article was chosen as the Cover Article for that issue of the journal (see below).



A new collaboration with Jan-Michael Rost was initiated during my stay in Dresden, also involving Panos and another collaborator Lev Khaykovich from Bar-Ilan University in Israel, studying non-adiabatic oscillatory effects in the radio frequency association and dissociation of ultracold molecules. This collaboration is attempting to explain some experiments that produce (and dissociate) molecules using an oscillating magnetic field. While the problem has resisted numerous attempted theoretical descriptions in the past, it looks promising that we were able to identify the crucial idea required to explain the relevant physics. It now appears as though this new formulation should produce a quantitative theoretical description of existing experiments, and also predict new, interesting phenomena that can be tested in the future. In a return visit to the MPI-PKS for 3 weeks in May of 2018, the collaboration on this project continued with Dr. Rost and Dr. Giannakeas, and extensive headway was achieved. This project is still in the process of being finalized.

While in residence at the Institute, I also attended numerous colloquia, seminars, and workshop talks, which have planted many ideas for future projects. I have also enjoyed several stimulating scientific discussions with several other current members of the Institute, especially Alexandra Landsman, Ulf Saalmann, Lukas Medisauskas, Nur Ünal, and Roderich Moessner, in addition to several collaborative conversations with Jan-Michael Rost.

Finally, I was able to finish extensive revisions to a major review article during my stay in Dresden, coauthored by myself, P. Giannakeas, and J. Perez-Rios, which was published in the journal *Reviews of Modern Physics* (volume **89**, article 035006, 2017) with the title *Universal few-body physics and cluster formation*.

Gutzwiller Fellowship 2018

(Prof. Werner Krauth)

Introduction Two years ago, in late 2016, I received the invitation to join the **mpipks**, as the 2018 Gutzwiller fellow. This great honor presented the opportunity to rediscover the institute which I had visited only once, for two days in 2009. Prof. Roderich Moessner then proposed me for the Research Award of the Alexander von Humboldt Foundation, which I was very fortunate to receive. My first long-term academic stay in Germany since 1986 thus got off to a great start.

I stayed at **mpipks** from 3 January to 28 June 2018 and again, very briefly in December 2018. (My next visit, in the context of my Humboldt fellowship, is scheduled for May 2019.) I quickly made my home in Dresden and at the institute, where I could work completely undisturbed when I needed to, but also exchange and discuss, collaborate and present results and overviews in seminars and colloquia. I participated in (parts of) many workshops at **mpipks** and meet new and old colleagues who came to **mpipks** for the weekly workshops. From the **mpipks**, I also traveled twice to the United States for invited conferences, and inside Germany to the University of Düsseldorf, the University of Leipzig, and several times each to the Free University and the Humboldt-University in Berlin, for colloquia and conferences. Several times, I returned very briefly to the Ecole normale supérieure (Paris), my home institution, for urgent university duties.

As a key element of the Gutzwiller program, the **mpipks** invited my PhD students at Ecole normale supérieure (J. U. Klamser, Z. Lei, L. Qin) and two of my junior collaborators (M. F. Faulkner, Bristol (Great Britain) and S. C. Kapfer, Erlangen (Germany)) to come for one month each, during my stay. All of them felt very welcome, and they were as much impressed by the infrastructure and the scientific environment as I was.

My six-month stay at **mpipks** was highly productive. Work on Coulomb systems [1] was meant to provide an entirely new perspective on computer simulation for long-range interacting systems that are studied by thousands of groups world-wide. Research on one-dimensional particle systems [2] resulted in a very surprising mathematically rigorous convergence theorem for irreversible Markov chains. A paper on thermodynamic phases in active matter [3], published in *Nature Communications*, clarified the continuity of equilibrium thermodynamic phases.

All-atom computations with irreversible Markov chains For more than ten years [4, 5], I have been convinced of the potential of irreversible Markov chains. While successful in statistical physics, the approach had not been applied in chemical and biological physics.

During my stay as a Gutzwiller-fellow, I applied the irreversible event-chain Monte Carlo (ECMC) algorithm to the simulation of dense all-atom systems with long-range Coulomb interactions. ECMC has astonishing properties: It is event-driven and exactly samples the Boltzmann distribution $\exp(-\beta U)$ without any time-step approximations nor spatial cutoffs, yet it need not evaluate the total Coulomb potential U . It thus circumvents the major computational bottleneck of traditional approaches that is associated with P. P. Ewald since the 1920s. ECMC only requires the derivatives of the two-particle Coulomb potential, a problem we solved trivially in 2018. ECMC breaks up the total interaction potential into factors (see Fig. 1).

For particle systems made up of neutral dipolar molecules, and in particular for the very popular “simple point-charge water model with flexible molecules” (SPC/Fw), we then broke up the potential into factors containing between two and six particles (see Fig. 1, again). For this all-atom liquid-water model, we demonstrated that the computational complexity of ECMC scales very well with the system size. This was achieved in a pure particle–particle framework, without the interpolating mesh required for the efficient implementation of the modern “particle-mesh Ewald” Coulomb algorithms.

The conceptual challenges posed by this project appeared out of reach in 2016/17, but were successfully met in an intensive research period during my 2018 stay at **mpipks** (and the visits of my co-authors). Besides overcoming technical problems, we also introduced a consistent mathematical language (see [1, Sect. II]), that I hope will be very fruitful in the future.

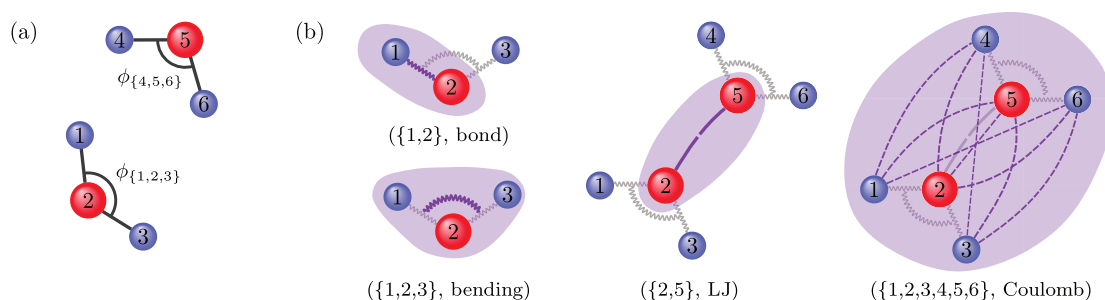


Figure 1: All-atom computations with irreversible Markov chains (see Faulkner et al., J. Chem. Phys. (2018) [1]). This project started shortly before W. Krauth’s stay as a Gutzwiller-fellow at **mpipks** (Jan–June 2018) and was completed there. All but one co-author visited **mpipks** during the project. Key achievement was the successful implementation of the long-range Coulomb potential into the event-chain algorithm. This publication is meant to open the way to the use of Monte Carlo methods in chemical and biophysical all-atom computations.

Mixing and perfect sampling in one-dimensional particle systems In computational physics, and especially in the analysis of Monte Carlo algorithms, the rigorous analysis of computing requirements (mixing times, convergence times), is often not achievable. New algorithms then take much time to impose themselves until empirical studies reach consensus on their correctness and speed. A few years ago, the irreversible Markov chains that I have long been interested in were in this uncomfortable situation, with the general public often doubtful about their correctness and merit.

During my stay at **mpipks** (and the visit of Z. Lei there), we studied the approach to equilibrium of the event-chain Monte Carlo algorithm for the one-dimensional hard-sphere model (see Fig. 2). Using the connection to the coupon-collector problem, we were able to prove rigorously that a specific version of this local irreversible Markov chain realizes perfect sampling in $\mathcal{O}(N^2 \log N)$ single steps for N spheres, whereas the reversible local Metropolis algorithm requires $\mathcal{O}(N^3 \log N)$ single steps for mixing. This confirmed a special case of an earlier conjecture about $\mathcal{O}(N^2 \log N)$ scaling of mixing times of ECMC and of the lifted forward Metropolis algorithm, its discretized variant. We also proved that sequential ECMC (with swaps), an algorithm that we introduced in this project, realizes perfect sampling in $\mathcal{O}(N^2)$ single events.

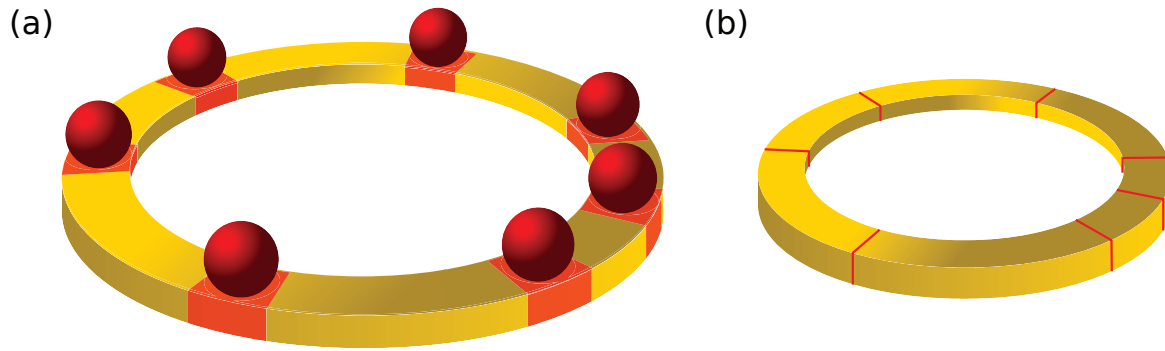


Figure 2: Mixing and perfect sampling in one-dimensional particle systems (see Lei and Krauth, EPL (2018) [2]). This project started during W. Krauth's stay as a Gutzwiller-fellow at **mpipks** (Jan-June 2018). Both co-authors were at **mpipks** during most of the project. Key achievements were the mathematically rigorous analysis of the convergence properties of an irreversible Markov chain, and the proposal of an improved algorithm.

A few months after the stay at **mpipks**, the paper proving the mixing time for the event-chain Monte Carlo's superior mixing time [2] has become a key element of my seminars and presentations, especially for mathematical audiences. Together with a subsequent paper [6], it forms the core of Ze Lei's thesis (2018) [7].

Thermodynamic phases in two-dimensional active matter In recent years, active matter has been much studied for its intriguing properties such as collective motion, motility-induced phase separation and giant fluctuations. However, it had remained unclear how the states of active materials connect with the equilibrium phases. For two-dimensional systems, this was also because the understanding of the liquid, hexatic, and solid equilibrium phases and their phase transitions is recent [8,9].

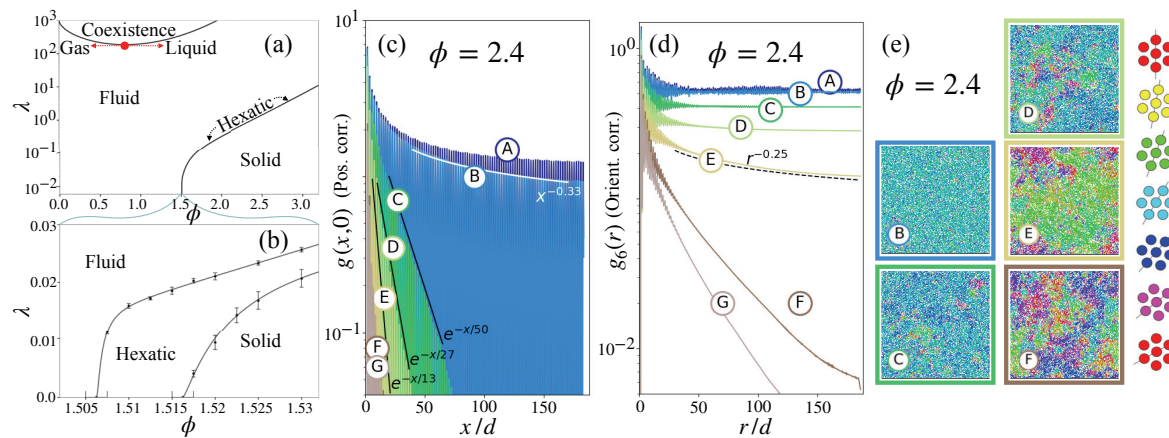


Figure 3: Thermodynamic phases in two-dimensional active matter (see Klamser et al., Nature Comm (2018) [3]). Essential parts of this project were completed, and the paper was written during W. Krauth's stay as a Gutzwiller-fellow at **mpipks** (Jan-June 2018). All co-authors of the publication visited **mpipks** during the project. Main achievement was the rigorous characterization of liquid, hexatic, and solid phases in a model of two-dimensional active matter in continuity with the passive systems described by equilibrium statistical mechanics.

During my stay at **mpipks** (and visits of J. U. Klamser and S. C. Kapfer there), we showed that two-dimensional self-propelled particles with inverse-power-law repulsions moving with a kinetic Monte Carlo algorithm without alignment interactions preserve all equilibrium phases up to very large activities. Furthermore, we were able to show that at high activity within the liquid phase, a critical point opens up a gas-liquid motility-induced phase separation region (see Fig. 3). In our model, two-step melting and motility-induced phase separation are thus independent phenomena.

In the paper (published in Nature Communications [3]), we thus clarified the behavior of a certain class of active materials and connected it to that of systems described by equilibrium thermodynamics. Together with a follow-up manuscript [10], it forms the core of J. U. Klamser's thesis (2018) [11].

Conclusion The 2018 Gutzwiller-fellowship at **mpipks** was a great honor, and it started a very productive period in my research career. The possibility to have junior collaborators join me at the pre-doctoral and post-doctoral level was very helpful. While I personally enjoyed this unique fellowship, I hope to also have

contributed to the liveliness and attractiveness of **mpipks**, where I would like to return to regularly, in the framework of my Humboldt fellowship. In one word, I had the best of times, amongst an outstanding senior and junior faculty and a dedicated and competent technical and administrative staff.

- [1] M. F. Faulkner, L. Qin, A. C. Maggs, and W. Krauth. All-atom computations with irreversible Markov chains. *The Journal of Chemical Physics*, 149(6):064113, 2018.
- [2] Z. Lei and W. Krauth. Mixing and perfect sampling in one-dimensional particle systems. *EPL*, 124(2):20003, 2018.
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- [4] E. P. Bernard, W. Krauth, and D. B. Wilson. Event-chain Monte Carlo algorithms for hard-sphere systems. *Phys. Rev. E*, 80:056704, 2009.
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- [6] Z. Lei, W. Krauth and A. C. Maggs. Event-chain Monte Carlo with factor fields. *arXiv e-prints*, 2018.
- [7] Z. Lei. *Irreversible Markov Chains for Particle Systems and Spin Models: Mixing and Dynamical Scaling*. PhD thesis, École Normale Supérieure, Paris, 2018.
- [8] E. P. Bernard and W. Krauth. Two-Step Melting in Two Dimensions: First-Order Liquid-Hexatic Transition. *Phys. Rev. Lett.*, 107:155704, 2011.
- [9] S. C. Kapfer and W. Krauth. Two-Dimensional Melting: From Liquid-Hexatic Coexistence to Continuous Transitions. *Phys. Rev. Lett.*, 114:035702, 2015.
- [10] J. U. Klamsner, S. C. Kapfer, and W. Krauth. A kinetic-Monte Carlo perspective on active matter. *arXiv e-prints*, 2018.
- [11] J. U. Klamsner. *Low-dimensional phase transitions in and outside equilibrium*. PhD thesis, Sorbonne University, Paris, 2018.

3.3.1.2 PKS-Fellows

Ultra-intense laser-matter interaction: From plasma physics to quantum electrodynamics

(Dr. Felix Mackenroth)

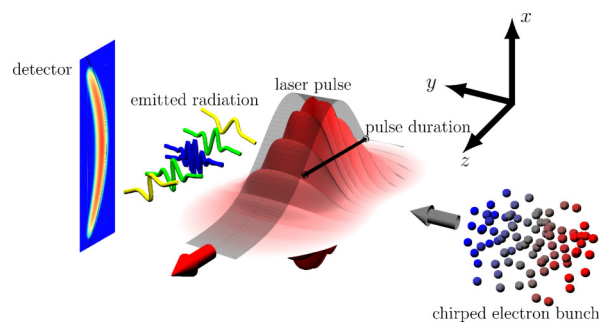


Figure 1: [from [1]] Schematic view of the a proposed scheme to measure the duration of an ultra-intense laser pulse directly in its focus from the emission patterns of an energy chirped electron bunch scattered from the laser.

Single-particle dynamics in ultra-intense electromagnetic fields As first pillar of my research agenda, I studied dynamics of single particles in ultra-intense electromagnetic fields in classical as well as QED regimes.

Together with a visitor at **mpipks** I developed a novel approach to perform metrology on ultra-intense laser fields [1] at full intensity inside their focus. In order to quantify such fields, precise knowledge of their spatiotemporal shape is required. Due to material damage, however, conventional metrology devices are inapplicable at highest intensities, limiting laser metrology thereby to indirect schemes at attenuated intensities. Direct metrology, capable of benchmarking these methods, thus far only provided static properties of short-pulsed lasers with no scheme suggested to extract dynamical laser properties. Most notably, this leaves the duration of an ultra-intense laser pulse in its focus unknown at full intensity. We demonstrated how the electromagnetic radiation pattern emitted by an electron bunch with a temporal energy chirp colliding with the laser pulse depends on the laser pulse duration and how this could be employed to determine the temporal pulse duration directly in its focus at full intensity.

Next to this applied study, I was involved in a pioneering study of a pure QED process: We studied nonlinear electron-positron pair production by an electron colliding with an arbitrary plane wave laser field (nonlinear trident pair production) analytically and numerically [2]. We could demonstrate that, while the full expression for the transition amplitude of the process as obtained from Wick's theorem is divergent and not manifestly gauge invariant, one can unambiguously gauge invariance effectively

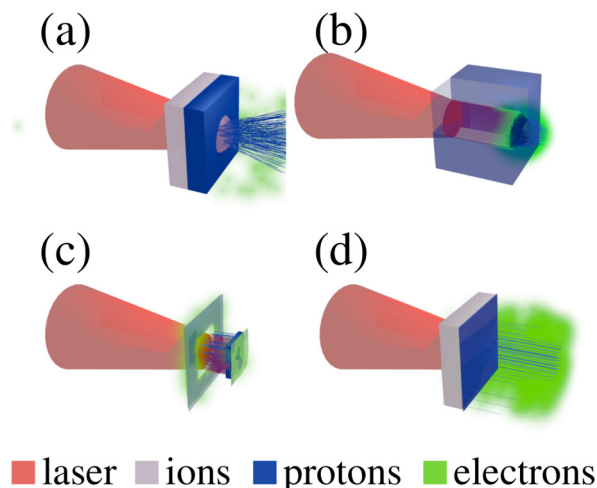


Figure 2: [from [5]] Laser (from left in red) impinging on optimized target designs driving standard high-power ion acceleration schemes: (a) Coulomb explosion of a double-layered target consisting of electrons (green), protons (blue) and heavier ions (light purple), (b) hole boring, (c) radiation pressure acceleration, (d) (thermal) target normal sheath acceleration.

regularizing the amplitude. As a consequence of this process, the amplitude split into a two-step and a one-step contributions, depending on the scaling dependence on the laser pulse duration. We studied both these contributions separately in the produced positron angular distribution and spectra and pointed out the possibility to measure the hitherto elusive one-step contribution experimentally. As a consequence of this work we could put stringent bounds on the applicability of commonly employed approximations in large-scale simulations of QED effects in laser-plasma interactions, which include only the two-step contribution.

Finally, in collaboration with researchers from the **mpipks** we could elucidate an long-standing, fundamentally important question of single-particle dynamics in ultra-strong magnetic fields using the same methods of nonlinear QED [3]. We provided first calculations of radiative transitions between states of an electron in a homogeneous magnetic field of arbitrary strength for low lying Landau levels, which are the relevant levels at ultra strong magnetic fields. In particular, we computed the rates of spin flip transitions at such low Landau levels and found them to be fundamentally different from the hitherto widely employed results obtained by Sokolov & Ternov. We found that the degree of spin polarization of the electron due to asymmetries in the radiative spin flip transitions is strongly underestimated by earlier calculations at low Landau levels and could provide quantitatively corrected rates.

Laser-ion acceleration As a second pillar of my research agenda, I studied and further optimized presently employed theoretical proposals of laser-plasma based ion acceleration schemes.

The most conventionally used scheme to accelerate ions with high-power lasers is to heat a plasma bulk and use the thermal expansion of the plasma electron to accelerate the residual ions. I contributed to an improved understanding of how lasers deposit their energy and how the detailed dynamics of this energy deposition may be used to control ion acceleration [4]. I provided theoretical modeling for a study that experimentally investigated the transverse expansion of the plasma electrons along the surface of a plasma heated by two laser pulses. If the pulses were spatially separated by less than three laser spot diameters, the resulting proton beam profiles became elliptical and the ellipses could be rotated by introducing a small intensity difference between the two pulses. My simple model described how the transverse shape of the electron sheath on the rear of the target depends on the relative intensity between the foci and its free parameters were estimated self-consistently through a series of high resolution, two-dimensional particle-in-cell simulations.

Next to studying such thermal ion acceleration schemes, I contributed to quantitatively comparing the basic laser-ion acceleration schemes going beyond thermal schemes (s. Fig. 2 for an overview). We could benchmark these schemes' performances at a given laser power against each other and identify the most promising schemes [5]. In contrast to earlier studies, in this work we used theoretical models and numerical simulations to systematically examine and compare the existing schemes of laser-based ion acceleration in their ability to provide high ion fluxes at varying ion energy levels. This was motivated by the observation that the ions' energy, which is usually optimized, is only one of several parameters

characterizing the beams' aptness for any desired application. For example, the usefulness of laser-based ion sources for medical applications such as the renowned hadron therapy, and potentially many more, can also crucially depend on the number of accelerated ions or their flux at a required level of ion energies.

Furthermore, we put an earlier proposal of controlling ion acceleration by a finely tunable laser pulse chirp on a solid foundation [6]. The proposal was that ions can be dragged by an electron bunch trapped in a controllably moving potential well formed by a standing wave generated in the reflection of laser radiation. In this work we analyzed general feasibility aspects of such standing wave acceleration and demonstrated its robustness against field structure imperfections, such as those caused by misalignment, ellipticity, and limited contrast.

Joint nonlinear plasma-QED theory framework Finally, it poses a long standing problem to unify the theoretical frameworks of strong field QED and classical plasma physics. The main reason for this challenge to persist over a long time is that classical plasma physics calculations are fundamentally incompatible with QED concepts, using wave functions instead of particle trajectories and projections on asymptotic states instead of continuously flowing time. These differences have not yet been reconciled, indicating a serious gap between high-power laser technology and theory. On the other hand, it is becoming increasingly apparent that at upcoming high-power laser facilities neither of these theory frameworks can be studied without accounting for the respective other: Collective plasma physics is predicted to be qualitatively altered by relativistic quantum phenomena and relativistic quantum dynamics will be affected by collective plasma effects. However, there does not yet exist a theory framework consistently describing relativistic quantum and plasma physics jointly.

We accomplished a first step in this direction by studying radiation emission triggered by a laser pulse traveling through a plasma [7]. Such a laser pulse can feature group velocities significantly differing from the speed of light in vacuum. This modifies the well-known Volkov states of an electron inside a strong laser-field from the vacuum case and consequently all quantum electrodynamical effects triggered by the electron. To develop a nonlinear QED description we solved the relativistic quantum equations of motion inside a laser field propagating through a nontrivial background plasma and used the found wave functions as basis for obtaining nonperturbative QED calculations. In particular, we studied photon emission from an electron scattered by the intense laser pulse inside the plasma, labeled nonlinear Compton scattering. We found the background plasma to significantly alter the emission's spectral properties, while leaving its angular distribution unchanged with respect to the vacuum case.

- [1] *Determining the duration of an intense laser pulse directly in focus*, F.M. and A. R. Holkundkar arXiv:1712.06898 (2017).
- [2] *Nonlinear trident pair production in an arbitrary plane wave: a focus on the properties of the transition amplitude*, F.M. and A. Di Piazza arXiv:1805.01731 (2018).
- [3] *Radiative spin polarization of twisted electrons in an ultrastrong magnetic field*, K. van Kruining, F.M., J.B. Götze, arXiv:1809.02133 (2018).
- [4] *Transverse expansion of the electron sheath during laser acceleration of protons*, K. Svensson, F.M. et al, *Physics of Plasmas* **24**, 123109 (2017).
- [5] *Reaching high flux in laser-driven ion acceleration*, F.M., A. Gonoskov and M. Marklund, *The European Physical Journal D* **71**, 204 (2017).
- [6] *Prospects for laser-driven ion acceleration through controlled displacement of electrons by standing waves*, J. Magnusson, F.M. et al., *Physics of Plasmas* **25**, 053109 (2018).
- [7] *Nonlinear Compton scattering of an ultra-intense laser pulse in a plasma*, F.M. et al., arXiv:1805.01762 (2018).

3.3.2 Conferences, Workshops and Symposia

1. *Charge Transfer meets Circuit Quantum Electrodynamics*
Workshop: June 29 - July 3, 2015 63 participants
Scientific coordinators: M. Blencowe, B. Huard, B. Kubala
2. *Mathematics and Physics of Multilayer Complex Networks*
Focus Workshop: July 6 - 8, 2015 45 participants
Scientific coordinators: A. Arenas, M. A. Porter
3. *Quantum Design*
Seminar and Workshop: July 13 - 24, 2015 66 participants
Scientific coordinators: A. Chubukov, P. Coleman, D. K. Morr, M. Vojta

4. *Dynamics of Coupled Oscillators: 40 Years of the Kuramoto Model*
Workshop: July 27 - 31, 2015 92 participants
Scientific coordinators: A. Pikowsky, A. Politi, M. Rosenblum
5. *Nanoscale Assemblies of Semiconductor Nanocrystals, Metal Nanoparticles and Single Molecules: Theory, Experiment and Application*
Workshop: August 24 - 28, 2015 81 participants
Scientific coordinators: A. Eychmüller, A. Govorov, V. May
6. *Synthetic Quantum Magnetism*
Workshop: August 31 - September 4, 2015 91 participants
Scientific coordinators: A. Eckardt, M. Lewenstein, I. Spielman, M. Ueda
7. *Quantum Transport in One Dimension*
Workshop: September 15 - 18, 2015 100 participants
Scientific coordinators: A. Mirlin, F. von Oppen
8. *Korrelationstage 2015*
Workshop: September 28 - Oktober 2, 2015 78 participants
Scientific coordinators: M. Garst, S. Kehrein, H.-H. Klauss
9. *Martin Gutzwiller's scientific Universe: From Wavefunctions over periodic Orbits to Sun, Moon and Earth*
Workshop: October 28 - 31, 2015 71 participants
Scientific coordinators: J.-M. Rost, S. Tomsovic, D. Vollhardt
10. *Atomic Physics 2015*
Workshop: November 23 - 27 86 participants
Scientific coordinators: A. Kuleff, A. Eisfeld, J.-M. Rost
11. *Topological Phenomena in Novel Quantum Matter: Laboratory Realization of Relativistic Fermions and Spin Liquids*
Workshop: Februar 29 - March 4, 2016 89 participants
Scientific coordinators: C. Broholm, M. Oshikawa, A. Rosch
12. *Two-Phase Continuum Models for Geophysical Particle-Fluid Flows*
Seminar and Workshop: March 14 - April 15, 2016 52 participants
Scientific coordinators: G. Bewley, J. McElwaine, A. Valance
13. *Prospects and Limitations of Electronic Structure Imaging by Angle Resolved Photoemission Spectroscopy*
Focus Workshop: April 25 - 27, 2016 38 participants
Scientific coordinators: S. Kera, S. Kümmel, A. Schöll
14. *Strong Correlations and the Normal State of the High Temperature Superconductors*
Seminar and Workshop: May 17 - 27, 2016 80 participants
Scientific coordinators: A. Chubukov, B. Keimer, M. Randeria, S. Sebastian
15. *FFLO-Phase in Quantum Liquids, Quantum Gases, and Nuclear Matter*
Workshop: June 20 - 24, 2016 53 participants
Scientific coordinators: A. Buzdin, M. Eschrig, J. Wosnitzer
16. *Topological Patterns and Dynamics in Magnetic Elements and in Condensed Matter*
Seminar and Workshop: June 27 - July 8, 2016 55 participants
Scientific coordinators: R. Ignat, S. Komineas, N. Papanicolaou
17. *Disorder, Interactions and Coherence: Warps and Delights*
Focus Workshop: July 13 - 15, 2016 63 participants
Scientific coordinators: S. Brazovskii, N. Kirova, L. Levitov
18. *Floquet Physics*
Focus Workshop: August 8 - 10, 2016 13 participants
Scientific coordinators: R. Moessner, S. Sondhi

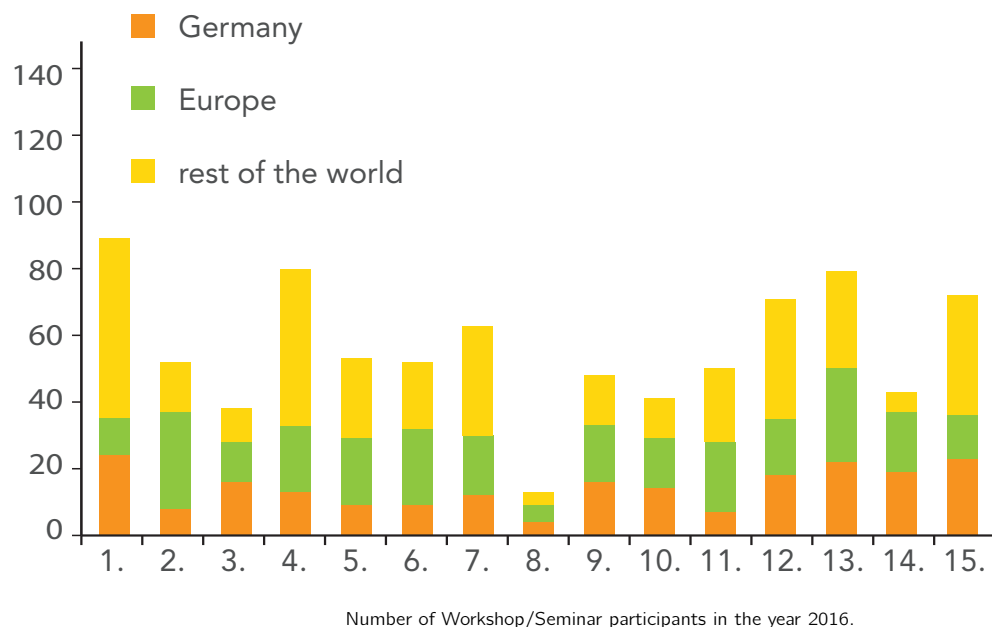
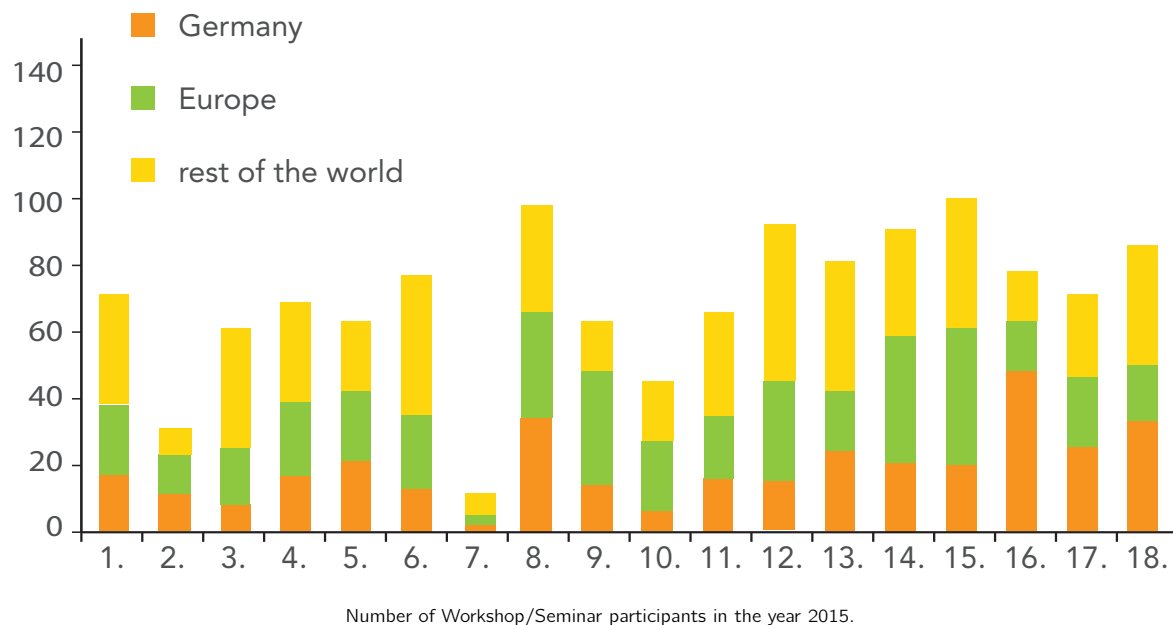
19. *Pattern Dynamics in Nonlinear Optical Cavities*
Workshop: August 15 - 19, 2016 48 participants
Scientific coordinators: N. Broderick, B. Krauskopf, K. Lüdge
20. *Principles of Biological and Robotic Navigation*
Focus Workshop: August 29 - 31, 2016 41 participants
Scientific coordinators: B. M. Friedrich, U. B. Kaupp, S. Sanchez
21. *Bridging-Time Scale Techniques and their Applications in Atomistic Computational Science*
Focus Workshop: September 12 - 15, 2016 50 participants
Scientific coordinators: M. Posselt, R. Smith, B. Uberuaga
22. *Multistability and Tipping: From Mathematics and Physics to Climate and Brain*
Seminar and Workshop: September 19 - October 14, 2016 71 participants
Scientific coordinators: U. Feudel, A. Pisarchik, K. Showalter
23. *Physical Biology of Tissue Morphogenesis - Mechanics, Metabolism and Signaling*
Workshop: October 17 - 21, 2016 79 participants
Scientific coordinators: Y. Bellaïche, S. Eaton, J.-F. Joanny, F. Jülicher
24. *Tensor Product State Simulations of Strongly Correlated Systems*
School: November 1 - 5, 2016 43 participants
Scientific coordinators: F. Pollmann, N. Schuch, F. Verstraete
25. *Atomic Physics 2016*
Workshop: November 28 - December 2, 2016 72 participants
Scientific coordinators: A. Landsman, J.-M. Rost
26. *Quantum-Classical Transition in Many-Body Systems: Indistinguishability, Interference and Interactions*
Workshop: February 13 - 17, 2017 85 participants
Scientific coordinators: A. Buchleitner, J.-D. Urbina
27. *Quantum Dynamics in Tailored Intense Fields*
Focus Workshop: February 27 - March 1, 2017 81 participants
Scientific coordinators: M. Lein, G. Paulus, J.-M. Rost
28. *Dynamical Probes for Exotic States of Matter*
Workshop: March 27 - 30, 2017 76 participants
Scientific coordinators: M. Knap, R. Moessner, F. Pollmann
29. *Joint IMPRS Workshop on Condensed Matter, Quantum Technology and Quantum Materials*
Workshop: April 3 - 7, 2017 80 participants
Scientific coordinators: S. Gzyl, A. Kenfack, M. König, H.-G. Libuda
30. *Many paths to interference: a Journey between Quantum Dots and Single Molecule Junctions*
Focus Workshop: April 18 - 20, 2017 38 participants
Scientific coordinators: A. Donarini, L. Zotti
31. *Discrete, Nonlinear and Disordered Optics*
Workshop: May 8 - 12, 2017 57 participants
Scientific coordinators: M. Segev, A. Szameit, S. Turitsyn
32. *Future Trends in DNA-based Nanotechnology*
Workshop: May 29 - June 2, 2017 102 participants
Scientific coordinators: Ch. Fan, M. Mertig, H. Yan
33. *Quantum Memory from Quantum Dynamics*
Symposium: June 15 - 17, 2017 42 participants
Scientific coordinators: J. S. Briggs, J.-M. Rost, W. T. Strunz

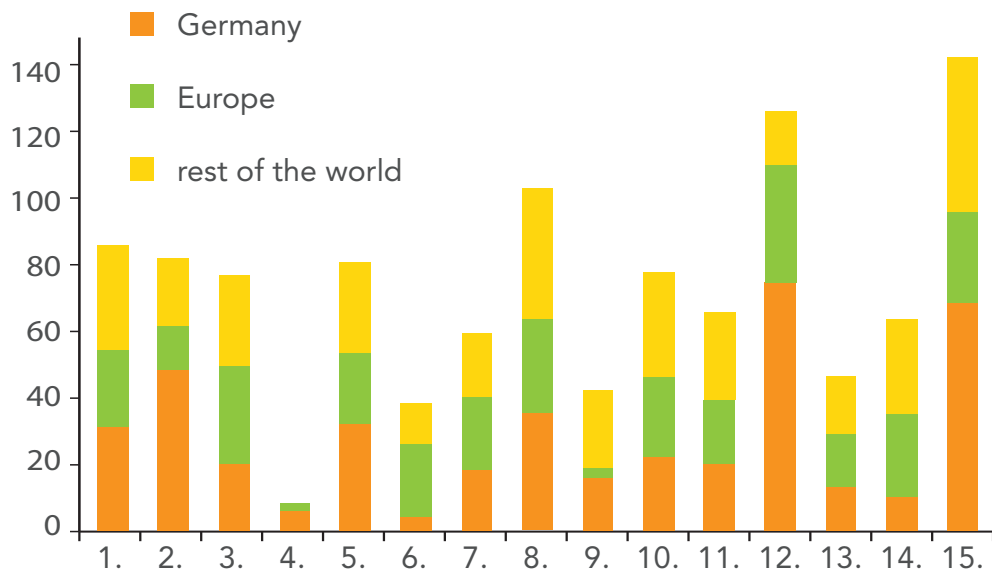
34. *Brain Dynamics on Multiple Scales - Paradigms, their Relations, and Integrated Approaches*
Workshop: June 19 - 23, 2017 77 participants
Scientific coordinators: P. Achermann, E. Olbrich, T. Wennekers
35. *Climate Fluctuations and Non-Equilibrium Statistical Mechanics: an Interdisciplinary Dialogue*
Seminar and Workshop: July 10 - August 4, 2017 55 participants
Scientific coordinators: J. Krug, B. Marston, J. Weiss, R. Zia
36. *Korrelationstage 2017*
Workshop: September 11 - 15, 2017 125 participants
Scientific coordinators: S. Eggert, A. Mackenzie, S. R. Manmana
37. *Quantum Sensing with Quantum Correlated Systems*
Workshop: September 25 - 29, 2017 46 participants
Scientific coordinators: M. Oberthaler, S. Rachel, A. Sanpera Trigueros
38. *Critical Stability of Quantum Few-Body Systems*
Seminar and Workshop: October 9 - 20, 2017 63 participants
Scientific coordinators: T. Frederico, A. Jensen, A. Kievsky, J.-M. Richard
39. *Atomic Physics 2017*
Workshop: November 27 - December 1, 2017 141 participants
Scientific coordinators: T. Pfau, J.-M. Rost
40. *Topological Matter in Artificial Gauge Fields*
School: February 26 - March 2, 2018 75 participants
Scientific coordinators: A. Eckardt, F. Heidrich-Meisner, C. Weitenberg
41. *Chaos and Dynamics in Correlated Quantum Matter*
Workshop: March 19 - 22, 2018 80 participants
Scientific coordinators: D. Luitz, R. Moessner, F. Pollmann
42. *Novel Paradigms in Many-Body Physics from Open Quantum Systems*
Workshop: March 26 - 29, 2018 89 participants
Scientific coordinators: E. Dalla Torre, S. Diehl, F. Piazza
43. *New Platforms for Topological Superconductivity with Magnetic Atoms*
Focus Workshop: April 9 - 11, 2018 50 participants
Scientific coordinators: T. Cren, K. Franke, P. Simon
44. *Predicting Transitions in Complex Systems*
Workshop: April 23 - 27, 2018 76 participants
Scientific coordinators: J. Hlinka, K. Lehnertz, C. Masoller
45. *Quantum and Semiclassical Trajectories*
Focus Workshop: June 12 - 14, 2018 26 participants
Scientific coordinators: B. Poirier
46. *Optimising, Renormalising, Evolving and Quantising Tensor Networks*
Workshop: June 18 - 22, 2018 55 participants
Scientific coordinators: A. G. Green, R. Melko, T. J. Osborne
47. *Machine Learning for Quantum Many-body Physics*
Workshop: June 25 - 29, 2018 76 participants
Scientific coordinators: R. Melko, T. Neupert, S. Trebst
48. *Frustration, Orbital Fluctuations, and Topology in Kondo Lattices and their Relatives*
Seminar and Workshop: July 16 - August 3, 2018 58 participants
Scientific coordinators: I. Sodemann, S. A. Parameswaran, S. Nakatsuji, D. E. Logan

49. *Synthetic Non-Hermitian Photonic Structures: Recent Results and Future Challenges*
 Workshop: August 13 - 17, 2018 52 participants
 Scientific coordinators: A. Eisfeld, R. El-Ganainy, T. Kottos, H. Schomerus
50. *Single Nanostructures, Nanomaterials, Aerogels and their Interactions: Combining Quantum Physics and Chemistry*
 Workshop: August 27 - 31, 2018 66 participants
 Scientific coordinators: A. Eychmüller, A. Govorov, A. Knorr
51. *Stochastic Thermodynamics: Experiment and Theory*
 Workshop: September 10 - 14, 2018 75 participants
 Scientific coordinators: J. Bechhoefer, S. Ciliberto, S. Pigolotti, E. Roldan
52. *Anderson Localization and Interactions*
 Workshop: September 24 - 28, 2018 78 participants
 Scientific coordinators: F. Evers, A. D. Mirlin
53. *Stochastic Dynamics on Large Networks: Prediction and Inference*
 Seminar and Workshop: October 8 - 26, 2018 41 participants
 Scientific coordinators: M. Opper, G. Sanguinetti, P. Sollich
54. *Correlated Electrons in Transition-Metal Compounds: New Challenges*
 Workshop: November 5 - 9, 2018 94 participants
 Scientific coordinators: M. Grüninger, G. Sawatzky, J. van den Brink
55. *Tensor Network based approaches to Quantum Many-Body Systems*
 School: November 13 - 17, 2018 70 participants
 Scientific coordinators: F. Pollmann, U. Schollwöck, N. Schuch, F. Verstraete
56. *Atomic Physics 2018*
 Workshop: November 26 - 30, 2018 75 participants
 Scientific coordinators: S. Popruzhenko, J.-M. Rost, U. Saalmann

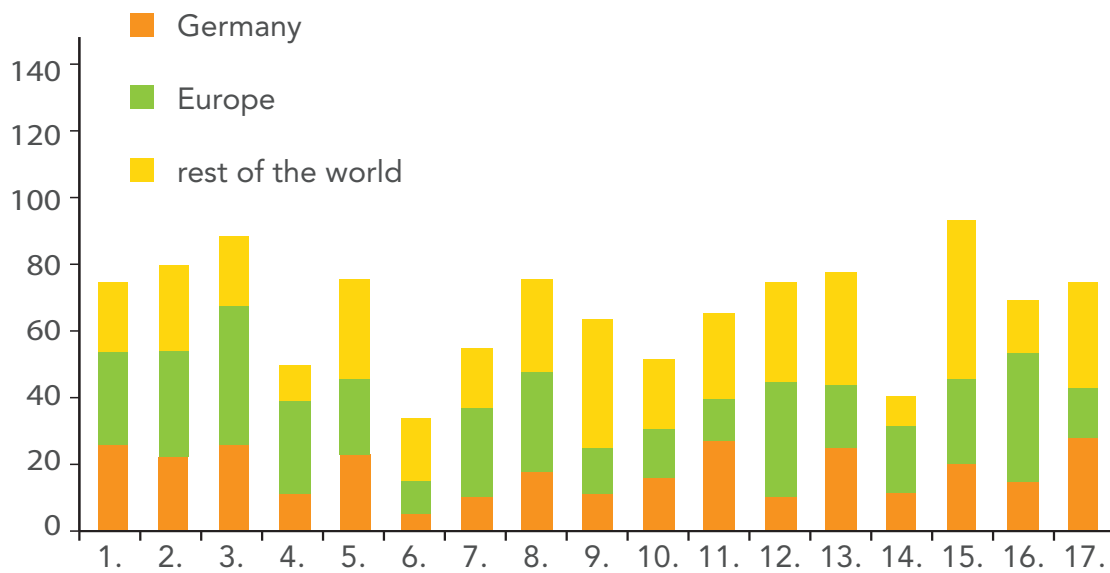
3.3.3 Workshop Participation and Dissemination of Results

Statistics of Workshop participation





Number of Workshop/Seminar participants in the year 2017.



Number of Workshop/Seminar participants in the year 2018.

Dissemination of Workshop Results

As the Workshop Program of the **mpipks** focuses 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 *Topological Patterns and Dynamics in Magnetic Elements and in Condensed Matter*
Sisodia, N., S. Komineas, P. K. Muduli: Chiral skyrmion auto-oscillations in a ferromagnet under spin transfer torque. arxiv: 1808.01436 (2016)
- Workshop *Multistability and Tipping: From Mathematics and Physics to Climate and Brain*
Feudel, U., A. Pisarchik and K. Showalter (Eds.): Multistability and Tipping Chaos. Focus Issue (2018)
- Seminar and Workshop *Climate Fluctuations and Non-Equilibrium Statistical Mechanics: An Interdisciplinary Dialogue*
Blencer, R., D. Gohlke, and F. Lunkeit: Fluctuation Analysis of the Atmospheric Energy Cycle. *Physical Review E* 98, 023101 (2018)
Buschow, S and P. Friedrichs: Local dimension and recurrent circulation patterns in long-term climate simulations. *Chaos* 28, 083124 (2018)
Friedrichs, P., S. Wahl and S. Buschow: Post-processing for extreme events. In: S. Vannitsem, D. Wilks, and J. Messner (Eds.): *Statistical Postprocessing of Ensemble Forecasts*. 127-154 (2018)
Henriksen, S. V.: Interannual oscillations and sudden shifts in observed and modeled climate. *Atmospheric Science Letters* 19, e850 (2018)
Majumdar, S. N., P. von Bomhard and J. Krug: An exactly solvable record model for rainfall. Submitted to *Physical Review Letters* (2018)
Pearson, B. and B. Fox-Kemper: Log-normal turbulence dissipation in global ocean models. *Physical Review Letters*, 120, 094501 (2018)
Stainfordth, D. A., S. C. Chapman and N. W. Watkins: The Consequences of Climate Model Evaluations. Submitted to *Nature Communications* (2018)
- International School and Workshop *Critical Stability of Quantum Few-Body Systems*
Frederico, T. and J.-M. Richard (Eds.): *Critical Stability. Few-Body Systems Special Issue* (2018)
- Workshop *Stochastic Thermodynamics: Experiment and Theory*
Special edition of *Journal of Statistical Mechanics: Theory and Experiments (JStat)*, to be published in early 2019

3.3.4 Workshop Reports

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 **mpipks**, 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 mesoscopic physics in a variety of regimes and systems.

Mathematics and Physics of Multilayer Complex Networks, Focus Workshop

Scientific coordinators: A. Arenas, M. A. Porter

The international workshop, Mathematics and Physics of Multilayer Complex Networks (MAPCOM15) was one of the highlight gatherings for the network-science community in 2015.

The 2.5-day workshop had a dense and exciting scientific program: more than a dozen of the world's leaders in the analysis of multilayer networks presented their latest work (either as invited speakers or as contributed speakers), and numerous rising stars in network science also presented talks. Talks by experts included the latest work by Shlomo Havlin and Peter Grassberger on percolation on multilayer networks (their perspectives differed, and the debate on this was lively), Marc Barthelemy on multilayer networks in transportation networks in cities, and Vittoria Colizza on using multilayer-network representations of temporal networks for the analysis of disease propagations in increasingly realistic networked structures. The talks by the young participants, who were from diverse backgrounds and nationalities, were very vibrant, and the network-science community clearly has much to which to look forward in the coming years. It was by design that so many young scholars were chosen as speakers, and they used the opportunity to discuss their work with scientific leaders and also to interact with them more generally. The workshop also included a very good gender balance, which tends to be uncommon in hard-science topics. The discussions at MAPCOM15 were plentiful and spirited (sometimes very spirited), and they spilled over into the coffee breaks, poster sessions, and social dinner and excursion.

As suggested by the title, the conference focused on the theory and applications of what has become known as "multilayer networks", which has quickly become arguably the most prominent area in network science during the last couple of years and which encompasses networks with multiple types of ties, multiple networks that are coupled to each other, and many other examples. Some talks focused on structural considerations, but many others focused on dynamical processes (such as percolation, oscillators, and epidemics) on multilayer networks. Still others, such Thilo Gross, focused on their potential use in disciplines — e.g. ecology — in which the language of multilayer networks is not yet very common. The participants left with a clear idea of the state of the field, where it is heading, and what are the outstanding open problems.

The workshop also included a vibrant journal session with a panel of editors from Nature Physics, Physical Review X (the editor in chief), and Physical Review E. The panel and the audience discussed both directly scientific issues, such as what types of articles are appropriate for those journals when undertaking interdisciplinary work (e.g. in complex systems) and other issues, such making data and code public (and privacy issues for human data), what work in interdisciplinary topics is also "physics", and so on. Another important issue that was discussed at the workshop was how to use ideas from developing fields, such as the study of multilayer networks, in inherently very messy scientific problems (e.g. in biological topics like neuroscience).

The short workshop demonstrated clearly that multilayer networks is an exciting field that has had many successes — especially recently — and which holds a great deal of additional promise in both theory and applications. There are clearly very big challenges that still need to be overcome, and the role of **mpipks** in bringing together leading scholars and rising young scientists for the MAPCOM15 workshop is an invaluable one. Plans for upcoming sequel workshops are already underway.

MAPCOM15 was a capstone workshop demonstrating research that was funded from a 2012–2015 proactive European Commission call on the Dynamics of Multi-Level Complex Systems. The workshop was coordinated scientifically by Alex Arenas and Mason Porter of the PLEXMATH consortium, and MAPCOM15's participants included many representatives from several of the funded consortia.

Quantum Design, Seminar and Workshop

Scientific coordinators: A. Chubukov, P. Coleman, D.K. Morr, M. Vojta

The seminar and workshop QUDES15 was held at **mpipks** during two weeks in July, from July 13 to July 24, 2015. The scientific program of the workshop week contained 28 invited and contributed talks and the colloquium by Prof. van der Marel from the University of Geneva. The second week was the seminar during which there were 8 longer and more detailed talks by mostly junior participants.

The main focus of seminar and workshop was to bring together theorists and experimentalists working on systems of interacting electrons with the focus of understanding and designing novel quantum materials with specific properties, both in the context of fundamental research and potential applications. The topics covered at the workshop included superconductors with unconventional properties and multiple broken symmetries, like Fe-pnictides, systems with topological order, systems far from equilibrium, strongly correlated systems, e.g., heavy fermions and novel correlated electron materials with tailored properties. During the second week we scheduled longer talks on the physics of cuprate and pnictide superconductors, bi-layer graphene, and on new correlated electron materials.

Many prominent scientists from Europe, US, Japan, Israel, and other countries attended the workshop and gave excellent talks. Well-known scientists among workshop and seminar participants included Y. Matsuda (Kyoto), A. Bernevig (Princeton, US), E. Demler (Harvard, US), J. Schmalian (Karlsruhe), H. Manoharan (Stanford, US), E. Berg (Weizmann, Israel), A. Kampf (Augsburg) and many others. In addition, there were many scientific newcomers – junior scientists from all over the world. Some of them, like O. Cyr-Choiniere (Sherbrooke, Canada) and C. Hicks (Dresden), gave talks at the workshop. Others, like D. Chowdhury (Harvard, US), M. Schütt and P. Orth (both from Karlsruhe/Minnesota, US) and B. Roy (Maryland, US) gave longer talks during the seminar week.

The organizers' primary goal was not to focus on one narrow sub-field of physics but bring people working on similar but non-identical problems (e.g., strongly correlated electron systems, novel unconventional superconductors, topological insulators and topological superconductors, novel materials with tailored properties) and not only have in-depth exchange of ideas, but also try to find common features of different materials and common physics. The responses we received from the participants indicate that this concept was successful.

We would like to thank the **mpipks** for its hospitality and excellent infrastructure provided to us and the participants. We would also like to thank the team of secretaries and, in particular, Mandy Lochar, for their kind assistance as well as friendly and efficient support in organizing the meeting.

Dynamics of Coupled Oscillators: 40 Years of the Kuramoto Model, Workshop

Scientific coordinators: A. Pikowski, A. Politi, M. Rosenblum

The main focus of the Workshop was the dynamics of large populations of interacting oscillatory units. The event was dedicated to the 40th anniversary of the first publication on the nowadays very popular Kuramoto model. This simple solvable model explains self-synchronization transition in large ensembles; it became a paradigmatic one and is used in many contexts, e.g. in computational neuroscience. It would not be an exaggeration to say that in studies of oscillatory dynamics the Kuramoto model plays the same central role as the Ising model in studies of phase transitions.

The main aspects addressed in invited and contributed presentations have been: analytical tools, such as the Watanabe-Strogatz theory and Ott-Antonsen ansatz; various extensions of the original Kuramoto model; dynamics on complex networks; analysis of chimera states; finite-size effects and scaling at the synchronization transition; effects of delayed connections; control of network dynamics; connections with phase transitions; experimental studies of lasers, electrochemical oscillators, and mechanical systems. Furthermore, the speakers addressed various aspects of neuronal dynamics modeling, including the analysis of systems with excitatory and oscillatory elements, pulse-coupled systems and firing-rate models, as well as the relationship with the circadian rhythm.

Generally, we believe that there has been a good balance between theoretical and experimental talks and that an appreciated aspect of the Workshop has been the opportunity for each participant to interact with members of different communities: experimentalists, theoretical physicists, and mathematicians. Finally, the friendly environment at the **mpipks** essentially contributed to fruitful discussions and helped to trigger new scientific collaborations.

The Workshop was very timely: it has allowed a fast spreading of recent rigorous mathematical results as well as of different theoretical techniques across the various disciplines. Many participants have indeed expressed a final positive opinion that goes beyond a formal congratulation. The impression of a successful

event is confirmed by the very few cancellations (mostly due to health and family problems). As a result, practically all leading experts in the field, coming from Europe, USA, Japan, and New Zealand, took part in the Workshop. Moreover, the number of applications for the contributed presentations essentially exceeded the limit so that we had to decline quite a number of otherwise meaningful applications. We are grateful to DFG for the additional financial support which made possible the participation of so many overseas speakers. Special thanks go to **mpipks**, its secretary team and especially to Maria Pätzold for her support and a very professional and efficient organization. As a weak point we mention that the breakfasts could have been better.

Nanoscale Assemblies of Semiconductor Nanocrystals, Metal Nanoparticles and Single Molecules: Theory, Experiment and Application, Workshop

Scientific coordinators: A. Eychmüller, A. Govorov, V. May

The Nanosa15 workshop focused on the theory and experiment of assemblies composed by semiconductor nano-crystals, metal nano-particles, molecules, bio-molecules and polymers. Nanosa15 brought together more than 80 scientists, both senior and beginners, from Europe, US, Canada and India. The meeting has covered cutting-edge research in the field of nanoscale physics with a strong inter-disciplinary character. A particular aim was to stimulate interactions and information exchange between theoretical and experimental experts working in this very dynamic field. The extremely productive scientific environment provided by the **mpipks** formed the ideal framework for this mutual interplay. During the five days of the workshop the participants could listen to lectures given by highly recognized speakers from solid state physics, from physical chemistry, from theoretical physics and also from theoretical chemistry. Two late afternoon sessions were dedicated to the discussion of the various posters. Young scientists could present their results in short invited talks or via posters. They took active part in the scientific discussion. This was the way the workshop promoted young active scientists. Another strong and productive side of this Workshop was its international character.

Nanosa15 addressed a multitude of questions on energy and charge transfer in nano-scale assemblies. Recent work has been presented on interfacial phenomena in hybrid systems with potential application in photovoltaics. Graphene nanocrystals were discussed and excitons and plasmons appearing in assemblies of nanocrystals could be described. One particular session was dedicated to recent advances in plasmonics. A specific subject was the discussion of the different facets of aerogels. This went along with the consideration of functional nano-materials including catalytic-, sensor- and bioapplications of nanocrystals. Most of the experimental questions which have been mentioned within the talks were confronted by modern theoretical and computational approaches to complex hybrid nanoscale systems as reported by other speakers.

Going back to their home institutions, all participants have been inspired by the exciting new ideas, the distributed knowledge and the specific information on cutting edge developments in the field of nanoscale assemblies. It is our particular pleasure to thank the local organizers, Katrin Lantsch and Dr. Ly Do, for their perfect organization of the meeting and the great support for its realization. This was very essential for the overall success of Nanosa15.

Synthetic Quantum Magnetism, Workshop

Scientific coordinators: A. Eckardt, M. Lewenstein, I. Spielman, M. Ueda

Quantum magnetism, as it results from the interactions between spin degrees of freedom, lies at the heart of many intriguing phenomena of condensed matter physics. Here strong quantum fluctuations do not only lead to fascinating physics, but also make a theoretical understanding challenging. This is a key motivation for the recent effort to experimentally emulate and study quantum magnetism in engineered synthetic quantum systems — such as trapped ions, atoms, and molecules — under very clean and highly controlled conditions.

During the one-week workshop "Synthetic Quantum Magnetism" (held from August 31 - September 04, 2015, at the **mpipks** in Dresden) experimentalists and theorists met to discuss recent achievements and prospects of this active and rapidly developing field. The workshop was truly international with invited speakers and participants from all over the world. It benefited greatly from having talks by both established senior scientists (Rainer Blatt, John Bollinger, Victor Gurarie, Randy Hulet, Chris Monroe, Frederic Mila, Roderich Moessner, Dan Stamper-Kurn, Peter Zoller, ...) and promising young researchers (such as Marcello Dalmonte, Ulrich Ebling, Igor Ferrier-Barbut, Shunsuke Furukawa, Tobias Grass, Christian

Groß, Philipp Hauke, Jonas Larson, Hsin-I Lu, Steven Moses, Shuta Nakajima, Juliette Simonet, Leticia Tarruell, Lei Wang, ...).

The workshop program covered the latest developments in different experimental platforms and approaches, among others: mimicking frustrated magnetism with hard-core bosons, superexchange magnetism (equilibrium and dynamics) of both fermions and bosons in optical lattices, orbital magnetism in optical lattices, spin-orbit coupling for neutral atoms using synthetic gauge fields, quantum Hall physics with spin degrees of freedoms forming synthetic dimensions, spin-imbalanced fermions with strong interactions, unconventional systems of fermionic atoms with large spin ($>1/2$) featuring either an enlarged $SU(N)$ -symmetry or spin-changing contact interactions, atomic systems with strong dipolar interactions, dissipative spin systems, the quantum engineering magnetism and spin-interactions in ion chains and lattices.

The Scientific coordinators, André Eckardt (Germany), Maciej Lewenstein (Spain), Ian Spielman (United States), and Masahito Ueda (Japan), are very grateful for the great support by the Max-Planck-Institut für Physik komplexer Systeme in Dresden, which made this event such a success; in particular, they are indebted to Amy Wright.

Quantum Transport in One Dimension, Workshop

Scientific coordinators: A. Mirlin, F. von Oppen

The quantum physics of interacting one-dimensional (1D) systems represents a fascinating research area. Theoretically, one of the main features of such systems is the emergence of a strongly correlated state, the Luttinger liquid. Experimentally, it has become possible to realize one-dimensional many-body systems in a surprising variety of ways, including electrons in 1D nanostructures (quantum Hall and topological insulator edges, carbon nanotubes, semiconductor quantum wires), quantum spin chains, as well as cold atoms (both bosonic and fermionic) in optical traps. A central direction of current research is the physics of transport phenomena in these structures, especially far from equilibrium.

The Workshop “Quantum transport in one dimension” involved a balanced participation of theorists and experimentalists, with 100 participants in total, and managed to collect many of the key researchers in the field. The focus was put on the fundamental physics exhibited by novel systems and on emergent phenomena, with a particular emphasis on 1D systems that are under active experimental investigation. The central topics of the Workshop and the corresponding key speakers were:

- integer and fractional quantum Hall edges, quantum Hall interferometry, neutral modes: M. Heiblum (Rehovot), Y. Gefen (Rehovot), C. Strunk (Regensburg);
- integer and fractional topological insulators, edge states, helical Luttinger liquids: K. Ensslin (Zürich), L. Molenkamp (Würzburg), R.-R. Du (Houston), A. Mitra (New York), A. Bernevig (Princeton), A. Kamenev (Minnesota), S. Carr (Kent U), Y. Oreg (Weizmann Inst.), A. Stern (Weizmann);
- topological superconductors and related hybrid structures, Majorana edge modes, and zero-energy Majorana states: A. Yazdani (Princeton), L. Glazman (Yale), R. Egger (Düsseldorf), A. Yacoby (Harvard), E. Berg (Weizmann Inst.), M. Houzet (Grenoble);
- transport properties of quantum wires (Luttinger liquids), including far-from-equilibrium phenomena, Kondo effects: F. Pierre (LPN-CNRS, France), A. Tsvelik (Brookhaven NL), M. Pustilnik (GeorgiaTech), I. Protopopov (Karlsruhe);
- quantum spin chains and ladders: C. Rüegg (Paul Scherer Inst. / Geneva U), M. Klanjsek (Ljubljana);
- cold atom realizations of 1D systems: S. van Frank (TU Wien), J. Catani (LENS, Florence), E. Demler (Harvard);
- 1D Josephson junction arrays: phase slips, interplay of disorder, interactions and superconductivity: D. Haviland (Stockholm), A. Shnirman (Karlsruhe);
- Anderson localization in many-body 1D systems: F. Pollmann (Dresden), I. Gornyi (KIT Karlsruhe), D. Abanin (Geneva).

One of highlights of the conference was the **mpipks** Colloquium talk on “The status of experiments to detect and control Majorana modes in Condensed Matter systems, towards the long-term goal of topological quantum computing” given by C. Marcus (Niels Bohr Inst., Copenhagen), one of pioneers of the field.

In addition to 32 invited talks, the conference program included 15 contributed talks as well as 50 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: A. Braggio (Genoa), H.-S. Sim (KAIST, Korea), D. Meidan (Ben Gurion U), I. C. Fulga (Weizmann Inst.), F. Pientka (FU Berlin), P. Lecheminant (U Cergy-Pontoise), Y. Baum (Weizmann), A. Rahmani (Vancouver), F. Hassler (Aachen).

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.

We would like to thank the Institute staff, and in particular Mandy Lochar, for outstanding organizational support.

Korrelationstage 2015, Workshop

Scientific coordinators: M. Garst, S. Kehrlein, H.-H. Klauss

The workshop "Korrelationstage 2015" was a meeting of physicists working in the field of strongly correlated phenomena. It presented an overview over recent important developments in the field with four invited international keynote speakers, and it also provided a platform for discussion, exchange and networking especially for the German community. During the week between 28 September and 2 October 75 participants attended in total 50 talks in 17 sessions.

The various themes of the sessions reflect the current hot topics in this research field. In six talks on *Fermionic quantum criticality* participants learned about new developments in the difficult problem of quantum critical Fermi surfaces. This is relevant to metals close to a magnetic, superconducting or nematic instability at zero temperature like, e.g., the pnictide superconductors. The sessions on *Spin-orbit Mott insulators* with six talks reported on novel types of Mott insulators with strong spin-orbit coupling, that may also realize unusual spin-liquid phases. In the colloquium talk, one of the keynote speakers *H. Takagi* reported on the experimental endeavour to uncover such exotic phases in certain iridate compounds. Traditionally, strong interest attract the *Frustrated spin systems*, and in four theoretical and three experimental talks we learned about the progress in understanding and experimentally realizing various magnetic phases on geometrically frustrated lattices. Concepts of entanglement, fractionalization and tensor networks were at the focus of the five talks in the sessions on *Topological order* where also keynote speaker *F. Verstraete* gave an overview over topological quantum phase transitions. Keynote speaker *M. Troyer* reported on the advance of simulating quantum systems in higher dimensions, while the problem of *Many-body localization* was elucidated in four talks with different numerical and analytical approaches. The strong correlations of *One-dimensional systems* were the topic of five talks, and keynote speaker *F. von Oppen* reported on the possibility to realize a Majorana bound state in the presence of a one-dimensional chain of magnetic atoms. In addition, there were sessions covering correlations in *Impurities & Kondo physics*, *Weyl & Dirac systems*, as well as phenomena of *Non-equilibrium systems*. Particular emphasis was given to young researchers, who delivered 32 talks, while 14 talks were delivered by senior researchers in addition to the four invited keynote talks. Moreover, 27 posters were advertised in a blitz poster session via 3 min talks and presented in three poster sessions in the evenings of Monday, Tuesday and Thursday. These evenings provided the important opportunity for gathering and discussion which was especially appreciated by the participants. The Korrelationstage again was an important event that was scientifically stimulating and promoted the exchange among the community.

The scientific organizers Markus Garst, Stefan Kehrlein and Hans-Henning Klauss would like to thank the **mpipks** for the support and, in particular, Katrin Lantsch and her team for the organization of this workshop.

Martin Gutzwiller's Scientific Universe: From Wavefunctions over Periodic Orbits to Sun, Moon and Earth, Workshop

Scientific coordinators: J.-M. Rost, S. Tomsovic, D. Vollhardt

This workshop was a special one honouring the work and life of Martin Gutzwiller, who has been closely linked to the **mpipks**. About 65 colleagues represented the wide range of Martin's scientific interest and expertise, from condensed matter physics to semiclassical theory to turbulence and classical chaos on scales from the microscopic world all the way to celestial mechanics. There were so many eminent scientists present that it is hard to pick individual contributions. One which stood out through

its character reviewing Martin Gutzwiller's life was given by Dionys Baeriswyl definitely striking a chord with his entire audience who asked for his talk to be made publicly available. This holds also true for the after dinner speech by Sir Michael Berry who gave in fact a brilliant full lecture on the history of semiclassical theory and Martin's contributions to it. Apart from the numerous deep reviews of periodic orbit theory, the Gutzwiller wave function and asymptotic expansions, there were also new significant developments reported: On the extension of the Gutzwiller wave function to the time-dependent domain for non-equilibrium processes (Marcus Kollar), on first successful attempts to take semiclassical propagation and periodic orbits from few particles to the many-body limit where the inverse particle number takes the role of (small) \hbar (Klaus Richter and Boris Gutkin), then on the formulation of a periodic orbit backbone to understand the onset of turbulence (Bruno Eckhardt) and on a novel scarring phenomenon in systems with a random potential component close to integrability (Esa Räsänen). The workshop made impressively clear the timelessness and elegance of Martin Gutzwiller's thinking and research. And it left those colleagues grateful and proud whose work attracted his attention which he often expressed in hand-written insightful and critical-encouraging letters commenting on their work - a number of such letters were cited during the workshop, whether formulated in English or German, always in a perfect elegant style, ready for print.

Topological Phenomena in Novel Quantum Matter: Laboratory Realization of Relativistic Fermions and Spin Liquids, Workshop

Scientific coordinators: C. Broholm, M. Oshikawa, A. Rosch

Topology is a field of mathematics which classifies properties of mathematical structures which are robust under deformations. This field has recently emerged as a powerful paradigm to discover, classify, and investigate quantum properties of materials. The international workshop, attended by 90 participants, has focussed on two classes of such topological quantum materials. First, in Dirac matter topological properties are often intrinsically linked to the relativistic Dirac equation. Second in spin systems geometry and spin-orbit coupling can suppress magnetic ordering and give rise to novel topological spin liquid states. The workshop brought together experimental and theoretical physicists working in the two fields. It gave an overview on the tremendous scientific development especially in the last one or two years focussing on synergies of the two fields, on experimental realizations of topological concepts and on future research directions shaping the field.

The experimental and theoretical investigation of new topological quantum materials was not only the main topic of the inspiring colloquium talk by S. Nakatsuji but also central to many key contributions to the workshop (Y. Ando, C. Felser, P. Gegenwart, Z. Hasan, Y.-B. Kim, O. Rader, K. Ross, M. Sato, H. Takagi, R. Valenti). Topological insulators, topological superconductors, and magnetic materials with strong spin-orbit interactions and frustration were some of the most discussed material classes. The classification of interacting topological states, which have not yet been realized experimentally, and routes towards their realization were also a major theme (e.g., in presentations of L. Balents, M. Daghofer, O. Erten, M. Hermanns, G. Jackeli, L. Savary, or T. Senthil). I. Bloch showed how experiments in ultracold atoms can be used to map topological Berry phases and gave a perspective of how concepts from solid state physics find their application in quantum optics experiments. The latest development on magnetic skyrmion materials (C. Pfleiderer, K. von Bergmann), including their controlled creation and destruction by electric fields, the quest for experimental signature of Majorana fermions in spin liquids in neutron scattering (S. Nagler, L. Balents), the observation of the topologically quantized electromagnetic response of topological insulators (P. Armitage), magnetic quantum oscillations without Fermi surfaces (J. Knolle) and anomalous magnetotransport (R. Arita, L. Balicas, Y. Ando) were presented in inspiring talks.

Overall, the workshop was characterized by lively and intensive discussions until late in the night. In particular the poster sessions offered a wealth of fresh experimental results and theoretical insights and highlighted the passion of young scientists for the field. A brainstorming session on the most important future research directions in topological quantum matter showed that this field is still at its infancy. Interacting topological states, experiments probing projective symmetries, strange metals and the experimental realization of emergent gauge fields were only some of the research areas where the participants expect major advances in the near future.

Besides the generous support by the Max Planck Society, the workshop was also supported by the TOPONET program of the Institute for Solid State Physics (University of Tokyo) and the profile area "Quantum Matter and Materials" of the University of Cologne.

Two-Phase Continuum Models for Geophysical Particle-Fluid Flows, Seminar and Workshop

Scientific coordinators: G. Bewley, J. McElwaine, A. Valance

A. Program Goals:

Progress in the study of granular materials, improvements in field measurements, and the increased capabilities of large-scale computer simulations have led to a better quantitative understanding of particle transport by a turbulent fluid, the interaction between transported grains and the bed, the development of surface feature on the bed, and their subsequent motion and interaction. Further progress requires advances in our understanding of particle-fluid interactions and the modification of particle-particle interactions in the presence of a fluid. This program attempted (i) to accelerate these advances by bringing together physicists and geophysicists with an interest in geological processes that involve the interaction between particles and fluids and (ii) to consolidate the development of a multi-disciplinary culture devoted to the description and prediction of geophysical flows that was initiated at a program entitled Fluid-Mediated Particle Transport in Geophysical Flows held at the Kavli Institute for Theoretical Physics in the fall of 2013.

B. Workshop structure:

The workshop took place during the first week of the program, from March 14th through 18th. The workshop served two purposes: it provide an opportunity to review what progress had been made since the Kavli program in 2013 and it gave researchers who could not participate in the seminar session an opportunity to present their work. The workshop consisted of 38, thirty-minute talks, each followed by ten minutes of discussion.

C. Seminar structure:

The backbone of the seminar program was a daily presentation by a participant concerning his or her relevant research. The talks were informal, often interrupted by questions from the audience, and, as a consequence, lasted for as long as two hours. Participants were scheduled to talk early in their visits. Extra, topical discussions were sometimes arranged and announced in the daily meetings.

Funding from the U.S. National Science Foundation was obtained for both the workshop and seminar. The funds were used to support the participation of US based scientists and included senior and junior scientists.

D. Program Outcomes: State of the Art and Future Research Directions:

The program dealt with various fluid-particle systems including Aeolian transport, turbidity currents, snow avalanches, clouds (i.e, liquid droplets in turbulent air flow), fluidized granular flows, debris flows, dense suspensions and pyroclastic flows. Issues related to erosion and deposition processes, segregation phenomena and bedform instability in aeolian, river and marine environment were also discussed.

The program evolved from proposals that focused on turbidity currents and Aeolian transport. The latter are dilute systems of particles in turbulent flows of water and air, respectively, that that we can describe accurately without considering the interactions between particles. The Navier-Stokes equations in their Boussinesq approximation provide a reasonable basis for numerical modeling of turbidity currents. Existing continuum and particulate descriptions of Aeolian sand transport can predict the steady-state profiles over flat beds of particle and wind velocities and particle concentration as a function of the strength of a steady wind. These are two examples of fluid-particle systems, one in water, the other in air, and both involving a turbulent shearing flow that are relatively well understood. The challenge was to build from these.

Sand particles in air are the simpler system. The flows are typically so dilute that collisions between particle above the bed are rare and the significant interaction is the drag between the wind and the particles saltating (jumping) above the bed. Because of the great difference in the mass density of the particles relative to that of the air, collisions of particles with the bed (the splash) are not influenced by the wind and the measured mass and momentum transfers in them can be employed to derive continuum boundary conditions. These features make Aeolian transport a model system. The issues that remain are:

1) to describe the transient evolution of flows in time and their development along the flow and, in particular, to understand the mechanisms that drive relaxation towards steady flows. This relaxation plays a key role in the development of sand patterns. Drag, splash, and mid-air collisions are expected to play a role, but their relative importance in winds of different strengths has not yet been identified.

2) to describe saltation transport over rippled surfaces. This issue is important in practice, because sand beds in Nature are rarely flat. Experimental and numerical investigations suggest that there is a

phase-locking between the length of the saltation hop and the spatial modulation of the ripple. Further studies are needed to capture the relevant mechanisms that are responsible for this.

3) to understand the transition between pure saltation and flows in which mid-air collisions are important. Several theoretical and numerical studies emphasize the role of mid-air collision in sand transport at higher wind speeds. Unfortunately, there is a lack of experiments to evaluate the importance of collisions and a clear need for further investigations in wind tunnels.

4) to describe polydisperse flows. Most theoretical approaches for modeling Aeolian sand transport assume particles of a single size. Wind-tunnel experiments and field observations indicate that the polydispersity of natural sand influences its transport and play a major role in the formation of mega-ripples.

5) to understand mechanisms for the development of steady bed forms, such as ripples and dunes. The origin of the instability of a planar sand bed is now well understood, but the mechanisms responsible for the wavelength selection of steady forms remain to be identified. Is such selection a linear process or is there a nonlinear mechanism at work? Further investigations that couple theory and experiment are necessary.

Sand particles are some three orders of magnitude denser than air. For systems in which the mass densities of the particles and fluid are not so different, such as sand in water, the situation is not so simple since much higher concentrations are encountered. Computational schemes to resolve individual particles in a realistic turbulent shearing flow are beginning to be developed. However, because of the length scales involved in a wide range of natural flows, fully-resolved simulations are unfeasible. Two-phase continuum models, with some averaged description of the turbulence, provide the best hope for describing natural, fluid-particle flows in the foreseeable future. However, the development of such descriptions requires modeling of the interaction between the particles and between particles and the flow and closure of terms that result from the averaging.

The power of modern computational schemes was made clear during the program, as was their present limitations. Direct numerical simulations and/or large eddy simulations that involve a discrete particle phase presently have the capacity to assist in the development of two-phase continuum models. Integration over the expertise expressed during the program indicates that something like this should be done. The activity should be carried out in conjunction with a program of laboratory experimentation, to test both the computations and modeling, and it should, of course, be informed by the phenomena in the field that it eventually hopes to describe.

Research results presented during this program promoted in-depth discussions concerning particle/turbulence interactions, particle/fluid and particle/particle interactions in dense suspensions, particle and fluid interactions at the bed, mechanisms of erosion and deposition, bed form dynamics and wavelength selection. These discussions resulted in the identification of several important challenges for aquatic particle-laden flows. Among them are:

1) the most important challenge for fluid-particle flows in water is to develop a better understanding of the interaction between the particles and the turbulent shearing flow over a range of different particle/fluid density ratios and particle volume fractions. Currently it is unclear what a minimal set of variables is that can accurately describe the flow. This can be done in laboratory experiments and, more and more, by direct numerical solution of turbulent shearing flows that include particles. Laboratory experiments and the further development of direct numerical schemes with this focus should be encouraged.

2) Most of theoretical approaches for modeling particle-laden flows deal with spherical particles of a single size while the poly-dispersity in size and shape is a common feature of natural flows. How do known results for mono-disperse suspensions of spherical particles need to be modified to be applicable to poly-disperse suspensions of irregularly shaped particles?

3) because the relevant physics near the particle bed are not known, ways must be found to study the particle-fluid interactions near, at, and in the particle bed during erosion and deposition. These are the regions of densest particle concentration and, as a consequence, they are, typically, opaque, so difficult to access experimentally. However, because the particle concentrations are so high, the fluid dynamics may be simplified. An elucidation of the appropriate physics will facilitate the development of continuum formulations for the transfer of mass, momentum, and energy at particle beds and provide the basis for the derivation of boundary conditions and the description of bed forms.

4) important challenges concerning bed forms dynamics are still to be addressed. Are there common morphodynamic organizing principles active across the entire range of particle/fluid density ratios and particle volume fractions, and between gas- and liquid-mediated flows? Which mechanisms dominate the wavelength selection of bed forms in different parameter regimes?

5) what is learned in physical and numerical experiments about the particle-turbulence interaction should

be employed to develop closures in continuum models. Such models will be employed to predict the evolution in time and space of the relevant particle and fluid variables. At the present time, two-phase continuum theories offer the best, and perhaps only, hope for treating geophysical fluid-particle flows over the time and space scales found in nature.

6) the predictions of two-phase continuum models must be tested against the results of physical experiments and direct and numerical simulations. This is the second role to be played by laboratory researchers and computational fluid dynamicists in the description of natural, fluid-particle flows.

7) the interaction between laboratory researchers, computational fluid dynamicists, theoreticians and those researchers working in the field must be facilitated and encouraged. A better understanding must be developed of how phenomena seen in the field are related to those studied in the laboratory – that is, an understanding of how geophysical fluid-particle flows scale. This should lead to field measurements that are informed by theory and field tests of theoretical prediction.

We are convinced that the cooperative venture between computational, theoretical, experimental and observational fluid dynamicists with the long-term goal of describing fluid-particle flows that occur in Nature is essential to conceive and launch novel research directions for advancing the field of two-phase flow modeling. We believe that the present program and the previous Kavli program provided an important step in this direction that we intend to pursue by seeking financial support from government and industry.

A proposal for a third program on fluid-mediated particle transport in 2019 will be submitted to the Mathematical Isaac Newton Institute in Cambridge, England. The intent is to involve as many of the participants in the past programs as possible, in order to continue to develop the multi-disciplinary culture devoted to geophysical flows that was initiated at the program.

E. Diversity:

While substantial progress has been achieved in recent years through field observation, laboratory experiments, numerical simulations and theoretical modeling, this progress has occurred in different communities that commonly do not interact closely. Hence, the program served the important function of bringing together researchers whose primary expertise lies in the physics of granular flows, in multiphase fluid dynamics, and in the geosciences. Intensive collaborations at the intersections of these disciplines led to stimulation, insights, and cross-fertilization during the workshop. The organizers believe, supported by early evidence, that this laid the foundations for sustained long-term collaborations among the program participants. Throughout the planning of the workshop and seminar the organizers attempted to contact a broad cross-section of researchers in the field, particularly with an eye toward inclusion of women. Though many were invited, of the 28 participants in the seminar only three were women. At the workshop, six (including a keynote) of the 38 speakers were women. The program included many international participants who were from Europe (49), United-State (13), India (2) and Canada (1).

F. Planning issues:

The staff of the Max Plank Institute was extraordinarily helpful in assisting the organizers and participants. The arrangement of accommodations and reimbursement and the organization of the program went very smoothly. Responses from participants to the organizers were very positive. The organizers thank Maria Pätzold and her colleagues for making their job relatively easy. A traditional hurdle is the length of stay requirement. We had only six participants who were able to attend for the entire four-week seminar session, including all of the organizers. We would have had long-term participants if the invitations had been sent out earlier. We would suggest at least one year in advance.

Prospects and Limitations of Electronic Structure Imaging by Angle Resolved Photoemission Spectroscopy, Focus Workshop

Scientific coordinators: S. Kera, S. Kümmel, A. Schöll

The focus workshop PLESI16 was held in spring 2016 from April 24 to 27 at the **mpipks**. The program consisted of 13 invited talks, 4 hot topic talks, one poster session and the colloquium of Prof. Michael Ramsey from the University of Graz, Austria.

The main focus of the workshop was to bring together researchers working in the field of orbital imaging by Angle Resolved Photoelectron Spectroscopy (ARPES) in experiment and theory. In recent years ARPES has seen a rapid development with a particular focus on imaging the electronic structure of ordered molecular layers. The contributions by Prof. Ueno and Prof. Ramsey gave a scientifically deep and historically fascinating perspective on the development of the field of photoemission spectroscopy, reminding everyone that it is not only allowed, but even fruitful to occasionally question the 'established

truth'. We learned with joy that "sometimes, one must sacrifice precision for clarity" (Bertrand Russell cited by M. Ramsey), and pondered the concept of "unnecessarily simplifying".

The combination of ARPES experiments and electronic structure calculations in the orbital imaging approach has become increasingly popular for investigating the structural, chemical and physical properties of molecular materials. However, despite its increasing popularity, the approach also leads to fascinating and pressing questions on the fundamental level. One prominent example is the plane wave final state approximation, which in the simplest interpretation of the photoemission process is often used to describe the outgoing electron. This approximation is too narrow for describing presently studied effects such as circular dichroism and raises the general question of how deviations due to the more complex final state manifest themselves and whether there is evidence for deviations particularly at low kinetic energies or for scattering at high energies. On the theoretical side the question arises how final state effects can be taken into account for systems with a complicated, possibly low-symmetry electronic structure such as seen in layers of organic molecules and whether explicit simulation of the emission process in real time can sidestep the problem. From a theoretical perspective, the interpretation of ARPES data by single particle orbitals raises the question, why and when the single-particle interpretation is appropriate and whether theory is available that goes beyond such a single orbital interpretation. Beyond this, the workshop was intended to fathom what can be learned from ARPES about systems such as e.g. graphene or other 2D or layered materials.

The talk by Prof. Wollenhaupt gave fascinating insights into time-resolved experiments with high-harmonic generation set-ups and broadened the workshop's perspective from solid-state systems to atomic and molecular physics. Other speakers pointed out new experimental possibilities with respect to spin-resolved experiments. The field of invited speakers was deliberately composed to cover these different aspects.

Well-known scientists from Europe, Japan, the US and Israel attended the workshop and provided excellent contributions. Beyond the aforementioned Prof. Ramsey (Graz, Austria), prominent researchers as Prof. Ebert (Munich, Germany), Dr. Ferretti (Modena, Italy), Prof. Höfer (Marburg, Germany), Prof. Kronik (Rehovot, Israel), Prof. Osterwalder (Zürich, Switzerland), Prof. Puschnig (Graz, Austria), Prof. Reinert (Würzburg, Germany), Prof. Rubio (Hamburg, Germany), Dr. Soubach (Jülich, Germany), Prof. Ueno (Chiba, Japan), and Prof. Wolf (Berlin, Germany) and others followed the invitation to Dresden and shaped this workshop with their excellent contributions.

Among the 36 participants were 14 scientific newcomers on the PhD and PostDoc level from all over the world. Amongst these, Simon Moser (Berkeley) and Matthias Dauth (Bayreuth) gave invited and hot topics talks, respectively, and all other young colleagues contributed by presentations at the poster session.

The workshop was a successful event and inspired very fruitful discussions. It summarized the recent progress in the field, helped to shape a perspective for the future, and triggered stimulating new ideas.

We would like to thank the **mpipks** for facilitating this focus workshop in their visitors program and for providing the excellent infrastructure to us and the participants. We particularly acknowledge the efficient organizational support and friendly assistance by the team of the visitors program, in particular Mandy Lochar, before, during, and after the workshop.

Strong Correlations and the Normal State of the High Temperature Superconductors, Seminar and Workshop

Scientific coordinators: A. Chubukov, B. Keimer, M. Randeria, S. Sebastian

The workshop and seminar on strong correlations and the normal state of high temperature superconductors was held at **mpipks** in Dresden from May 17 to May 27, 2016. The first week (May 17-20) was the workshop week, with around 70 participants and around 8 talks per day. The talks were 35 min. long. There was discussion at the end of each talk, and we allocated additional time for discussions at the end of every session. The session chairs directed the discussion and some presented summary slides. We had two evening poster sessions on Tuesday and Wednesday, and there was a lively discussion around posters on both days. During the second, seminar week, we had 4-5 talks per day, mostly by junior participants. We also had three talks by the organizers (Chubukov, Keimer, Sebastian), and one informal blackboard talk by Subir Sachdev, who also gave a colloquium at **mpipks** on Monday, May 23.

The goal of the workshop was to bring together leading experimentalists and theorists working in the field of strongly correlated systems, mostly cuprates and Fe-pnictides/chalogenides, with the goal to advance our understanding of the role of correlations in these materials, particularly of the origin of the pseudo-

gap and charge-density-wave state in the cuprates, and nematic state in Fe-based systems. Arriving at a theoretical understanding of the normal state in both these materials is particularly challenging given the likely involvement of multiple of these contributing factors. Within the last few years, however, an infusion of new experimental results has finally made a resolution of normal state physics in the family of high temperature superconductors a tangible possibility.

The discussion at the workshop and the seminar chiefly focused on two main issues:

- The origin of the pseudogap in the cuprates and its interplay with the charge order
- The origin of the nematic state in Fe-based systems.

The first issue included the discussion on: (i) Is the pseudogap in the cuprates a phase with a broken symmetry, or does it represent a crossover to Mott physics as suggested by some DMFT- based theoretical studies? (ii) If the pseudogap involves a broken symmetry (most likely related to charge order), can the symmetry-breaking order be better described in terms of charge order (or strong fluctuations), or pair-density order (a pairing instability with a non-zero total momentum of a pair)? (iii) Which instability is stronger for a realistic fermionic dispersion? Is there a single phase transition at $T = T^*$, or a series of transitions at different temperatures involving for example the breaking of time-reversal symmetry and U(1) translational symmetry? (iv) What is the interplay between the description of the pseudogap in the metallic scenario and in the strong coupling scenario describing a doped Mott insulator? (v) How can we reconcile the breakdown of the Fermi liquid paradigm when superconductivity is suppressed by elevated temperatures, with Fermi liquid behavior observed at low temperatures when superconductivity is suppressed by a magnetic field? (vi) What is the role of the quantum critical points associated with density wave order that underlie the maxima of the two-dome superconducting structure? (vii) Does the Fermi arc represent a nodal quasiparticle density of states at the Fermi energy, or does it just reflect a strong incoherence of excitations at the antinodal region?

The discussion on the nematicity was focused on the following topics: (i) What is the origin of the nematic phase in iron pnictides? Is it due to orbital order or is the result of magnetic fluctuations? (ii) If orbital order is the primary one, what gives rise to an attraction in the orbital space and is orbital transition continuous or discrete? (iii) If nematic phase is the result of a composite spin order (a four-fermion condensate), what is the effect of such order on single electron properties? (iv) Can nematic fluctuations mediate an attractive pairing interaction? If yes, in what channel? (v) Is it possible to have a non-superconducting phase with time-reversal symmetry breaking in Fe-pnictides? (vi) Is Mott physics and the concept of “orbital selective Mott transition” relevant for at least some Fe-pnictides?

For the workshop, 30 speakers gave talks, and for the seminar, 15 speakers gave talks. The senior speakers at the workshop were L. Taillefer, A. Kapitulnik, D-H Lee, R. Greene, M. Rice, Y. Matsuda, H. Kontani, B. Buechner, C. Varma, W. Metzner, A. Mackenzie, J. Schmalian, and M. Vojta. S. Sachdev gave a colloquium and informal talk during the seminar week. A number of junior scientists gave talks during the workshop and the seminar week. All these talks went very well and generated a lot of questions. There wasn't a single talk without at least 10 min discussion.

The key scientific results of the workshop and seminar is (i) the broad understanding that the emergence of the pseudogap in the cuprates gives rise to strong reconstruction of electronic states, consistent with the idea that the density of carriers sharply changes from $1+x$ to x , where x is the doping, and (ii) the understanding that there exists two mechanisms for nematic order in Fe-based systems — one is a spontaneous orbital ordering, and the other is an Ising-nematic order due to magnetic fluctuations. Most, but not all researchers believe that for Fe-pnictides magnetic scenario is realized, but for FeSe a spontaneous orbital order is a clear possibility.

FFLO-Phase in Quantum Liquids, Quantum Gases, and Nuclear Matter, Workshop

Scientific coordinators: A. Buzdin, M. Eschrig, J. Wosnitza

The workshop was held at **mpipks** in Dresden from June 20 to June 24, 2016.

The discovery of the so-called Fulde-Ferrell-Larin-Ovchinnikov (FFLO) effect had its 50-year anniversary in 2014, and enjoys a renewed interest during the past decade in superconductivity, cold fermionic gases, as well as nuclear and quark matter. It describes the appearance of Cooper pairs with a finite center of mass momentum as a result of a spin polarization arising either from an externally applied magnetic field, from a spin imbalance, or from an internal exchange field. The appearance of such a state shows intriguing properties, as singlet-triplet mixtures, spatially inhomogeneous order parameters, and unconventional pairing.

The aim of this workshop was to bring together the communities working on FFLO effects in heavy-fermion systems, in organic superconductors, in superconductor-ferromagnet hybrid structures, in spin Peierls systems in magnetic fields, in cold atomic gases, and in nuclear matter. With the unifying theme of FFLO pairing states in such a diverse number of fields in physics a fruitful exchange between otherwise rather disjoint communities was possible.

The workshop started, after welcome words by Roderich Moessner, with short historical notes by Profs. Fulde and Ovchinnikov, who both were guests of honor, and an introductory presentation by Gertrud Zwicknagl. On Monday evening, a Colloquium was presented at the Festsaal Dülferstraße by Wilhelm Zwerger - a common event of TU Dresden, the **mpipks**, and all other physics-related institutions in Dresden. The large lecture hall was filled to the last seats, and the Colloquium was followed by a reception with lively discussions between the participants of the workshop and audience members from TU Dresden.

The workshop was special in the broad spectrum of topics it covered, with the FFLO mechanism as unifying theme. We had a number of high-level speakers in spin-imbalanced cold atomic gases (Zwerger, Zwierlein, Hu), in the fields of quantum chromodynamics (Mannarelli) and nuclear matter (Sedrakian), in layered organic superconductors (Uji, Brown, Mitrovic, Agosta), in superconductor-ferromagnet hybrid systems (Blamire, Annett, Melnikov, Linder), in quasi-one-dimensional systems (Brazovskii, Orso), and in strongly correlated superconductors (e.g. Mitrovic, Kasahara, Machida, Brison). Several interesting theoretical methods and predictions were discussed (e.g. Agterberg, Zhitomirsky), as well as exotic states of matter and applications, like odd-frequency pairing states (Fominov), ϕ -junctions (Goldobin), topological superconductivity (Houzet), or antiferromagnetic superconductors (Bulaevskii).

We had two extended poster presentations on Tuesday and Thursday, and a spectrum of early-carrier participants and students. In addition we had presentations by early carrier speakers (e.g. Mazzone, Gukelberger, Croitoru), as well as involvement of students and younger scientists in the technical organization (Gronemann, Coniglio). There was also lively communication between junior and senior participants during the workshop excursion to the Baroque castle Moritzburg on Wednesday afternoon.

The scientific results of the conference in the broader sense include a higher awareness of similar methods and phenomena in fields describing as diverse systems as quark matter, nuclear matter, cold atomic gases, superconductors, hybrid structures, charge density wave order, and antiferromagnetic materials, and covering an extraordinary energy range from 10⁻⁹ to 10⁹ Kelvin. The FFLO effect thus proved to have a great integrative power between scientific communities.

Apart of giving a broad overview over imbalanced Fermi systems in physics, the conference also accelerated the development of the field and was conducted in a highly inspiring atmosphere.

Several speakers and participants as well as guests of honor expressed their gratitude for the throughout high quality of the presentations, the broad range of topics brought together by a unifying theme, as well as the relaxed atmosphere during scientific discussions and poster sessions. We would like to add that **mpipks** and the workshop administrator Amy Wright excellently handled the organizational and other administrative formalities of the workshop.

Topological Patterns and Dynamics in Magnetic Elements and in Condensed Matter, Seminar and Workshop

Scientific coordinators: R. Ignat, S. Komineas, N. Papanicolaou

The event has focused on nontrivial topological patterns observed in magnetic elements, such as vortex singularities, domain walls and traveling waves. The relevant micromagnetic models were based on the Landau-Lifshitz equation. In parallel, some contributions were on theories developed for mesoscopic condensed matter systems, such as a Bose-Einstein condensates (BEC), which present similar patterns. At the event, experts from physics (mainly theoretical but also experimental and computational) and mathematics have been brought together. These communities have worked in similar problems, for example, on the topological features of micromagnetic and condensed matter systems. Since there has been hardly any communication between these communities, our event had the aim to foster the interaction and collaborations between physicists and mathematicians.

In the first week (seminar week) lecture series were given by

- Felix Otto, on “Domain and wall patterns in thin-film ferromagnets” (4 lectures).
- Hans-Benjamin Braun, on “Topology, thermal fluctuations and quantum effects in nanomagnetism” (3 lectures).

- Nicolas Vukadinovic, on “Numerical methods for the Landau-Lifshitz equation in the frequency domain” (1 lecture).

These were attended by a number of young researchers (10 PhD students and 6 postdoctoral researchers) as well as by the senior participants. The program was complemented with research talks (one per day). In the second week a workshop was held with about 50 participants and 25 research talks. The results presented showed that the subject of micromagnetics is going to be further developed because (a) significant theoretical questions remain to be studied and (b) technological problems with industrial impact are connected to them.

Two poster sessions were organized, on Wednesday the 29th of June (seminar week) and on Tuesday the 5th of July (workshop week). In the former poster session the researchers have presented their work in short (5-10 minutes) talks before the poster session.

The meeting was successful in bringing together communities of researchers from Physics and from Mathematics. Common research interests were identified at the level of technical and applied problems. It promoted the level of understanding between these researchers to such a degree that a permanent line of communication has now been established. It has become apparent that most of the participants are interested in contributing further to the objectives of the event, so that an event of similar format can be organised in the next two year period.

Disorder, Interactions and Coherence: Warps and Delights, Focus Workshop

Scientific coordinators: S. Brazovskii, N. Kirova, L. Levitov

Financial support from other sources than **mpipks**: Cavendish laboratory and Trinity College of the Cambridge University covered travel, local expenses and conference fees for three their participants.

Structure of the event: Talks (25 minutes) on advanced topics, while keeping the pedagogical aim with respect to the young audience. Poster session.

Participant's details:

Total number of participants: 60.

Among them: Professors - 35, PhD - 21, PhD students - 4.

Geography: USA -16, France - 9, Germany - 8, UK - 6, Israel - 4, Russia - 4, Italy - 2, The Netherlands - 4, Switzerland - 2, Australia - 1, Belgium- 1, India - 1, South Korea -1, Slovenia-1.

The Workshop was centered around major modern directions in physics of disordered systems such as Many-Body Localization, Decoherence and Noise, Multifractality and Integrability, Disorder versus Superconductivity and Interactions or Nonlinearity. There were also more auxiliary modern subjects such as quantum Hall effect (QHE, integer and fractional), topological states and phase transitions, Majorana and Weyl fermions, chiral anomaly, quantum critical points, hydrodynamics of electrons, high-Tc superconductivity, etc. Most of talks at the workshop were based upon very recent results and even unpublished yet papers.

The workshop has been initiated in honor 50 years in science of David Khmelitskii, now the emeritus professor at Cambridge UK and formerly at the Landau Institute in Russia. His alumnae from these fabulous institutes and his very successful former students strongly contributed to the accomplishment of the workshop.

At the core of the meeting, several talks have been presented by senior scientists from leading laboratories over the world, who have contributed substantially to the proposed research field. Among them are J. Chalker, M. Dyakonov, K. Efetov, M.V. Feigelman, A. Finkelstein, P. Fulde, L. Glazman, L. Ioffe, P. Littlewood, Yu.N. Ovchinnikov, V.L. Pokrovskii, A.M.M. Pruisken, G. Schön, B. Spivak, P. Wiegmann, and others.

The sessions were followed by vital discussions during the breaks and, especially, during the poster session which was remarkably well attended by all participants. Beyond the mature scientists, there was a large contingent of young people in their 20th and early 30th. Most of young people contributed significantly to success of the workshop by both presenting their original research and participating in discussions.

The Workshop went on very friendly: hot scientific discussions facilitated learning and understanding. At the end, many participants expressed their satisfaction by the atmosphere and exceptionally high scientific level of the Workshop.

Pattern Dynamics in Nonlinear Optical Cavities, Workshop

Scientific coordinators: N. Broderick, B. Krauskopf, K. Lüdge

As the first part of a set of Tandem workshops between the Max Planck Institute in Dresden, and the New Zealand Institute for Advanced Study (NZIAS) together with the Dodd-Walls Centre for Photonics and Quantum Technologies (DWC) in Auckland, the PDNOC workshop in August 2016 brought together about 50 scientists from different fields of research in optics. The common interest and, thus, the overall connection between the communities was the phenomenon of pattern formation that can happen in optically active media, e.g., in different semiconductor cavities, in fiber laser setups or in materials with nonlinear optical properties. The patterns analysed during this week were, on the one hand, temporal patterns that emerge due to the coupling of different cavities, i.e. mode-locking pulses, Q-switching pulses or chaotic spiking, and, on the other hand, spatial patterns that build up due to spatial inhomogeneities. The communities engaged in these different fields were so far well separated from each other and the aim of the workshop was to bring them together and locate synergies by exchanging ideas. Further, the presence of mathematicians, theoretical physicists as well as experimental physicists at the workshop was designed to start discussions that are sometimes hindered by the different scientific languages used within different communities.

The workshop allowed every invited speaker to present and discuss their work within 45 minutes. During the coffee breaks and the social events, including the excursion, the workshop dinner and BBQ, we had numerous discussions both between people who already work together and between participants who just got to know each other. Moreover, participating early-stage researchers got a very broad introduction into the different fields, and they did a very good job in presenting their own research results during the poster session and the contributed talks. Vital discussions emerged at the posters. Overall the workshop was a great success and we could achieve the goal of building bridges between the communities. All speakers gave their utmost best to present their ideas and research results. During the discussion session and informal meetings we received very positive and encouraging feedback from the participants.

In a broader sense the improved understanding of the underlying mechanisms behind the optical phenomena discussed at the workshop may lead to smaller, more energy efficient optical devices that are able to generate, store and process optical data. During the workshop, especially during the discussion session on Friday afternoon, we identified three main topics that are worth of being studied even further in the second dedicated Tandem workshop in Auckland:

- (1) optical computing beyond the von Neumann paradigm,
- (2) dynamics of complex micro laser systems for processing and storing optical data,
- (3) ultra short pulse generation via nonlinear processes in active media.

The workshop is presently being organized with 8-10 invited speakers over a 2 week period in June 2017.

Principles of Biological and Robotic Navigation, Focus Workshop

Scientific coordinators: B.M. Friedrich, U.B. Kaupp, S. Sanchez

The BioNav workshop was held at the **mpipks** in Dresden from August 29 to August 31, 2016. The workshop was special in its cross-disciplinary focus and format, as it brought together physicists, mathematicians, biologists, and robotic engineers interested in principles of navigation. The common theme was the reliable control of directional motion in response to environmental cues with sparse computational resources.

After welcoming words by Frank Jülicher, the workshop started with sessions on 'sensori-motor coupling' and 'mechanisms of gradient-sensing'. We highlight a few of the contributions to the workshop. Massimo Vergassola gave a key note lecture on gradient sensing in turbulent environments and their information-theoretic basis. These concepts were applied to both pheromone-guide navigation of moths and mobile robots that had to find the maximum of an odor plume distorted by turbulent air flow. Matthieu Louis demonstrated a chemotaxis mechanism of *Drosophila* larvae based on head casting, which remains operative even if all but one sensory neurons are deactivated. Gaspar Jékely discussed three different phototactic steering strategies in *Platynereis* larvae and linked those to the neuronal connectome in these larvae. Luis Alvarez presented impressive 3D-tracking data of navigating sperm cells, revealing a distinct chemotaxis strategy along helical paths. Interestingly, all these three biological navigation strategies rely on active exploratory motion of the swimmer themselves, whereby a spatial stimulus is converted into a temporal signal. This concept is known as 'information self-structuring' in the robotics field, and was the topic of the talk by Fumiya Iida. Barbara Webb impressively combined both topics of the workshop in her talk: she presented experimental data on path-learning in ants, together with a computational model

of vector integration that turned out to match the neuronal morphology of the relevant structure in the ant brain. Eberhard Bodenschatz gave a lively PKS colloquium talk on Monday afternoon, speaking about cilia-generated fluid flow in the brain. Surprisingly, these flows reverse direction depending on the signaling state of the brain.

The majority of speakers followed our suggestion to start their talk with a brief overview of their field and a short introduction of the relevant general concepts. This allowed the highly interdisciplinary audience to connect to the work of the other disciplines and revealed the commonalities between biological and robotic navigation. A number of theoretical talks e.g. by Nihat Ay and Peter Thomas showed how general questions of minimal information processing capacity and trade-off choices for optimal navigation can be approached by formal methods. This approach is very important for the field as it allows to distill generic principles from specific systems, yet the formal language of presentation can sometimes present a barrier for efficient communication. In this respect, it was very useful that the speakers illustrated the mathematical theorems presented by specific applications, allowing for example experimental physicists and biologists to connect to this theoretical research. On the other hand, several theoreticians emphasized in discussions how the talks by biologists sparked new ideas for their theoretical work. This positive experience highlights how biological systems can inspire the advancement of theoretical concepts.

As a novel element of the workshop, targeted at young scientists, we included a "poster flash-mob" into the workshop. Thus, in addition to the poster session on Monday evening, we scheduled an extra session, where each poster presenter had 60 seconds to present his project in 1 or 2 slides. This format also emphasized the poster presentation as integral part of the workshop, as well as allowed the participants to directly approach the posters of maximal interest to them during the poster session. For the junior participant among the poster presenters, this "poster flash-mob" presented an opportunity to be on stage, even if only briefly, and to train their oral presentation skills.

The scientific results of the conference in the broader sense include a higher awareness of similar concepts concerning navigation strategies both in the field of biological and robotic navigation, and to foster new theory-experiment collaborations. Thereby, the workshop contributed to better connect said communities and to highlight the emerging field of bio-inspired robotics. Conversely, engineering concepts can prove useful to describe key principles of biological navigation. Information-theoretic concepts provide a unifying theme that connects both fields. Apart of giving a broad overview over various navigation strategies, the conference also accelerated the development of the field and was conducted in a highly inspiring atmosphere.

Several speakers and participants expressed their gratitude for the throughout high quality of the presentations, the broad range of topics brought together by a unifying theme, as well as the relaxed atmosphere during scientific discussions and poster sessions. We would like to add that **mpipks** and the workshop administrator Mandy Lochar excellently handled the organizational and other administrative formalities of the workshop.

Bridging-Time Scale Techniques and Their Applications in Atomistic Computational Science,

Focus Workshop

Scientific coordinators: M. Posselt, R. Smith, B. Uberuaga

The BRITS International Workshop was held from 11-15 September 2016 with 50 participants from 14 different countries. In total we had 39 contributions (1 Colloquium, 30 oral presentations and 8 Posters). The theme of the meeting was the subject of how to perform dynamical simulations in atomic systems over time scales that are longer than those computationally accessible by Molecular Dynamics (MD). At the meeting were a mixture of disciplines and talks and posters varied from descriptions of new algorithms and theoretical underpinning of the techniques, to exciting new applications in materials science, chemistry, biology and physics. The applications included chemical reactions on surfaces, transport mechanism across cells and the long-term evolution of radiation damage.

Many techniques were discussed including new ideas of parallel trajectory splicing, using the power of modern computers with their thousands of processors, adaptive kinetic Monte-Carlo (KMC) methods, stochastic surface walking techniques, course graining using metadynamics and free energy methods.

For the KMC methods, the determination of saddle points on n-dimensional surfaces is still the subject of current research since the algorithms that are used are always a compromise between speed and robustness. Algorithms described by mathematicians that work for small systems are not always practical to use for large systems. Even after the meeting it was still not clear how to extend precise results obtained using transition state theory on small systems to the larger practical systems that many materials

scientists wish to study, despite this being a topic of the discussion session.

For the larger systems where free energy methods are used rather than detailed atomistics, the use of collective variables and the metadynamics technique was discussed in detail. An interesting new development in this area was the discussion of how an algorithm might be used to determine the best collective variables for the systems but more work needs to be done to provide a consistent link to the atomistic level.

Presentations by Established Scientists:

The colloquium talk was given by David Landau of the University of Georgia, who gave an excellent overview of the Wang-Landau method and its application to Monte Carlo techniques. This technique was applied in a number of problems described by the other participants of the meeting. The colloquium was very well attended by many of the local members of the MPI and lively discussion followed the talk. A large group of participants from Los Alamos National Laboratory, led by Art Voter presented significant advances in the use of multiprocessors to advance new techniques while others applied these techniques to important systems in materials science.

Similarly, Normand Mousseau described recent advances with his ART method, which was used in other presentations in practical applications.

Presentations by Young Scientists:

There were a number of presentations that were from younger participants. There were excellent talks from Fudan university from chemists who had used their in-house methods, to determine reaction pathways and to investigate the structure of molecular crystals.

The metadynamics methodology mentioned above was the idea of a young researcher, Pratyush Tiwary about to start his first academic staff position at the University of Maryland.

In addition Abhijit Chatterjee from Mumbai presented an interesting variation of temperature accelerated dynamics where the temperature was raised in steps to speed up the rare event processes.

Posters from PhD students included a description of how events with low transition barriers can be included in a mean rate theory in a lattice-based KMC method to model the growth of thin films.

The organisers received a number of positive comments from the workshop participants many of whom have uploaded their presentations to the workshop web site. However, the success of the meeting was not just because of the quality of the scientific programme but also in a large part due to the **mpipks** for the wonderful facilities offered, including a very nice outing along the river with dinner at the Fortress Koenigstein and especially to Amy Wright for her perfect administrative input.

Multistability and Tipping: From Mathematics and Physics to Climate and Brain, Seminar and Workshop

Scientific coordinators: U. Feudel, A. Pisarchik, K. Showalter

According to the goal of this workshop/seminar we brought together scientists from various disciplines of natural sciences, such as mathematics, physics, climate science, neuroscience, ecology, systems biology and network science. Multistability has been presented in various disciplines of science including electronics, optics, mechanics, laser physics, chemistry, genetics, neuroscience, in the climate system and in ecology. Of particular interest for many applications were transitions between the different states, also called regime shifts or tipping points, which can be either due to changes in the internal parameters of the system, changes in the forcing or the influence of noise. According to the nature of the transitions they have been classified as R-tipping, B-tipping, and N-tipping. Besides studies of the dynamics depending on environmental parameters, the focus was on developing methods how to estimate the distance from a regime shift/tipping point in models as well as from time series. The concept of critical slowing down, i.e. the increase in the times necessary to return to the original state after a perturbation, has been proven to be suitable for this task.

Almost all speakers which have been invited accepted this invitation, so that most of the major players in this field were present in the workshop, some of them gave also lectures in the seminar. Due to the extremely high quality of the program we had an overwhelming number of applications and it was a pity that we were unable to accommodate all the people who were interested because of the strict number of 70 participants. We had 18 worldwide well-known invited speakers who attracted so many applications. The most famous ones among them are James A. Yorke (USA), Celso Grebogi (UK), Alan Hastings (USA), Egbert van Nes (The Netherlands), Kunihiko Kaneko (Japan), Juergen Kurths (Germany), Tamas Tel (Hungary) and Eckehard Schoell (Germany). The participants came from 19 countries. Due to this highly competitive participation at the conference the level of all talks was very high and we had lively

interdisciplinary discussions leading to the intended cross-fertilization between the different fields. The two poster sessions included in the program were very busy and the young participants benefitted a lot from the discussions with the well-known senior scientists. A committee, consisting of A. Hastings, T. Tel, J.A. Yorke, E. van Nes, selected 5 posters to be awarded with a poster price. As a result of this workshop it can be expected that several joint papers with different participants of the workshop will appear in the future. We plan a Focus Issue of the international peer-reviewed journal CHAOS with 20-25 invited papers.

The seminar was equally successful thanks to the excellent lecturers we had. Lecture series have been given by J. A. Yorke, C. Kuehn, K. Kaneko, J. Kurths and the two organizers A. Pisarchik and U. Feudel. Since we had again an overwhelming number of application and could only accept 20 participants, the participation was highly competitive, so that the young people selected were extremely motivated and took part very actively. All of them used the unique opportunity to talk with the lecturers about their PhD projects. Particularly, it is worth mentioning that the students also talked a lot with each other trying to figure out topics of joint interest. Several people started new collaborations based on their interaction in the seminar.

Tensor Product State Simulations of Strongly Correlated Systems, School

Scientific coordinators: F. Pollmann, N. Schuch, F. Verstraete

The **mpipks** International School "Tensor Product State Simulations of Strongly Correlated Systems" (TENSOR16) was held from November 1-5, 2016. The goal of the school was to teach young PhD students the basics of tensor-product states as well as the most recent technical developments. This is particularly important given the increasing number of groups working on this quickly evolving topic. The lectures were given by researchers who work actively both on the development and the application on tensor-product state based methods.

The TENSOR16 school provided pedagogical introductions to matrix-product state based methods and discussed the most recent numerical and analytical developments in the field. The school comprised of five lectures and tutorials on different topics:

- Entanglement, matrix-product states, simple algorithms, some Python basics (Lecturer: Frank Pollmann, Dresden)
- Time dependent variational principle (Lecturer: Laurens Vanderstraeten, Ghent)
- Applications of MPS in condmat and AMO (Lecturer: Fabian Heidrich-Meisner, Munich)
- Introduction to Projected Entangled Pair States and the multi-scale entanglement renormalization ansatz (Lecturer: Phillippe Corboz, Amsterdam)
- Topological orders in tensor networks: Analytical approaches (Lecturer: Norbert Schuch, Munich)

The school was very well received by the students and the feedback given was extremely positive. The tutorials and hands-on sessions were particular popular as these allowed a direct application of the theory taught during the lectures. All lectures notes and tutorials are public and can be accessed from the website of the European Tensor Network (quantumtensor.pks.mpg.de).

The students participated very actively throughout the entire program and the questions asked led to stimulating discussions. We were also happy to see that the school helped students from different groups to get to know each other which will foster future scientific exchange (the students in fact formed an independent Facebook group to stay in touch).

All students had the opportunity to present their own work during a poster session. The poster session was very well attended and the students discussed their work among each other and with the lectures until late night.

Quantum-Classical Transition in Many-Body Systems: Indistinguishability, Interference and Interactions, Workshop

Scientific coordinators: A. Buchleitner, J.-D. Urbina

The international workshop "Quantum-classical transition in many-body systems: Indistinguishability, interference and interactions" took place at **mpipks** during Feb. 13-17. In terms of our initial objective to open an space for communication and interactions between several different communities that deal with various aspects of the quantum-classical transition in many-body systems- the meeting was highly successful.

The conference was very intensive and roughly organized in blocs of talks, dealing with the following specific aspects:

- Multiparticle correlations in non-interacting many-body scattering: In this area we have the opportunity to hear the state of the art in the experimental implementation of photonic circuits with many-body states and its relevance in the context of a proposed realization of Quantum supremacy (the BosonSampling problem) and its certification. Several applications and extensions of suppression laws for many-body scattering through networks were also presented.
- Exciton transport in complex networks: During the meeting, we enjoyed talks from world-leading experts in the experimental and theoretical study of quantum effects in the transport of excitations through biomolecular complexes, with emphasis in the effects of decoherence, dissipation and disorder.
- Interplay between single-particle and many-body effects in the properties of cold atom systems in the mesoscopic and macroscopic domain. A major theme during the conference was the emergence of local equilibration due to interactions in many-body systems, a problem where several timely discoveries play a role, like many-body localization, path interference in Fock space and the quantum signatures of mean-field solitons.

The strongly inter-disciplinary character of the conference was very well received by all participants, and the general opinion was that the subjects and the speakers were well appropriate for the task of presenting the sometimes rather technical concepts and results in an accessible manner for people from different communities.

We are happy to mention that a good half of the talks were given by young scientists, showing the healthy state of the communities working on the different aspects of the quantum-classical transition and its interplay with many-body interference.

The poster sessions were lively and in general, the mood was that of open mindedness and readiness to discuss the implications of the new results in the broad context of many-body interference.

Quantum Dynamics in Tailored Intense Fields, Focus Workshop

Scientific coordinators: M. Lein, G. Paulus, J.-M. Rost

The workshop focused on the dynamics of microscopic systems under the influence of strong tailored laser waveforms. The systems under investigation range from atoms over molecules to nanostructures and solids. The applied laser fields are shaped on the sub-cycle scale for example by using two- or multi-colour fields or few-cycle pulses with stable carrier-envelope phase. Besides bringing together a number of international speakers, the workshop served as the Annual Meeting of the Priority Programme "Quantum Dynamics in Tailored Intense Fields" (QUTIF) of the German Research Foundation DFG. The programme consisted of seven invited talks, a substantial number of talks by QUTIF network members as well as two contributed talks from external participants. One invited talk was given by Isabelle Auffret-Babak as a representative of IOP Publishing, providing information about peer review and the publication landscape in Europe.

Among the invited speakers, Professor Zenghu Chang (University of Central Florida) reported the most important scientific news in the sense that he presented a new record in making the shortest coherent light pulses produced until today. In the talks by QUTIF members, particularly interesting progress was reported by Matthias Wollenhaupt (University of Oldenburg) on a new setup that allows to generate polarization controlled multicolor fields over an octave-spanning spectrum. New theoretical results by Armin Scrinzi (Ludwig-Maximilians-Universität München) on photoelectron momentum distribution from ionization of helium atoms by circularly polarized pulses ("attoclock"), now including electron-electron interactions, could not resolve the longstanding discrepancy between experiment and theory regarding the emission angle of electrons. He thus inspired and renewed the debate on the attoclock method.

About one third of the list of speakers consisted of young scientists, many of them being PhD students in the QUTIF network. They did an excellent job in reporting the status of the QUTIF network nearly one and a half years after its beginning. Noteworthy scientific newcomers include Giulio Vampa (invited speaker from Stanford University), showing exciting results of high-harmonic generation from various types of solid systems, Alvaro Jiménez-Galán (Max Born Institute Berlin), reporting a theoretical framework for high-harmonic generation in bicircular laser fields and shedding light on the polarization properties of individual harmonic peaks, and Sebastian Eckart (Goethe University Frankfurt), showing pump-probe measurements that experimentally confirm the dependence of strong-field ionization on the direction of the initial-state angular momentum. Although not using tailored fields, this work provides a knowledge basis for other projects that rely on bicircular fields or angular momentum states.

The workshop gave a broad view on physics and chemistry driven by tailored light fields on ultrafast time scales. Clearly, one important subject was the observation and control of matter on sub-femtosecond time scales, while another intensely discussed aspect was the response of matter to non-linearly polarized fields. Overall, the workshop showed how the manipulation of microscopic phenomena on short time scales has become surprisingly accurate through recent developments in the field.

Dynamical Probes for Exotic States of Matter, Workshop

Scientific coordinators: M. Knap, R. Moessner, F. Pollmann

The **mpipks** workshop “Dynamical probes for exotic states of matter” was held from 27 - 30 March 2017. The aim of the workshop was to bring together leading scientists working on dynamical and non-equilibrium properties of quantum many body systems. Dynamical properties have shown to provide characteristic fingerprints of exotic phases of matter such as topologically ordered and fractionalized phases. Furthermore, quantum matter out of equilibrium can exhibit novel phases that cannot occur in equilibrium settings. The talks and poster contributions mainly followed the main themes:

- Dynamical properties of quantum spin liquids
- Floquet engineering of novel orders and their dynamics
- Dynamics of the many-body localization transition
- Many-body localization beyond one-dimension
- Efficient algorithms for the simulation of quantum many-body dynamics
- Decoherence in open systems and stability of quantum orders
- Diagnostics of topological phases and transitions
- Dynamics of fractionalised particles

The organizers attempted to have a wide representation of invited talks from different field, including established as well as junior scientists: Dynamical properties of quantum spin liquids (Claudio Castelnovo, Sasha Chernyshev, Radu Coldea, Matthias Gohlke, Matthias Punk, Ioannis Rousochatzakis, and Yuan Wan). Many-body localization (Jens Bardarson, Immanuel Bloch, John Chalker, Johannes Knolle, David Luitz, Maksym Serbyn, Mari Carmen Bañuls, and David Pekker). Floquet engineering of novel orders and their dynamics (Arnab Das, André Eckardt, Netanel Lindner, Gil Refael). Non-equilibrium properties quantum many-body systems (Fabian Heidrich-Meisner, Michael Messer, Leonid Pryadko).

The talks were well attended and discussions to these topics were very lively. The longer lunch and coffee breaks were useful as they led to many stimulating discussions between the participants.

The poster sessions, which gave in particularly young researchers the chance to present their results, were well attended and discussion in front of the posters lasted until late in the night.

Stephen Nagler (Oak Ridge, USA) accepted our invitation as the distinct speaker of the institutes colloquium in which he gave a overview talk on “Magnons, spinons, Majorana fermions and quantum spin liquids”. His very inspiring talk highlighted many of the recent theoretical advances in the understanding of quantum magnets.

Joint IMPRS Workshop on Condensed Matter, Quantum Technology and Quantum Materials, Workshop

Scientific coordinators: S. Gzyl, A. Kenfack, M. König, H.-G. Libuda

The Joint IMPRS Workshop on Condensed Matter, Quantum Technology and Quantum Materials took place from 3 - 7 April 2017 at **mpipks**. The workshop was a joint initiative of four International Max Planck Research Schools - the IMPRS for Condensed Matter Science (Stuttgart), the IMPRS for Chemistry and Physics of Quantum Materials (Dresden), the IMPRS for Quantum Science and Technology (Garching), and the IMPRS for Many-particle Systems in Structured Environments (Dresden) - which have a scientific overlap in the research areas mentioned in the workshop title. The topics presented and discussed at the workshop covered all aspects of research performed at the participating programs, ranging from fundamental theoretical concepts in quantum information theory to experimental studies of novel quantum materials.

The workshop brought together approximately 60 PhD students and senior scientists from the four programs as well as a few external participants, i.e. PhD students and young postdocs from research institutions not affiliated with any of the IMPRS. The main goals of the workshop were to give the junior scientists, in particular, insight into the different research topics pursued at the participating institutions,

and also foster direct interaction and discussion among all participants. To achieve these goals, the program of the meeting was predominantly made up of talks from the students themselves, with a good balance between the different IMPRS, together with overview talks from the MPI directors and group leaders and with a good amount of discussion time.

In addition, poster sessions gave all participants an opportunity to present their own results. In particular, students in the early stages of their PhD projects were encouraged to discuss the ideas of their projects enabling them to receive feedback. The poster sessions sparked a lot of discussions between participants from different research fields and thus contributed significantly to the desired exchange between students.

Discrete, Nonlinear and Disordered Optics, Workshop

Scientific coordinators: M. Segev, A. Szameit, S. Turitsyn

The **mpipks** workshop "Discrete, Nonlinear and Disordered Optics" (DINDOS17) was held from 8 - 12 May 2017. The aim of the workshop was to present the latest experimental and theoretical results in the fast developing field of discrete nonlinear and disordered optical systems. The recent merging of nonlinear photonics and disordered system physics promises a considerable impact on various disciplines in science, from physics to biology and chemistry. Nonlinear disordered optical systems offer new platform for numerous engineering applications: random lasers for imaging, random fibre lasers for material processing, ranging, metrology and telecommunications, disordered fibre gratings for various applications (ultra-broadband or very narrow filtering) and other applications. The workshop brought together 60 leading experts and students from the fields of photonic lattices, disordered systems, nonlinear photonics, meta-surfaces, random laser science and discrete systems to timely discuss recent progress and interdisciplinary synergy emerging at the interface of these fields, and gave an overview to young scientists of exciting possibilities of interdisciplinary research in these fields with the special focus on the practical applications of fundamental science. The talks and poster contributions mainly followed the main themes:

- Photonic simulators of quantum physics
- Disordered quantum physics
- Synthetic photonic lattices
- Nonlinear photonics
- Disordered photonics
- Meta-surfaces
- Random lasers
- Discrete optical systems

We were in particular delighted to welcome Prof. Nader Engheta, Prof. Immanuel Bloch and Prof. Federico Capasso as plenary speakers.

The talks were well attended and discussions to these topics were very lively. Extended lunch and coffee breaks were useful as they led to many stimulating discussions between the participants. Also, the poster sessions, which gave in particularly young researchers the chance to present their results, were well attended and discussion in front of the posters lasted until late in the night.

Future Trends in DNA-based Nanotechnology, Workshop

Scientific coordinators: Ch. Fan, M. Mertig, H. Yan

Nucleic acid-based nanotechnology employing basic biological principles such as molecular recognition and self-assembly for advanced materials synthesis is now a pioneering field. This year's DNATEC17 meeting reflected the enormous progress in this rapidly growing cross-disciplinary field. Moreover, DNATEC17 focused on a profound discussion of its future trends. By bringing experts from the field and related fields of physics, biophysics, chemistry, biology, computer science and materials science together, the meeting enhanced the exchange of ideas and understanding. This way, DNATEC17 has become an international widely recognized event in the field of DNA nanotechnology. It brought together more than 100 scientist from 22 nations.

The meeting showcased the most recent progress in nucleic acid-based nanotechnology with invited speakers who are pioneers and key players of the field. Ned Seeman, Ebbe Anderson, Mark Bathe, Yonggang Ke, Chengde Mao, William Shih and Peng Yin discussed the amazing capability to design and construct DNA and RNA nanostructures of increasing complexity. Robust RNA folding into predesigned structures is demonstrated in cells. Automated design features and modelling of the structure dynamics,

as presented by Aleksei Aksimentiev, are more widely introduced to the field to enable scientists to design their own structures. Such design capabilities enable more applications to follow. Guillermo Acuna, Sebastien Bidault, Frank Cichos, Baoquan Ding, Oleg Gang, Tim Liedl, Philip Tinnefeld and Qiangbing Wang discussed their progress in using DNA nanostructures to direct the assembly of photonic structures to build plasmonic nanodevices and nanoswimmers. Ashwin Gopinath from Caltech showed the amazing capability to precisely position single DNA origami containing chromophores to create defects in photonic crystals. Oleg Gang presented his groundbreaking results of using DNA origami to build 3D arrays to organize nanoparticles. Programmable as well as large-scale assembly of nanoparticles and proteins was shown by Yossi Weizmann, Hendrik Dietz and Andreas Fery.

DNA nanostructure provides excellent molecular pegboards to position molecular imaging probes for super-resolution fluorescence imaging. Ralph Jungman and Peng Yin talked about their results of using DNA pegboard to achieve super-resolution imaging down to 5 nm resolution.

DNA-directed lipid assembly is an emerging hot topic in the field. Chenxiang Lin from Yale, Dongsheng Liu from China, Stefan Howorka and Ulrich Keyser from UK discussed their work on using DNA nanostructures to engineer shapes of lipids and liposomes to create artificial membrane nanopores and nuclear nanopores. These would lead to new methods in synthetic biology to control material transport in and out of cellular systems.

Dynamic nucleic acid nanotechnology was another new and fascinating topic of the meeting. Andrew Turberfield and Yonggang Ke discussed their work on using DNA to building molecular devices and transformers. Yonggang Ke presented an amazing work of reconfiguring DNA origami by utilizing conformational isomerization of DNA junctions.

Nucleic acid nanotechnology has provided its potential for programmable molecular circuitry, intracellular biocomputation and synthetic biology. Alex Green and Yannick Rondelez showcased their work on using DNA and RNA toehold switches to control and construct biological circuitry.

Functional nucleic acid nanotechnology for biological systems was another important topic in the meeting. Yamuna Krishnan, Kurt Gothelf and Itamar Willner presented their results of using DNA nanostructures to deliver, image and sense events in and outside of cells. The first application of DNA origami in dynamic biosensors was reported by Ulrich Rant.

Young scientists could present their results in short invited talks or via posters. Two evening sessions were dedicated to the discussion of the various posters. These sessions have been a good venue for young scientists to interact with world leading scientists in the field. The last day of the meeting was focused on tutorials on photonic systems and controlled surface immobilization for young students and beginners in the field.

It is a particular pleasure of the scientific coordinators of the meeting, Chunhai Fan (Chinese Academy of Sciences, Shanghai, China), Michael Mertig (Technische Universität Dresden and Kurt-Schwabe-Institut für Mess- und Sensortechnik e.V., Germany) and Hao Yan (Arizona State University, USA), to thank the local organizers, Katrin Lantsch and Dr. Michael Genkin, for their perfect organization of the meeting and the great support for its realization. The meeting was further financially supported by a DFG grant to Michael Mertig and a NSF and an ONR grants to Hao Yan.

Quantum Memory from Quantum Dynamics, Symposium

Scientific coordinators: J. S. Briggs, J.-M. Rost, W. Strunz

This was a concentrated symposium with around forty-five participants from some ten different countries. The conference began on Thursday 15 June at 16:00 and ended on Saturday 17 June around 12 noon. The aim of the conference was to assess the progress made in the theory of quantum dynamical processes of complex atomic and molecular systems over the last ten years. Of particular interest, as the name of the symposium suggests, was the role played by “quantum memory” on the time evolution of dynamical systems on a microscopic level. Indeed the role of time propagation in general was a theme throughout most of the conference talks and the importance of time dependence in physics, whether atomic, molecular, nuclear or solid state, was made evident.

The role of quantum memory in general time propagation was outlined in the talk of Strunz (Dresden) and examples of Markovian or non-Markovian behavior treated in two further talks. Helm (Freiburg) discussed the question of phase memory in quantum processes and Richter (Regensburg) introduced the intriguing possibility of quantum time mirrors. The role of time in the quantum to classical transition was the subject of three further talks.

There was a strong representation from the group of Keitel at the MPI fuer Kernphysik in Heidelberg

with talks on all aspects of time-dependent processes in extreme laser-matter interactions extending to the relativistic regime and nuclear processes. Thumm (Kansas) described how time resolution can now be extended to surface photoemission.

Additionally there were several contributions on the time evolution of quantum dynamics in few-body systems from atoms to molecules, clusters and solids, indicating the breadth of application of rather similar theoretical approaches developed by the participants.

The symposium was undoubtedly a great success and all attendees carried away happy (quantum) memories of the occasion.

Brain Dynamics on Multiple Scales - Paradigms, their Relations, and Integrated Approaches, Workshop

Scientific coordinators: P. Achermann, E. Olbrich, T. Wennekers

Motivation for the workshop was that previous research in the brain sciences frequently focused on a single spatial or temporal scale, often related to just one specific paradigm, experimental technique, or theoretical approach. Only as a more recent trend, that we wished to foster, have integrated approaches been put forward, which, for example, provide mathematical or experimental links between the dynamics on different brain scales, combine different experimental or modelling methods, analyse large and heterogeneous data sets in multiple ways or at different resolution, or simulate multiple area models of cognitive functions and whole subsystems of the brain. It seems plausible that understanding a multiple-scale system made up of complex interacting dynamical elements like the brain, likewise requires a science that puts emphasis more on the relations between its building blocks, its scales, methods, and paradigms, rather than individual such entities alone.

The main aim of the conference was therefore to identify and nurture bridges or connections between two, three or more "elements of brain science". "Elements" here was understood in a broad sense (disciplines, methods, paradigms, scales, levels, etc.) – emphasis was on combining different elements in novel ways, as well as the expected benefits of the proposed links, that is, how they might contribute to the goal of understanding brain function.

The 5-day workshop was attended by 75 participants, and comprised 16 invited and 15 contributed talks as well as 37 posters. We had a good mix of experienced senior researchers, aspiring younger scientists, postdoctoral fellows and graduate students. It is noteworthy that we had more than twice as many applications than places available. Many attendants brought posters that hung for the whole duration of the conference and were presented in 3 lively and open-ended evening sessions. This and also the intensive discussion sessions were very well received.

The workshop gave a comprehensive overview in the area of the workshop topics. The participants appreciated in particular the breadth of the program. We observed an extraordinary amount of interaction between participants from different fields and backgrounds which may lead to future collaborations.

The workshop identified several lines of research that may serve important integrating functions and see growth in the future, for example, networks of phase oscillators (Kuramoto model and its extensions), models for large scale and systems level simulations, or standardized platforms for data sharing, analysis and simulation. However, to close the gap between mechanisms of information processing and cognition and macroscopic brain dynamics as it is reflected by EEG and MEG oscillations remains a challenge for the future.

Climate Fluctuations and Non-Equilibrium Statistical Mechanics: an Interdisciplinary Dialogue, Seminar and Workshop

Scientific coordinators: J. Krug, B. Marston, J. Weiss, R. Zia

Climate change requires that we better understand coming changes to the planet. Since climate is the result of complex interactions between the atmosphere, oceans, polar ice, and life, it is very challenging to predict future conditions, including shifting extremes in variability or fluctuations of climate. A fundamental difficulty is that the solar radiation drives the climate system far away from thermal equilibrium, into a regime where the well established principles of thermodynamics developed in the 19th century cannot be reliably applied. Non-equilibrium statistical mechanics is a rather young branch of theoretical physics that aims to identify overarching principles governing the behavior of such strongly driven systems, an endeavor that has been remarkably successful in recent years. The statistical analysis of long time series, such as records of temperature or flooding, has a longer history but new mathematical ideas are now

transforming the field. So far there has been only limited interactions between researchers in climate science, non-equilibrium statistical mechanics, and time series analysis, despite important implications of the work in each of the three fields for the other. In the workshop and seminar held at **mpipks**, senior and junior scientists in all three fields engaged in dialogues that benefitted from cross-fertilization.

55 participants from 11 countries attended, 19 of which were at the graduate student or early postdoc level. Invited speakers represented the three areas, including Petra Friederichs (Bonn, DE), Christopher Jarzynski (Maryland, USA), Udo Seifert (Stuttgart, DE), and Cecile Penland (NOAA, USA). The Workshop program comprised 19 invited and 24 contributed talks as well as 8 poster presentations, and 24 lectures were scheduled during three weeks of the Seminar. All the young scientists attending the Seminar were given the opportunity to deliver hour-long presentations of their work, thus allowing for detailed feedback from the more senior participants. This emerging generation of scientists will be the ones to bring the fields of climate science, statistical mechanics, and time-series analysis together.

The program was very successful in establishing new contacts between participants with different backgrounds and identifying key questions for future interdisciplinary work. Examples include the application of principles of nonequilibrium statistical mechanics to the optimization of subgrid parametrizations of climate models, and the use of dynamical models of intermediate complexity to provide a physical underpinning of time series analysis.

A public lecture, entitled “Neue Daten aus der Klimaforschung: Bekommen wir die Klimakrise noch in den Griff?” was given by Prof. Stefan Rahmstorf (Potsdam, DE) to a full auditorium on 18 July. The many questions that Prof. Rahmstorf received at the end of the talk was one indication of the keen interest by the audience in the ideas that he presented.

Korrelationstage 2017, Workshop

Scientific coordinators: S. Eggert, A. Mackenzie, S.R. Manmana

The meeting Korrelationstage is one of the central meetings in Germany for the strongly correlated quantum systems' community taking place every 2 years. The goal is to give an overview over the most important developments in the field, and to provide a lively platform for discussion, exchange and networking especially for the German community. In this year's event, ca 120 participants presented their results in ca. 80 talks distributed over 18 sessions and ca. 40 poster presentations on Tuesday and Wednesday evening. The topics covered by this workshop had a wide range, including nonequilibrium many-body physics, disorder and impurities, frustrated magnetism, reduced dimensions, topology, superconductivity, computational methods, and developments towards applications of correlated systems.

Particular emphasis was given to young researchers (> 40 participants), who presented their work in oral and poster contributions. In addition to the sessions, time for free discussions was available, which was used in a lively way and which helped to stimulate and promote exchange between young and senior researchers.

The Korrelationstage again was an important event that was scientifically stimulating and promoted the exchange among the community. The scientific organizers Salvatore R. Manmana, Sebastian Eggert and Andrew Mackenzie would like to thank the **mpipks** for the support and, in particular, Katrin Lantsch and her team for the organization of this workshop.

Quantum Sensing with Quantum Correlated Systems, Workshop

Scientific coordinators: M. Oberthaler, S. Rachel, A. Sanpera Trigueros

Focus of the Workshop:

The focus of the workshop “Quantum sensing with quantum correlated states” has been to joint together worldwide experts in the many facets involving quantum metrology. Quantum metrology with strongly correlated systems is a truly multidisciplinary area and we aimed at putting together scientist working in quantum information processing, condensed matter, ultracold gases, quantum dots etc.. in order to explore how quantum correlations, on their broader sense, can be used for improved sensing beyond classical limits.

Quantum information theory has helped developing a precise language with an ample vocabulary for the characterization of quantum systems based on quantum correlations. Undoubtedly, the theory of entanglement has provided a new set of powerful tools to gain understanding about many-body strongly correlated systems by explicitly considering the tensorial product structure of the composite states. Quantum correlations put in evidence the importance of such tensorial structure. Therefore, the workshop

has also been very useful to question fundamental topics about characterization and quantification of highly entangled quantum states in interacting many particle systems. The combination of fundamental theoretical aspects with experimental activities in the context of metrology and synthetic quantum matter provides a unique opportunity to explore new possibilities. Sensing is one of the tasks in which quantum correlated states can over perform the efficiency of classical systems to determine a parameter and has applications in many other areas of science. Special emphasis on magnetometry and magnetic gradients using strongly correlated systems has been discussed.

Participants:

The list of invited speakers included both, very relevant and established figures in different disciplines, both experimental and theoretical, with young scientist with already promising contributions on the field. In experiments, particularly remarkable were the contributions of J. Bollinger (NIST, USA), Steve Girvin (Yale, USA), D. Budker (Germany), E. Polzik (Univ. Copenhagen), Monika Schleier-Smith (MIT, USA) and several others. In the theory, the work of A. Smerzi (Florence, Italy), Ana Maria Rey (NIST, USA), Israel Klich (USA), M. Heyl (Germany) where also very remarkable. In general, we have prioritized the scientific contact and discussions between the participants allowing to this aim a lot of time for discussions. To achieve this goal we enhanced scientific exchange and reduced the number of talks. Invited speakers were asked to spend 10' of their time slot to introduce their subject to the audience and to present their results in the frame of quantum sensing. A large majority of the speakers did so, as a consequence, in a large part of the invited talks, questions from the participants extended far away from the allocated discussion of time. That has helped to the newcomers to feel in a very open and relaxed atmosphere and to discuss together very vividly.

Unfortunately, due to the fact that the workshop time-slot was allocated on the third week of September of 2017, and on the first week of September, the biannual conference on Bose-Einstein Condensation took place in Spain, few remarkable scientists outside Europe which were initially accepted had to decline due to the impossibility of doing two trips to Europe within two weeks. be an invited speaker, decline because travelling twice to Europe was not possible for them.

Expected Outcomes:

Several outcomes are to be expected as a consequence of the workshop, mostly motivated from (i) A timely research topic, (ii) First interdisciplinary workshop on quantum metrology, (iii) The talks presented by the invited speakers, (iv) The interdisciplinary participation with people from distinct scientific areas. The possibility of opening common projects have been discussed at length by the European participants. In general, we believe that the potential outputs of the workshop are very high. A lot of different ideas about quantum sensors with many different applications are now starting to be developed and new collaborations between different groups is a reality due to the workshop. To give some examples, Prof. A. Smerzi (Italy) has been invited by Prof. A. Sanpera (Spain) in January 2019 to initiate a joint work on metrology. The student A. Yuste (Barcelona) has been invited by Dr. P. Hauke (Heidelberg) for a research stage based on quantum sensing. A lot of discussion were also devoted to prepare joint common projects for the next European calls.

Finally, we would like to mention that the organization and facilities offered by the M. Planck Institute at Dresden were very helpful. We truly appreciated this invaluable help regarding financial support, infrastructure, and last but not least the efficiency before, during and after the workshop of Mrs. C. Domaschke.

Critical Stability of Quantum Few-Body Systems, Seminar and Workshop

Scientific coordinators: T. Frederico, A. Jensen, A. Kievsky, J.-M. Richard

School:

The first week was organized as a school for mature students, postdocs, and young researchers. There were four lecturers, each giving three lectures of one hour, and a follow up of twice two hours of discussion and exercise sessions. This resulted in four full days of teaching activities. The topics and teachers were chosen to present a broad pedagogical introduction to the subjects expected at the workshop, namely momentum and coordinate space few-body techniques, the concept of universality, and the transition from few- to many-body degrees of freedom. The lecture notes by the teachers were made available before the presentations.

The last day was reserved for the contributions of the participants. Each of them had twenty minutes to present a project he had himself chosen and respond to questions. The organizers were present at all lectures and talks on the last day of the school. It was a good surprise that the talks by the participants were of very high quality both by their scientific content and pedagogical aspects.

The school participants were asked to evaluate the lectures and the exercises, through an e-mail questionnaire. The responses were in general very positive with evaluations ranging from excellent to above the average. Without exceptions, the responses indicated that the school was a very fine preparation for the specialized workshop talks. Also the individual project presentations and the subsequent discussions on the last day were unanimously very positively received. The lectures were deemed very well presented while the exercises in general were less popular and less helpful probably because they were too often made at generalizations and further applications of the concepts introduced in the lectures, and less often devoted to immediate and direct applications. The amount of content in the four series of lectures probably added up to be too large for four days. The week was intense but overall the participants were satisfied.

Workshop:

The second week was organized as a workshop with 39 contributions of 40 minutes by all participants split as 30 minutes for the talk and 10 minutes for the discussion. In addition, the Colloquium by the recipient of the Gutzwiller award was included in the program of the workshop. The 9 groups of topics, 1. Universality, 2. Finite-range corrections, 3. Few and many-body degrees of freedom, 4. One and two dimensions, 5. Dimensional crossover, 6. Multicomponent systems, 7. Dynamics, 8. Reactions with weakly bound systems, 9. Mathematical few-body problems. All topics received attention through several talks.

Most workshop contributions are planned to appear in a special issue of Few-Body Systems entitled "Special issue on Critical Stability of Quantum Systems" where also the lectures at the school will be included.

There were 63 participants at the workshop, coming from 17 different countries, including almost all 21 school participants who stayed for the workshop. A number of subfields of physics with focus on few-body quantum problems were represented, such as quantum chemistry, mathematical, atomic, molecular, condensed matter, hadron and nuclear physics. Apart from the school participants (very young) and the organizers (rather senior) the average age of the workshop participant was about 43 years. This corresponds to a generation ready to take over from the very well established physicists. They all presented convincing and mature talks about the diverse topics they had been working on, expressing vitality and new avenues to be explored on the boundaries and within the different subfields of physics.

The topics of universality in various disguises were probably the most prominent issue discussed at the workshop. It is not easy to select specially interesting contributions, but if pressed consensus probably would be, (i) the experiments by Reinhard Dörner where the probability distribution of the excited atomic helium trimer is mapped out, (ii) the zoo of Efimov towers of excited states by Yusuke Nishida, (iii) the topological classification of symmetries of few-body structures in different spatial dimensions by Nathan Harsmann.

The overall goals of the workshop were achieved, that is exchange of ideas and techniques across the barriers of subfields, updating and distributing research results, and initialization of new collaborations perhaps based on the ideas exchanged at the meeting. The school served both as basic education but also as a preparation for the more specialized workshop talks.

The organizers are plainly satisfied by the success of the school and workshop, which came across different subfields of physics and in broad sense each with its set of concepts applied to finite and many-body quantum systems in different dimensions. At the workshop the underlying relevance of the long range quantum correlations brought by some selected degrees of freedom to the complex finite or infinite quantum systems were tackled in the presentations. This common universal basic concept, was raised in different forms during the discussions through the fruitful questions and answers, where the participants were prompted to make an effort to go over distinctions and find the subtle links between the conceptual complexity coming across the boundaries of different subfields of physics.

All this was made possible by the generosity of the **mpipks** in Dresden. This is of course part of the purpose of the Institute but the organizers are nevertheless very grateful for the support which includes not only financial but also the quiet and stimulating environment, the well-functioning infrastructure and the efficient secretarial assistance.

Atomic Physics 2017, Workshop

Scientific coordinators: T. Pfau, J.-M. Rost

This year's workshop was special since it hosted as a focus the status workshop of the DFG SPP 1929 GiRyd priority program which brought two unusual circumstances with it: (i) A number of slots were devoted to present progress in the projects. For this reason additional international speakers were invited in part of the general workshop in the field of the focus. (ii) Due to the structure of the SPP an unusual large number of young investigators attended the meeting. Among them there is considerable interest to gain insight into machine learning. Therefore, we organized in the general part of the workshop a tutorial on machine learning (given by Dr. Stehphan Bialonski on Thursday evening) followed by a session on applications of different machine learning techniques in AMO physics on Friday morning. The focus part of the workshop (Monday to Wednesday) we describe in the following in more detail.

Theme of the focus workshop:

The combination of ultra-cold atoms and high-resolution laser spectroscopy of Rydberg atoms has enabled the observation of very strong interactions between Rydberg atoms, the so-called Rydberg Blockade. Triggered by this milestone a new research field emerged which is branching out from atomic physics to molecular physics, physical chemistry, many-body physics, quantum information processing, quantum simulation, quantum optics, and semiconductor physics as well as surface physics and sensor applications. These topics are explored under the umbrella of the DFG priority program SPP 1929 "Giant Interactions in Rydberg Systems" (GiRyd) established in 2016. The annual GiRyd Status Workshop featured talks from all current GiRyd project groups as well as a number of invited international speakers. The workshop program was designed to bring members of the wide-spread Rydberg community together for networking, discussion and the exchange of up-to-date results and development of new projects. An additional half-day workshop was aimed specifically at young researchers on PhD level in GiRyd projects.

Participants:

A total of 140 delegates participated in the workshop. A majority of them is involved as scientific staff or PIs in active or associate GiRyd research projects. Next to the principal investigators of all GiRyd projects (see giryd.de/en/projects.php) a number of distinguished invited speakers presented talks: Hannes Bernien (Harvard University, USA), Michel Brune (CNRS, Laboratoire Kastler Brossel, France), Matthew Jones (Durham University, UK), Tom Killian (Rice University, USA), Thierry Lahaye (CNRS, Laboratoire Charles Fabry, France), Frederik Merkt (ETH Zürich, Switzerland), Hossein Sadeghpour (Harvard University, USA), Richard Schmidt (Harvard University, USA), James Shaffer (University of Oklahoma, USA).

General Scientific Outcome and Perspective:

When designing the program of the workshop the organizers had the following principal aims in mind:

- to exchange of up-to-date research results in the field of Rydberg physics;
- to discuss new joint projects and collaborations;
- to create coherence and strengthen the network between members of the widespread GiRyd community (22 research groups funded under the DFG priority program SPP 1929 plus numerous associated research groups and scientists from all over Germany);
- to foster the contact between PhD students and postdocs and leading experts in the field.

The workshop has been highly successful with regards to the above mentioned aims. Among other things numerous exchange projects between GiRyd groups were discussed to be realized in 2018 and a plan for a GiRyd PhD School held in Israel in collaboration with Weizmann Institute of Science was formed (preparations are continuing for the event to take place in late September/early October 2018).

We would like to thank Gabriele Makolies for her excellent organization which made this workshop a full success.

Topological Matter in Artificial Gauge Fields, School

Scientific coordinators: A. Eckardt, F. Heidrich-Meisner, C. Weitenberg

The PhD School entitled "Topological Matter in Artificial Gauge Fields (TOPART18)" took place from February 26th to March 2nd at the **mpipks** in Dresden. The school focused on a very timely area of research: artificial gauge fields, which can now be experimentally realized with ultracold atoms and other physical systems and which thereby allow a new view on this central concept of modern physics. In particular, these realizations allow studying topological states, which also lie at the heart of the quantum

Hall effect in solid state physics.

The school had 65 participants from 17 countries in Europe, Asia and America, most of them PhD students working in related fields. 8 internationally distinguished researchers introduced the topic in 13 lectures and 3 tutorials: Monika Aidelsburger, Jan Budich, André Eckardt, Fahad Mahmood, Belén Paredes, Frank Pollmann, Ian Spielman and Alexander Szameit. The program was completed by a poster session, an excursion and time for discussions. In the poster session, the participants presented their own research and used this opportunity to present themselves as a promising new generation of researchers in the field of topological physics.

The PhD School was organized by the MPI-PKS in collaboration with the Research Unit FOR 2414 of the German Research Foundation (DFG). The scientific result of the school is a contribution to the education of young researchers in the field of topological quantum matter and an exchange between the different experimental platforms for the realization of artificial gauge fields.

Chaos and Dynamics in Correlated Quantum Matter, Workshop

Scientific coordinators: D. Luitz, R. Moessner, F. Pollmann

The international **mpipks** workshop “Chaos and Dynamics in Correlated Quantum Matter” was held from 19 - 22 March 2018. The aim of the workshop was to bring together leading scientists working on the dynamics of quantum many body systems. The dynamics of complex systems is apparently irreversible, seemingly in contradiction with the intrinsic reversibility of the microscopic laws of nature. The effective formation of an arrow of time by complex dynamics is an ongoing debate lasting over more than a century. Chaos plays a crucial role in resolving this paradox, and the past decade has seen a great revival of interest in this question concerning the foundations of quantum statistical mechanics and how chaos arises in quantum many-body systems due to enormous computational, theoretical and experimental progress in the field. Important milestones are theoretical findings involving the long sought demonstration that many-body localization (MBL) exists as well as the derivation of exact bounds on chaos and the discovery of spontaneous time translation symmetry breaking. On the experimental side, significant advances have been made in the study of cold atomic gases which provide examples of closed macroscopic quantum systems for which the foundational questions of quantum statistical mechanics are particularly relevant:

- Operator spreading
- Out-of-time-order correlations
- Dynamic entanglement formation
- Quantum thermalization
- Novel quantum phases out of equilibrium
- Spatio-temporal orders
- Efficient numerical simulation of quantum many-body dynamics
- Many-body localization

The organizers attempted to have a wide representation of invited talks from different fields, including established as well as junior scientists: Operator spreading (Adam Nahum, Curt von Keyserlingk, Tibor Rakovszky and Vedika Khemani), Out-of-time-order correlations (Balazs Dora, Yevgeny Bar Lev, Michael Knap, Victor Galitski, Adam Green, Klaus Richter and Subhro Bhattacharjee), Many-body chaos and thermalization (Lea Ferreira dos Santos, Marcos Rigol, Alexey Gorshkov, Tomaz Prosen and Jorge Kurchan), Spatio-temporal orders (Shivaji Sondhi, Achilleas Lazarides, Sthitadhi Roy), Many-body localization (Thorsten Wahl, Janez Bonca and Adam Smith), Statistical Mechanics and high energy Physics (Peter Reimann, Hong Liu, Mukund Rangamani).

The talks were well attended and discussions to these topics were very lively. The longer lunch and coffee breaks were useful as they led to many stimulating discussions between the participants. In particular, the provided up to 6 discussion rooms were very well received and used for smaller group discussions which contributed to a collaborative atmosphere.

The poster sessions, which gave particularly young researchers the chance to present their results, were well attended and discussion in front of the posters lasted until late in the night.

Shivaji Sondhi (Princeton, USA) accepted our invitation as the distinct speaker of the institute’s colloquium in which he gave a overview talk on “Statistical mechanics, localization and periodically driven quantum systems”. His very inspiring talk highlighted many of the recent theoretical advances in the understanding of driven quantum systems and attracted a very large audience.

Novel Paradigms in Many-Body Physics from Open Quantum Systems, Workshop

Scientific coordinators: E. Dalla Torre, S. Diehl, F. Piazza

Strongly-correlated open systems generically violate basic paradigms of many-body physics in thermal equilibrium and therefore require novel concepts and methods to be studied. The goal of this workshop was to provide an overview of the state-of-the-art of this field, both in terms of theoretical approaches as well as experimental realizations. To achieve this goal, we asked 6 of the invited speakers to deliver introductory lectures of 2-3 hours, and limited the other 10 invited and contributed talks to 30 minutes. The total number of participants was 80.

The workshop was dealing with a novel direction of research that crosses different fields, ranging from quantum optics to condensed matter. Consequently, one of our main goals was to provide an overview of the field, especially for young students who are interested in exploring this topic during their graduate and post-graduate studies. Thanks to the growing interest around the themes of the workshop, we expect that in the long term, this will lead to an international scientific community working on this topic. In this sense, we believe the PhD students (33 in number) were probably the most important participants, along with the 6 lecturers, who provided the broad introductions to different aspects of the field, namely Alberto Amo (C2N, Marcoussis), Andrew Daley (University of Strathclyde), Michael Fleischhauer (University of Kaiserslautern), Jonathan Keeling (University of St. Andrews), Tomaž Prosen (University of Ljubljana), Jonathan Simon (University of Chicago).

As said above, the workshop was especially addressed to young researchers entering the field. We had several postdocs and junior PI's among the speakers who provided very clear presentations and represented the large number of diverse directions emerging in this area. We also had more than 60 posters mostly from PhD students presenting the results of their work so far. The two poster sessions were organized in the evenings and provided the basis for intensive and lively discussions among scholars from different areas.

We believe the main result of the workshop was the success of the introductory lectures, especially among the young researchers. The lecturers had the difficult task to coordinate among one another and bridge between different areas of research, and they did a very good job. We think this was a unique opportunity for participants, who could additionally interact with people from different areas based on the common denominator of quantum many-body open systems.

New Platforms for Topological Superconductivity with Magnetic Atoms, Focus Workshop

Scientific coordinators: T. Cren, K. Franke, P. Simon

Topological superconductors have received much attention in the past years, because they may host exotic low energy excitations such as Majorana bound states (MBS). The fact that these obey non-Abelian statistics renders them very attractive for topological quantum computation. Several different platforms to realize topological superconductivity are currently the subject of intensive research.

Among them, a rather simple recipe combining arrays of magnetic atoms or nanoparticles on top of a superconducting surface has been proposed to engineer topological superconductivity. Recent developments in scanning tunneling microscopy (STM) now permit probing and fabricating magnetic structures and many other artificial spin systems on top or embedded in superconductors. The goal of this focused workshop was to gather the main specialists in this growing field in order to discuss the key experimental advances (material preparation, measurements), and to view how the exotic bound state excitations associated with these new superconductors may be unambiguously detected, manipulated and used within this scheme.

Ali Yazdani (Princeton) who was the first to find some possible signatures of Majorana bound states in chains of iron on lead gave the colloquium. He described the recent progress of his group to find unambiguous fingerprints using spin-polarized STM as a way to distinguish standard (Shiba) bound states from the Majorana bound states. His results were based on some general sum rules that the spin-resolved density of states has to satisfy. These sum rules and their derivation were presented by B. Bernevig (Princeton) earlier in the workshop. B. Bernevig also presented some evidence that Bismuth is a second-order 3D topological insulator with protected 1D hinge states. R. Wiesendanger (Hamburg) demonstrated a fully-controlled bottom-up fabrication of artificial 1D atomic chains from individual magnetic Fe adatoms on a superconducting Rhenium substrate, which are also suggested to host Majorana bound states at their ends. Experimental results which probe the structure and Majorana wave function of mono-atomic Fe chains on superconducting lead with atomic force spectroscopy were shown by E. Meyer (Basel). Some more detailed theoretical frameworks to describe chains of magnetic atoms or

more complicated clusters were explained by B. Braunecker (St Andrews) and T. Ojanen (Helsinki). F. von Oppen (Berlin) presented results of a successful experiment-theory collaborative work to scrutinize the physics of Shiba multiplets and associated wave functions taking into account the different orbitals of the adsorbed magnetic atoms. The theoretical picture of single impurities was further complemented by R. Zitko (Ljubljana).

Alternative platforms have also been discussed extensively along the workshop. A. MacDonald (Austin) exposed recent results on thin-film magnetically-doped topological insulators that are placed on a superconducting substrate as a promising route. C. Brun (Paris) showed experimental results on a system composed of magnetic Co clusters below a monolayer of lead which may offer an interesting route for 2D topological superconductivity. D. Loss (Basel) proposed a critical interpretation of the recent achievements of the physics of topological semiconducting wires. B. Sacepe (Grenoble) presented recent results on the ac Josephson effect in the 3D topological insulator Bi_2Se_3 . The physics of iron-based superconductors has also been covered by other invited speakers such as P. Wahl (St Andrews) and C. Hess (Dresden). J. Hoffman (Harvard) presented SmB_6 as an interesting topological material, whereas H. Suderow (Madrid) showed topological aspects of vortex states.

Finally, the program was considerably enriched by contributed talks of high quality on all of these topics together with a lively poster session.

Predicting Transitions in Complex Systems, Workshop

Scientific coordinators: J. Hlinka, K. Lehnertz, C. Masoller

Complex dynamical systems, ranging from the heart and the brain to ecosystems, financial markets and the climate, can show sudden transitions to contrasting and, at times, even disastrous dynamical regimes. Both reliable detection and prediction of transitions are of utmost importance in many scientific fields. If catastrophic transitions occur in an unexpected way, they often do not allow for developing adaptation and/or mitigation strategies. It is thus crucial to identify early-warning signals of such transitions.

The main focus of the workshop was therefore to bring together scientists from various disciplines of natural sciences who investigate transitions in complex systems and their predictability either from the methodological point of view or through applications. The workshop aimed to bridge the different disciplines by stimulating the discussion about new advances in data-driven approaches for identifying, characterizing and predicting regime transitions.

The 5-day interdisciplinary workshop was attended by 71 experienced senior researchers, aspiring younger scientists, postdoctoral fellows and graduate students from 21 countries. It is noteworthy that we had more than twice as many applications than places available. The workshop gave a comprehensive overview in the area of the workshop topics through 27 invited and 22 contributed talks as well as 31 posters presented in two lively and open-ended evening sessions, all of which were very well received. The participants appreciated in particular the breadth of the program. Excellent presentations of the different approaches developed in the context of the wide-spread areas of applications generated an extraordinary amount of interactions between participants from different fields and backgrounds, which initialized new international and interdisciplinary collaborations.

Quantum and Semiclassical Trajectories, Focus Workshop

Scientific coordinator: B. Poirier

Twenty-seven interdisciplinary participants from fifteen countries came together to discuss the core question of how best to reconcile the wave and particle (trajectory) pictures in quantum mechanics. Over the decades, substantial progress has been made, but from a broad range of disciplines that often have little interaction with each other.

The aim of this workshop was therefore to bring together researchers from these diverse communities—e.g., atomic and molecular physics, chemical dynamics, extremely high resolution spectroscopy, mathematics, nuclear physics, scientific philosophy, quantum foundations, and relativistic quantum mechanics—to share ideas and expertise, and to foster exciting new interdisciplinary collaborations.

This focus workshop was highly unusual in that most participants did not know each other beforehand. However, through carefully coordinated discussion sessions, shared meals, etc., there were many lively discussions, and much interdisciplinary cross-fertilization. Not all participants were formal speakers, but all were encouraged to take part in the discussions. There were a number of faculty who participated in this fashion, i.e. not as formal speakers. Conversely, several postdocs and assistant faculty members

gave formal presentations.

In the short term, the most important broader impact was that a meaningful dialog was established, in an area of common interest, among disciplines that ordinarily have little to no contact with each other. In the long-term, this may lead to new research areas and collaborations. Also, many participants shared their enthusiasm for holding more meetings of this kind in the future.

Optimising, Renormalising, Evolving and Quantising Tensor Networks, Workshop

Scientific coordinators: A. G. Green, R. Melko, T. J. Osborne

The guiding focus of the workshop EVONET18 was the study of the varied methods and applications of tensor networks in quantum physics and beyond. In particular, the meeting was intended to explore key directions organised under several broad, physically-motivated themes. These included, chaos and hydrodynamics in quantum thermalisation, quantizing tensor networks, representing and evolving open quantum systems, renormalizing tensor networks, and new network structures. Another key goal of the workshop was to intensify research on connections between tensor networks and machine learning networks, to which end, the meeting benefitted from the machine learning conference organised in the following week.

There were several key participants of the workshop. Here we were lucky to have Miles Stoudenmire present the colloquium, who gave an excellent overview of both the fields of tensor networks and machine learning. This played a crucial role during the remainder of the workshop as the participants could relate to each other via the common vocabulary Miles introduced. Further significant participants included Robert Konik who gave a guiding talk on thermalization, Ehud Altman who gave an important contribution on hydrodynamics of thermalization, and Zohar Ringel who gave an excellent talk on connections between machine learning, tensor networks, and quantum information ideas.

The scientific newcomers provided some of the most interesting and inspiring contributions to the workshop. Here notable talks include those of Gemma De las Cuevas, Andrew James, Andrew Hallam, Sebastian Wetzl, and Thorsten Wahl. The speakers made extra efforts to make their work accessible while also managing to touch on advanced research topics.

The scientific results reported on during EVONET18 provided a broad cross-section of the cutting edge research taking place in the rapidly diversifying field of tensor networks. Several key areas of very active research were discussed thoroughly, including many body localization, hydrodynamics and thermalization, and machine learning. In addition, state-of-the-art numerical methods were intensively reported. Multiple guiding problems were discussed and newly arising research areas at the intersection of machine learning and tensor networks were explored.

Machine Learning for Quantum Many-body Physics, Workshop

Scientific coordinators: R. Melko, T. Neupert, S. Trebst

This one-week workshop covered the emerging research area that applies machine learning techniques to analyze, represent, and solve quantum many-body systems in condensed matter physics. Over the last few years, researchers with diverse backgrounds in theoretical condensed matter physics used artificial intelligence algorithms for a variety of purposes including phase classification and characterization, state compression, feature extraction, wavefunction representation with neural networks, and to draw connections between tensor networks and machine learning. All these approaches were represented at the workshop. Each day started with an overview lecture on one of these subjects, delivered by Roger Melko (University of Waterloo), Eun-Ah Kim (Cornell University), Juan Carrasquilla (Perimeter Institute), Lei Wang (Chinese Academy of Sciences), and Miles Stoudenmire (Flatiron Institute). These talks were complemented by shorter invited and contributed talks and two poster sessions. As part of the workshop, Giuseppe Carleo from the recently founded Flatiron Institute in New York gave a **mpipks** colloquium on "Neural-Network Quantum States: from Condensed Matter to Quantum Computing".

The event allowed for plenty of discussions and exchanges between the participants, which is vital in this rapidly developing yet already rather complex field. It became clear that this young field has a lot of potential, for instance with regards to the connections between machine learning and tensor network methods as well as in developing the most useful applications for quantum machine learning. Furthermore, the dialogue between the field of computer science and the field of quantum physics can be beneficial for both sides. Physicists clearly profit from taking advantage of the latest and best performing algorithms for their problems. On the other hand, they may contribute to making algorithms less prone to failure

and to a deeper understanding of the inner workings of machine learning algorithms. The workshop demonstrated not only that the field of machine learning is very young, but also that a number of the key players are early career scientists. In addition, a large number of PhD students and young postdocs showed their first results in this field of research and indicated that they will be focussing on machine learning applications in their upcoming work. This, together with the large number of applications for the workshop, points toward an expansion of this vibrant research area in the near future.

Synthetic Non-Hermitian Photonic Structures: Recent Results and Future Challenges, Workshop
Scientific coordinators: A. Eisfeld, R. El-Ganainy, T. Kottos, H. Schomerus

For this workshop, the **mpipks** welcomed a diverse group of 52 participants from all inhabited continents, representing leading experimental and theoretical groups that work on the fundamental and applied aspects in gain/loss engineered optical and quantum-optical systems, as well as extensions to analogous physical settings.

Under the general theme of non-hermitian physics, the workshop covered new developments in the research of Parity-time reversal symmetry, Exceptional points, Topological effects, Supersymmetry, Non-linear interactions, Unidirectional invisibility, Microlasers and Optical sensors.

These issues were covered by 24 invited speakers, representing roughly in equal parts closely interconnected experimental and theoretical activities and including the founding figure of the field, Max-Born medalist Demetrios Christodoulides (University of Central Florida, Orlando), as well as contributed talks and a very lively poster session highlighting the important contributions of the junior participants. Professor Christodoulides also delivered an inspiring colloquium on thermodynamic interpretations of multimode propagation in optical fibres.

Of particular note transpiring through all contributions was the rapidity in which novel theoretical ideas find their way into experimental realizations and practical applications. Throughout the workshop, this was emphasized in the dedicated discussions over the breaks and continuing into the evening, where participants forged new links and exchanged ideas, thereby significantly shaping the future course of this active field. Examples include the upcoming realization of supersymmetric lasers and the pursuit of higher-order degeneracies, topological robustness, time-domain realizations and quantum-optical fingerprints of nonhermitian symmetries, as well as the transfer of ideas to phononic, polaritonic and electronic settings and systems operating in the THz regime.

Single Nanostructures, Nanomaterials, Aerogels and their Interactions: Combining Quantum Physics and Chemistry, Workshop

Scientific coordinators: A. Eychmüller, A. Govorov, A. Knorr

With its great and inspiring scientific atmosphere, the **mpipks** forms an ideal environment for the mutual discussion of experts in complementary fields of nanostructure physics and nano-chemistry. The workshop on Single Nanostructures, Nanomaterials, Aerogels and their Interactions (CQPC18) brought together theoreticians and experimentalists in the fields of materials physics, spectroscopy and chemistry to exchange and develop ideas on the physical and chemical properties of nano-structures and nano-materials. The topics covered investigation, preparation and theory of nano-materials with a focus on their non-equilibrium collective dynamics. Typical examples included nanostructured assemblies such as atomically thin semiconductor materials, perovskites, nanocrystal solids, metamaterials, and aerogels. This choice of materials allowed for a direct knowledge exchange between well established and newly emerging nanoscale systems: highly debated examples included the interplay of bright and dark excitations in strained and stacked materials, nano-crystals and nano-platelets as well as magnetic spin effects in semiconductor quantum dots.

Within these emerging topics, CPQC2018 brought together more than 70 scientists, both experienced and early stage researchers from all over Europe, the US, Israel and Asia, including China, India, Pakistan and Singapore, providing a productive, international and diverse character of the meeting. This way, the meeting has covered cutting-edge research in the field of nano-scale physics with a strong interdisciplinary character including five days of lectures filled with lively discussion sections and three evening sessions that were dedicated to flash presentation and the discussion of the various posters. In particular, young scientists could present their results in talks or posters to promote their career and connect to mature scientists.

The topics of the talks and posters addressed a multitude of aspects of excitation transfer on the nano-

scale such as ultrafast relaxation and high excitation phenomena, cavity photon dynamics, nano-scale chirality, pump-probe and high harmonics spectroscopy, electron capture in strain induced potentials up to functionality in medicine and nano-particle assembly, applications of nanocrystals for lighting and capturing of solar light, the unique properties of aerogels, the art of assembly of a single nanocrystals and nanocrystal architectures, etc.

Most of the experimental questions which have been addressed were accompanied by theoretical and high-end computational work, such as path integrals, new integration schemes and ab-initio theoretical optical spectroscopy, allowing an extensive discussion of the underlying physics and chemistry across the disciplines. This way, all participants have been inspired by exchanging ideas from different fields and cutting-edge developments in the field of nanoscale assemblies.

We really need to thank the local organizers for this, very successful scientific event, in particular Katrin Lantsch for her absolutely perfect organization of the meeting and the great, always sustained support in the process of preparation and while running the meeting. Her support was essential and the overall success of CPQC2018 would not have been possible without her.

Stochastic Thermodynamics: Experiment and Theory, Workshop

Scientific coordinators: J. Bechhoefer, S. Ciliberto, S. Pigolotti, E. Roldan

Stochastic thermodynamics was initiated in the late 90s as a framework to describe the fluctuating behaviour of thermodynamics fluxes that occur at the mesoscale. While much of the initial discussion was theoretical or focused on thought experiments (e.g. Maxwell's demons), impressive technological advances in the last two decades have enabled tests of many of the fundamental principles.

The main focus of this workshop, then, was to bring together representatives from a number of experimental groups, combined with leading theoreticians in the field. The goal was to both summarize the state of the art and to chart further progress.

The Stochastic Thermodynamics: Experiment and Theory (STET) workshop was held over five days and was attended by 74 researchers, divided among senior and junior academics, postdoctoral fellows, and graduate students. The participants were drawn from 22 countries. There were nearly twice as many applications as could be accommodated, indicating the strong interest in the community in these topics. The experimentalists represented worked on a wide range of systems, ranging from colloidal model systems to low-temperature quantum dots to biological motors to gravitational-wave detectors. The theorists presented a range of current views, with much discussion of recent hot topics in nonequilibrium thermodynamics such as: thermodynamic uncertainty relations; the role of phase transitions in various aspects; universal fluctuations of work and entropy production; thermodynamics with strong coupling; and optimization protocols at the nanoscale. The number of invited 32 and contributed 7 talks were kept relatively low to allow ample time for discussions, an aspect of the workshop that was very well received. Conversely, a relatively large number of posters (40) were explored in two evening poster sessions that provoked lively discussion.

The list of invited speakers included some of the most relevant researchers in the field of stochastic thermodynamics, both from theoretical and experimental communities. The scientific newcomers attending the workshop participated actively in discussions with leading experts of the field and had the opportunity to present their most recent work in the two evening poster sessions.

The workshop provided a broad overview of the state-of-the-art of the different research lines developed within the field of stochastic thermodynamics, both experimental and theoretical. The results presented at the workshop may open new avenues in the research areas of nonequilibrium physics of strongly-coupled systems, fluctuations of gravitational-wave detectors, statistical mechanics approaches to cosmology and thermodynamics of biological systems. Furthermore, the discussions between experimentalists and theorists seem to have launched a number of new collaborations, many of them international.

We also organized a special edition of *Journal of Statistical Mechanics: Theory and Experiment (JStat)*, that accepts contributions from participants to the workshop, to be published in early 2019. We expect the special edition to gather the fruits of these new interactions and collaborations and we already received very positive feedback about it from the participants.

Anderson Localization and Interactions, Workshop

Scientific coordinators: F. Evers, A. D. Mirlin

The focus of the Workshop was put on the interplay of Anderson localization and many-body effects. Anderson localization, which is one of the most fundamental and ubiquitous phenomena in modern condensed matter physics, remains a vibrant research area sixty years after its discovery. Recent years have witnessed an outstanding interest in Anderson localization effects in the context of quantum many-body physics. Experimentally, it has become possible to explore localization phenomena in a variety of quantum many-body systems, including disordered semiconductors, electron glasses in amorphous systems, graphene and other Dirac materials, topological insulators, disordered superconducting films and wires, and cold-atom systems in magneto-optical traps. The Workshop involved a balance participation of experimentalists and theorists, with 80 participants in total, and collected many of the key researchers in the field. The central topics of the Workshop and the corresponding key speakers were:

- Many-body localization: W. De Roeck (KU Leuven), S. Bera (IIT Bombay), S. Flach (Daejeon), U. Schneider (Cambridge), D. Abanin (Geneva), G. Pagano (Maryland), D. Luitz (**mpipks**), H. Pichler (Harvard)
- Superconductor-insulator transitions: D. Shahar (Weizmann Inst.), I. Gornyi (KIT Karlsruhe), A. Fridman (Bar Ilan U), C. Strunk (U Regensburg), D. Popovic (Nat MagLab Tallahassee), T. Vojta (Missouri)
- Localization and topology: H. Buhmann (Würzburg), R.-R. Du (Rice U), A. Po (MIT), M. Foster (Rice U), I. Gruzberg (Ohio)
- Anderson localization in driven systems: R. Moessner (**mpipks**), S. Parameswaran (Oxford)
- Anderson localization on random graphs modeling interacting systems: K. Tikhonov (KIT Karlsruhe), M. Tarzia (Sorbonne)
- Disordered interacting quantum systems: A. Altland (Cologne), I. Burmistrov (Landau Inst.)
- Anderson transitions: novel settings, advanced numerical approaches: G. Lemarié (Toulouse), V. Gurarie (Boulder), M. Pretko (Boulder), T. Ohtsuki (Sophia U), K. Slevin (Osaka)

One of highlights of the conference was the **mpipks** Colloquium talk on "Probing many-body localization using ultracold atoms" given by I. Bloch (MPI für Quantenoptik, Garching), one of pioneers of the field. In addition to 28 invited talks, the conference program included 10 contributed talks as well as 32 posters presented at two poster sessions. Several invited talks, as well as 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: E. Doggen (KIT Karlsruhe), S. Bera (IIT Bombay), M. Serbyn (IST Austria), D. Luitz (**mpipks**), Z. Lenarcic (Cologne), K. Tikhonov (KIT Karlsruhe), I. Protopopov (Geneva), H. Pichler (Harvard), M. Tezuka (Kyoto), X. Wan (Zhejiang), I. Khaimovich (**mpipks**).

In our view, the Workshop was a highly successful event; there are several reasons why we think so. First, it offered a possibility of very fruitful discussions of the progress in the field and future perspectives. Without exception, each talk has been followed by an intensive sequence of questions and answers as well as comments. The discussions sometimes uncovered scientific controversies but were always constructive. This has given everyone in the audience a chance to monitor the status of affairs in different directions of the field. Second, we can definitely say from our own observations that the meeting promoted many collaborations and certainly also stimulated new ones. Third, we have received feedback from many participants who fully substantiated our impression. Our colleagues emphasized that the Workshop was very useful and stimulating for them.

We would like to thank the Institute staff, and in particular Maria de Haas, for outstanding organizational support.

Stochastic Dynamics on Large Networks: Prediction and Inference, Seminar and Workshop

Scientific coordinators: M. Opper, G. Sanguinetti, P. Sollich

Stochastic dynamical systems are increasingly playing a central role across many disciplines, with applications in fields as diverse as systems biology, meteorology, computational neuroscience and the quantitative social sciences. Statistical physics has a long tradition of developing approximate methods for forward prediction of the dynamics of a given model. However, researchers are often faced with inverse problems, where parameters of the models may not be known or there are different models competing to explain the

same phenomenon. Hence efficient methods of statistical inference, i.e. the estimation of unobserved states and parameters, are highly relevant in fields such as experimental biology, finance and other areas where very large data sets are available but there is a shortage of modern theoretical techniques for analysing them.

There is a close relationship between statistical inference and the statistical physics of disordered systems, which can be characterized as large systems of simple units linked by a complex network of interactions. This relationship has so far mainly been exploited in the area of developing equilibrium tools that can be used to analyse data from systems at stationarity. More recently, the community has seen a growing awareness of the importance of moving beyond this towards dynamic models, for two main reasons:

(a) Many interesting systems for which statistical analysis techniques are required, e.g. networks of biological neurons, gene regulatory networks, protein-protein interaction networks, stock markets, exhibit very rich temporal or spatiotemporal dynamics; ignoring this can lose interesting information or lead to even qualitatively wrong conclusions.

(b) Current technological breakthroughs in collecting data from complex systems are yielding ever increasing temporal resolution, allowing the fundamental temporal aspects of their functioning to be analysed if combined with strong theoretical methods.

The last few years have seen an increasing development of such methods in computational statistics, machine learning and statistical physics. DyNet18 was set up to exploit the resulting opportunities for cross-fertilisation between ideas and techniques that have up to now been largely developed in distinct communities, with the potential for broad impact across a number of application domains. Its goal was to bring together researchers from different fields such as statistical physics, statistics, numerical mathematics, machine learning and their applications in order to discuss the new challenges originating from dynamical data and how recently developed techniques can be used to tackle them.

DyNet18 successfully provided a forum for exploring possible synergies between solutions to inference problems studied in different communities, with topics ranging across state and parameter estimation in stochastic differential equations; inference in spatio-temporal e.g. reaction diffusion models; path integral approaches; Monte Carlo methods, particle filter based inference; inferring networks from dynamical data; inference and stochastic control/rare event simulations; and agent systems and traffic models.

The workshop brought together a number of successful senior and young scientists, the former including Eric vanden Eijnden (Courant Institute, US), Ron Meir (Technion, Israel), David Saad (Aston University, UK), Sebastian Reich (Potsdam, DE) and Ben Leimkuhler (Edinburgh, UK). PhD students and post-doctoral researchers were particularly encouraged to present their results, both as 20-minute talks and at poster sessions to give them maximal exposure to interaction and scientific discussion. Interesting insights arose for example on the links between non-equilibrium (driven, irreversible) dynamics in physical systems and Monte Carlo samplers that mix more rapidly by breaking detailed balance; on the connections between optimal transport problems and data assimilation; on applications of inference and simulation to crowded stochastic systems; and on new perspectives on the complexity of learning with large neural networks provided by the theory of stochastic dynamical systems.

Correlated Electrons in Transition-Metal Compounds: New Challenges, Workshop

Scientific coordinators: M. Grüninger, G. Sawatzky, J. van den Brink

Strongly correlated transition-metal compounds show very rich physics based on competing interactions and competing phases. The interplay of spin, charge, orbital, and lattice degrees of freedom has been viewed as the main driving force for many years. More recently, this has been complemented by investigations of the role of relativistic spin-orbit coupling, which can result in the emergence of novel phases and topological states of matter. Transition-metal compounds were the binding factor of this workshop, bringing together theoretical model Hamiltonian approaches, first principles density functional theory based calculations, spectroscopic, magnetic, transport, and structural measurements, and the synthesis of new materials. The interplay and mutual frustration of electron-electron interactions and relativistic spin-orbit coupling effects have been the main focus of this workshop held from November 5 to 9, 2018. With 50 invited talks, this workshop attracted a large number of leading scientists from all over the world with a balanced share of theoretical and experimental physics. In total, the 97 participants from 17 countries formed a highly interacting well-focused group of senior researchers and younger scientists. In addition, the workshop profited from the attention of many further colleagues from different institutes in Dresden who complemented the audience. Many participants mentioned the striking coherence of the talks and the very inspiring atmosphere.

The four keynotes were given by Bob Cava (Princeton), Antoine Georges (Paris & New York), Yoshinori Tokura (Tokyo), and Maxim Mostovoy (Groningen). The **mpipks** colloquium was contributed by George Sawatzky (Vancouver). Particularly noteworthy were the three very clear talks given by Judit Romhányi (Okinawa), Alessandro Revelli (Cologne), and Oleg Janson (Dresden), three younger scientists who made excellent use of the chance to present themselves and their fascinating results. Other young colleagues were strongly involved in the lively discussions during the extended lunch break, in the coffee breaks, and after 17:00, for instance during the poster sessions. 40 posters were presented and discussed until late in the night. The **mpipks** is the perfect place fostering such extensive discussions, laying ground for intense collaborations.

The promise held by the prominently staffed list of speakers very nicely materialized during the workshop. Both talks and posters were very well received. The latest developments in both theory and experiment were put in perspective, including in particular topics such as topological quantum spin liquids, exotic quantum states dominated by strong spin-orbit coupling, Kugel-Khomskii-type spin-orbital physics, negative charge-transfer gap compounds, multiferroics, topological defects, or Dirac and Weyl semi-metals.

Tensor Network Based Approaches to Quantum Many-Body Systems, School

Scientific coordinators: F. Pollmann, U. Schollwöck, N. Schuch, F. Verstraete

The **mpipks** International School “Tensor Network based approaches to Quantum Many-Body Systems” (TENSOR18) was held from 13 - 17 November 2018.

Tensor networks provide a new paradigm for describing quantum many-body systems. This school covered recent progress in the fast moving field of tensor network based simulations of quantum many-body systems. The main goal of the school was to teach young PhD students the basics of tensor-product states as well as the most recent technical developments. This is particularly important given the increasing number of groups working on this quickly evolving topic. The lectures and tutorials were given by researchers who work actively both on the development and the application on tensor-product state based methods.

The TENSOR18 school provided pedagogical introductions to matrix-product state based methods and discussed the most recent numerical and analytical developments in the field. The school had lectures and tutorials on different topics:

- Introduction to tensor networks and DMRG (Lecturer: Steven R. White, UC Irvine)
- Tangent space methods for matrix product states (Lecturer: Jutho Haegeman, Ghent)
- Two dimensional tensor networks (Lecturer: Philippe Corboz, Amsterdam)
- Mathematical results and tools on Tensor Networks (Lecturer: David Pérez Garcia, Madrid)
- MPS methods for open systems (Lecturer: Corinna Kollath, Aachen)
- MPS for Lattice Gauge Theories (Lecturer: Mari Carmen Bañuls, Munich)
- Global Symmetries in Tensor Networks (Lecturer: Claudius Hubig, Munich)

The school was very well received by the students and the feedback given was extremely positive. The tutorials and hands-on sessions were particular popular as these allowed a direct application of the theory taught during the lectures.

The students participated very actively throughout the entire program and the questions asked led to stimulating discussions. We were also happy to see that the school helped students from different groups to get to know each other which will foster future scientific exchange.

All students had the opportunity to present their own work during a poster session. The poster session was very well attended and the students discussed their work among each other and with the lecturers until late night.

3.4 Collaboration with Experimental Groups

- *Understanding the physics of dormancy* with S. Alberti MPI-CBG and J. Guck, BIOTEC (Dresden, Germany)
- *Bacterial microcolonies* with N. Biais, CUNY Brooklyn College (New York, USA)
- *RNA-polymerase transcription* with S. Grill, MPI-CBG (Dresden, Germany)
- *Metabolic pathways of dauer worms* with T. Kurzchalia, MPI-CBG (Dresden, Germany)
- *Chromosome organisation during meiosis* with I. Tolic, Ruder Bovskovic Institute (Zagreb, Croatia)
- *Genome activation and chromatin architecture during early embryo development* with N. Vastenhouw and A. Honigmann, MPI-CBG (Dresden, Germany)
- *Quantum dynamics of ultracold atoms* with J. Sherson, Aarhus University (Denmark)
- *Many-body physics with ultracold atoms in optical resonators* ETH Zürich (Switzerland)
- *Characterizing topology by dynamics: Chern number from linking number* with K. Sengstock, University of Hamburg (Germany)
- *Controlling and characterizing Floquet prethermalization in a driven quantum system* with D. Weld, University of California (Santa Barbara, USA)
- *Pump-power-driven mode switching in a microcavity device and its relation to Bose-Einstein condensation* with S. Reitzenstein, Technical University of Berlin (Germany)
- *Interaction dependent heating and atoms loss in a periodically driven optical lattice* with I. Bloch, LMU of Munich (Germany)
- *Quantum phase transitions in ZnO two-dimensional electron systems in the quantum Hall regime* with J. Falson, group of K. von Klitzing and group of J. Smet, MPI-FkF (Stuttgart, Germany)
- *Logarithmic transport anomalies in topological insulator films* with D. Nandi and group of A. Yacobi and P. Kim, Harvard University (USA)
- *Reconstitution of genome activation in synthetic nuclei* with J. Guck, MPI-MPL (Erlangen, Germany), with T. Hyman, MPI-CBG (Dresden, Germany) and with C. Zechner, CSBD (Dresden, Germany)
- *Shape and mechanics of mitotic spindles* with I. Sbalzarini, CSBD (Dresden, Germany)
- *Scaling of spindles during embryogenesis* with J. Huisken, Morgridge Institute for Research (Madison, USA)
- *Harmful algae blooming* with S. Morthi and H. Hillebrand, University of Oldenburg (Germany)
- *Electric power grids* with J. Peinke, University of Oldenburg (Germany)
- *P granule segregation in living cells* with A. Hyman, MPI-CBG (Dresden, Germany)
- *Physics of the formation of the tight junction* with A. Honigmann, MPI-CBG (Dresden, Germany)
- *Ripening in active emulsion* with J. Boekhoven, Technical University of Munich (Germany)
- *Physical principles of replication at the onset of life* with D. Braun and C. Mast, Ludwig Maximilian University of Munich (Germany)
- *Ageing of phase separated compartment* with S. Alberti, MPI-CBG (Dresden, Germany)
- *Controlling and characterizing Floquet prethermalization in a driven quantum system* with D. Weld, University of California (Santa Barbara, USA)
- *Measuring a Dynamical Topological Order Parameter in Quantum Walks* with G.-C. Guo, CAS Center for Excellence in Quantum Information and Quantum Physics (China)
- *Direct Observation of Dynamical Quantum Phase Transitions in an Interacting Quantum Many-Body System* with R. Blatt, Institute for Quantum Optics and Quantum Information (Innsbruck, Austria)
- *Organic monolayers on dielectric surfaces and superradiance* with M. Sokolowski, University of Bonn (Germany)
- *Phase-modulated femtosecond spectroscopy* with F. Stienkemeier, University of Freiburg (Germany)
- *Dynamics of driven Rydberg assemblies* with S. Whitlock, Universite de Strasbourg (France)
- *Localization in photonic molecules* with A. Yacomotti, CNRS UPR 20 (France)
- *Evolution of exceptional traits in bats* with E. Teeling, University College Dublin (Ireland)
- *Evolution of limb proportions in the jerboa* with K. Cooper, UCSD San Diego (USA)
- *Genomic basis of phenotypic differences in primates* with T. Capellini, Harvard University (USA)
- *Genome assembly and annotation of the axolotl* with E. Tanaka, IMP (Vienna, Austria)
- *Current-induced strong diamagnetism in the Mott insulator Ca_2RuO_4* with C. Sow, S. Yonezawa,

Y. Maeno, Kyoto University (Japan), K. Kuroki, Osaka University (Japan), F. Nakamura, Kurume Institute of Technology (Japan)

- *Probing spin correlations using angle resolved photoemission in a coupled metallic/Mott insulator system* with A. Mackenzie, MPI-CPFS (Dresden, Germany) and P.D.C. King, University of St. Andrews (UK)
- *Self-organization of growth* with M. Gonzales, Universite de Geneve (Switzerland)
- *Pattern formation by genetic oscillators* with A. Oates, EPF Lausanne (Switzerland)
- *Collective behavior of molecular motors* with Pascal Martin, Institute Curie (Paris, France)
- *Morphogenesis of epithelia* with S. Eaton, MPI-CBG (Dresden, Germany)
- *Protein phase separation* with T. Hyman, MPI-CBG (Dresden, Germany)
- *Balance of Matter and Energy during growth and degrowth* with J. Rink, MPI-CBG (Dresden, Germany)

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 1143 *Correlated magnetism: from frustration to topology*, Prof. R. Moessner, Dr. F. Pollmann
- *Quantum Control mit intensiven Pulsen im Röntgenbereich: Ein theoretischer Zugang*, Prof. U. Saalman
- Exzellenzcluster *Center for Advancing Electronics Dresden*, Prof. F. Jülicher
- Exzellenzcluster *Physics of Life*, Prof. F. Jülicher
- Exzellenzcluster *Complexity and Topology in Quantum Matter*, Prof. R. Moessner
- *Abbildung nichtlokaler Photonen-Wechselwirkungen mit strukturiertem Licht*, Dr. T. Pohl
- *Schnittstellen-induzierte Kohärenz und Verschränkung von Rydberg Einheiten*, Prof. J.-M. Rost, Dr. A. Eisfeld
- Gottfried Wilhelm Leibniz-Preis 2017, Prof. F. Jülicher
- Priority Program 1840 *Quantum Dynamics in Tailored Intense Fields*, Prof. J.-M. Rost
- Priority Program 1929 *Giant Interactions in Rydberg Systems*, Prof. J.-M. Rost, Dr. A. Eisfeld
- Research Unit 2414 *Artificial Gauge Fields and Interacting Topological Phases in Ultracold Atoms*, Dr. A. Eckardt

Individual Projects

- *Kontrolle der epithelialen Zellschichtausbreitung im Zebrafisch*, Dr. S. Grill, Dr. G. Salbreux
- *Microswimmers - from single particle motion to collective behavior*, Dr. B. Friedrich
- *Development of a computational approach to accurately detect gene losses in genome sequences*, Dr. M. Hiller
- *Ultrakalte Atome in dynamisch erzeugten Eichfeldern*, Dr. A. Eckardt
- *Quantum dynamics of topologically nontrivial systems with Coulomb blockade effects*, Dr. I. Khaymovich

3.5.2 EU Funding

- 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 *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 Horizon 2020 *Rydberg quantum simulators*, Prof. J.-M. Rost, Dr. T. Pohl
- EU Horizon 2020 *Dynamics and transport of quantum matter - exploring the interplay of topology*, Dr. J. H. Bardarson

3.5.3 Additional External Funding

- AvH Programm: Förderung von Institutspartnerschaften, Prof. F. Jülicher, Dr. A. Basu
- BMBF Grant *Collective organization of cells and tissues: systems biology of tissue size and shape*, Prof. F. Jülicher
- BMBF SysBioll - Gewebe- und Organbildung: ein systemmikroskopischer Ansatz, Prof. F. Jülicher
- Boehringer-Ingelheim Foundation *Discovering novel genes underlying human eye disorders by comparative genomics in mammals with degenerated eyes*, Dr. M. Hiller
- DAAD Programm PROALMEX 2016 (PPP Mexiko), Dr. A. Eisfeld
- HFSP Human frontiers science program career development award, Dr. J. Bruges
- Leibniz-Gemeinschaft e.V. *Identifying the genomic loci underlying mammalian phenotypic variability using Forward Genomics with Semantic Phenotypes*, Dr. M. Hiller
- The Royal Society Newton fellow: *singularimetry in light-matter interaction*, Dr. J. Götze
- Volkswagen Foundation *To the edge of life and back again: Unlocking the secrets of dormancy to preserve human life*, Dr. V. Zaburdaev
- Volkswagen Foundation *Unterstützung zu Tutorial und finales Statussymposium "Extremes 2018"*, Prof. H. Kantz
- 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

3.5.4 Scholarships

- Aguilar-Hidalgo, Daniel; Université de Geneve
- Blackburn, George; ONR
- Briffa, Amy; CCQCN
- Cairolì, Andrea; Queen Mara, University of London Postgraduate Research Fund
- De, Arinjoy; DAAD
- Deng, Qimin; Peking University
- Dias, Laercio; CNPq/ Conselho Nacional de Desenvolvimento Científico e Tecnológico
- Guzzo da Costa, Fausto; CNPq/ Conselho Nacional de Desenvolvimento Científico e Tecnológico
- Hofmann, Cornelia; Swiss National Science Foundation
- Leitao, Jorge; FCT / Fundaco para a Ceincia e Tecnologia
- Li, Xikun; Aarhus University
- Lim, Lih-Kung; Tsinghua University, Scientific Research Program
- Liu, Jinlein; Tsinghua University, Scientific Research Program
- Medrano Sandomas, Leonardo Rafael; DAAD
- Mikkelsen, Troels Bogeholm; Niels-Bohr-Institut
- Mizoguchi, Tomonari; Gakushuin University
- Ni, Hongcheng; AvH
- Nishida, Naoki; Osaka University
- Prelovsek, Peter; AvH
- Quail, Thomas Duncan; EMBO
- Ramaswamy, Rajesh; AvH
- Sondhi, Shivaji; AvH
- Sato, Yuzuru; Japan Society for the Promotion of Science (JSPS)
- Tada, Yasuhiro; University of Tokyo
- Traillero-Giner, Carlos; AvH

3.5.5 External Cofunding of Workshops and Seminars

2015

- Focus workshop *Mathematics and Physics of Multilayer Complex Networks*
(31% of budget)
- Workshop *Dynamics of Coupled Oscillators: 40 years of the Kuramoto Model*
(25% of budget)
- Workshop *Nanoscale Assemblies of Semiconductor Nanocrystals, Metal Nanoparticles and Single Molecules: Theory, Experiment and Application*
(31% of budget)

2016

- Workshop *Topological Phenomena in Novel Quantum Matter: Laboratory Realization of Relativistic Fermions and Spin Liquids*
(28% of budget)
- Seminar and Workshop *Multistability and Tipping: From Mathematics and Physics to Climate and Brain*
(14% of budget)

2017

- Focus workshop *Quantum Dynamics in Tailored Intense Fields*
(76% of budget)
- Workshop *Joint IMPRS Workshop on Condensed Matter, Quantum Technology and Quantum Materials*
(29% of budget)
- Workshop *Future Trends in DNA-based Nanotechnology*
(53% of budget)
- Workshop *Atomic Physics 2017*
(11% of budget)

2018

- School *Topological Matter in Artificial Gauge Fields*
(22% of budget)
- Workshop *Predicting Transitions in Complex Systems*
(19% of budget)
- Workshop *Single Nanostructures, Nanomaterials, Aerogels and their Interactions: Combining Quantum Physics and Chemistry*
(42% of budget)
- School *Tensor Network based approaches to Quantum Many-Body Systems*
(7% of budget)

3.5.6 Patents and Licenses

- J. Götze, R. Cameron, S. Barnett
International patent **PCT/EP2016/076742**
Chiral rotational spectrometer, since 11/2015
- A. Pollakis, L. Wetzels, D. J. Jörg, W. Rave, F. Jülicher, G. Fettweis
European patent **EP 2 957 982**
Self-synchronizable network, since 08/2017

3.6 Teaching and Education

3.6.1 Lectures at Universities

Wintersemester 15/16

- *Quantum information and computation* Dr. J. H. Bardarson, Dr. F. Pollmann, Prof. Dr. R. Moessner, TU Dresden
- *Biological Hydrodynamics* Prof. Dr. S. Grill, Dr. J. Bruges, TU Dresden

Sommersemester 2016

- *Fluctuations and transport in biology* Dr. V. Zaburdaev, Prof. Dr. S. Grill, TU Dresden
- *Biological Hydrodynamics* Prof. Dr. S. Grill, Dr. J. Bruges, TU Dresden
- *Biophysik III, Theoretical Biophysics* Prof. Dr. F. Jülicher, Prof. Dr. S. Grill, TU Dresden
- *Reading group on machine learning* Dr. S. Bialonski, TU Dresden
- *QUTIF research School: Electron dynamics in strong fields* Prof. Dr. U. Saalman, University of Rostock

Wintersemester 2016/2017

- *Time-periodically driven many-body systems: Theory and recent experiments* Dr. A. Eckardt, TU Dresden
- *Biological Hydrodynamics* Prof. Dr. S. Grill, Dr. J. Bruges, TU Dresden
- *Stochastic processes* Prof. Dr. H. Kantz, TU Dresden
- *Reading group on machine learning* Dr. S. Bialonski, TU Dresden

Sommersemester 2017

- *Fluctuations and transport in biology* Dr. V. Zaburdaev, Prof. Dr. S. Grill, TU Dresden
- *Statistical Physics* Dr. A. Nielsen, Aarhus University
- *Biological Hydrodynamics* Prof. Dr. S. Grill, Dr. J. Bruges, TU Dresden
- *Biophysik III, Theoretical Biophysics* Prof. Dr. F. Jülicher, Prof. Dr. S. Grill, TU Dresden
- *Reading group on machine learning* Dr. S. Bialonski, TU Dresden
- *Proseminar on Theoretical Physics* Dr. M. Heyl, TU Dresden
- *Molecular Aggregates* Dr. A. Eisfeld, TU Dresden
- *Genome Engineering class* Dr. M. Hiller, TU Dresden

Wintersemester 2017/2018

- *Many-body quantum dynamics in and out of equilibrium: From thermalisation to new types of border* Dr. A. Eckardt, Dr. M. Heyl, Prof. Dr. R. Moessner, TU Dresden
- *Biological Hydrodynamics* Prof. Dr. S. Grill, Dr. J. Bruges, TU Dresden
- *Atmospheric physics* Prof. Dr. H. Kantz, TU Dresden
- *Reading group on machine learning* Dr. S. Bialonski, TU Dresden

Sommersemester 2018

- *Statistical Physics*, Dr. A. Nielsen, Aarhus University
- *Biological Hydrodynamics* Prof. Dr. S. Grill, Dr. J. Bruges, TU Dresden
- *Pattern formation and phase transitions in Soft Matter and Biophysics* Dr. Ch. Weber, TU Dresden
- *Biophysik III, Theoretical Biophysics* Prof. Dr. F. Jülicher, Prof. Dr. S. Grill, TU Dresden
- *Quantum phase transitions go dynamical* Dr. M. Heyl, University of Regensburg

Wintersemester 2018/2019

- *Thermalization and its absence in closed and open systems*, Dr. F. Piazza, Dr. A. Lazarides, TU Dresden
- *Quantum simulators: A Theory perspective onto experimental platforms and prospects* Dr. A. Eckardt, Dr. M. Heyl, TU Dresden
- *Biological Hydrodynamics* Prof. Dr. S. Grill, Dr. J. Bruges, TU Dresden
- *Nonlinear dynamics and chaos* Prof. Dr. H. Kantz, TU Dresden
- *Atomic and molecular systems in strong laser fields* Prof. Dr. U. Saalman, TU Dresden

3.6.2 Professional Skills Training

Talk series on professional skills topics (since July 2015)

- *Just enough Unix to be dangerous*
Hagen Fuchs, **mpipks** and IFW (November 2015)
- *Careers in quantitative finance: An introduction for graduate students of physics and Co.*
Dr. Christian Gnodtke, **mpipks** alumnus, now at Citibank London (December 2015)
- *Inside Nature Physics*
Dr. Andrea Taroni, Chief Editor Nature Physics (February 2016)
- *Scientists in Risk-Management Consulting*
Dr. Stefan Winkelmann, d-fine (April 2016)
- *A Quantum Physicist: From TU Dresden to Intel Labs*
Dr. Sarah Mostame, **mpipks** alumnus, now Research Scientist at Intel Labs (September 2016)
- *A very limited and completely subjective comparison between research in industry and academia*
Dr. Peter Borowski, **mpipks** alumnus, now Manager at Characterization AVANCIS GmbH, Munich (November 2016)
- *A Physicist in Silicon Valley: Google Search*
Dr. Ionut Georgescu, **mpipks** alumnus, now at Google, USA (November 2016)
- *An overview of technology consulting*
Dr. Wladimir Tschischik, **mpipks** alumnus, now at TNG Technology, Munich (May 2017)
- *Science Management: An Experience report on managing an NSF Physics Frontiers Center*
Dr. Lena Simon, JINA (June 2017)
- *A random walk from physics to AI*
Dr. Oliver Tieleman, Google DeepMind Technologies (October 2017)
- *From exciton dynamics to grocery dynamics: Data science tales from e-commerce*
Dr. Bas Vlaming, Picnic Supermarkets (December 2017)
- *The Technology Industry in Saxony*
Dr. Uwe Lienig, Wirtschaftsförderung Sachsen GmbH (January 2018)
- *Complex Physics Insights in R&D Applications*
Dr. Mykola Maksymenko, SoftServe, Kiev (April 2018)
- *Career perspective for physicists in machine learning and biometrics*
Dr. Christopher Gaul, Cognitec Systems GmbH (June 2018)
- *Venturing into industry - My journey so far*
Dr. Kai Dierkes, **mpipks** alumnus, now at Pupil Labs UG, Berlin (September 2018)
- *Data Science and e-commerce at Wayfair*
Dr. Florian Fruth & Benjamin Schröder, Wayfair, Berlin (November 2018)

3.6.3 Degrees

Habilitation

- Altmann, E.G.: *Transient Chaos in Physical Systems*. Dresden, 2016
- Eckardt, A.: *Controlling atomic quantum gases by strong time-periodic driving*. Dresden, 2017

Dissertations

- Erzberger, A.: *Actomyosin mechanics at the cell level*. Dresden, 2015
- Gerlach, M.: *Universality and variability in the statistics of data with fat-tailed distributions: the case of word frequencies in natural languages*. Dresden, 2015
- 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
- Roychowdhury, K.: *Aspects of many-body systems on a kagome lattice : strong correlation effects and topological order*. Dresden, 2015
- Sartori, P.: *Effect of curvature and normal forces on motor regulation of cilia*. Dresden, 2015

- Alt, S.: *Epithelial mechanics in 3D - how form follows force*. Dresden, 2016
- Camacho Garibay, A.: *Dynamics of Highly Charged Finite Systems Induced by Intense X-ray Pulses*. Dresden, 2016
- Diesen, E.: *Low-Energy Electrons in Strong-Field Ionization*. Dresden, 2016
- Werner, S.: *Growth and Scaling during Development and Regeneration*. Dresden, 2016
- Leonhardt, K.: *Interplay of excitation transport and atomic motion in flexible Rydberg aggregates*. Dresden, 2016
- Motruk, J.: *Characterization of topological phases in models of interacting fermions*. Dresden, 2016
- Schneider, J.A.M.: *The interplay of the cell membrane with the cytoskeletons*. Dresden, 2016
- Zamani, F.: *Local quantum criticality in and out of equilibrium*. Dresden, 2016

- Abdussalam, W.: *Dynamics of Rydberg atom lattices in the presence of noise and dissipation*. Dresden, 2017
- Bagheri, M.: *Dynamics of Driven Quantum Systems: A Search for Parallel Algorithms*. Dresden, 2017
- Celestino, A.: *Tuning coupled electronic and nuclear dynamics in the nanoscale*. Dresden, 2017
- Lee, J.-H.: *Detecting signatures of convergent evolution genome-wide*. Dresden, 2017
- Klindt, G.S.: *Hydrodynamics of flagellar swimming and synchronization*. Dresden, 2017
- Popovic, M.: *Continuum mechanics of developing epithelia: shaping a fly wing*. Dresden, 2017
- Schönleber, D.: *Controlling system dynamics through reservoir engineering*. Dresden, 2017
- Sträter, C.: *Many-Body Floquet Engineering in Periodically Driven Optical Lattices*. Dresden, 2017

- Behrends, J.: *Transport and Quantum Anomalies in Topological Semimetals*. Dresden, 2018
- De Tomasi, G.: *Characterization of Ergodicity Breaking in Disordered Quantum Systems*. Dresden, 2018
- Gohlke, M.: *Emergent Gauge Fields in Systems with Competing Interactions*. Dresden, 2018
- Huang, W.: *Theoretical study of pulled polymer loops as a model for fission yeast chromosome*. Dresden, 2018
- Javanmard, Y.: *Strongly Correlated Systems: Transport, Entanglement and Dynamics*. Dresden, 2018
- Langer, B.: *Phenotype-related regulatory element and transcription factor identification via phylogeny-aware discriminative sequence motif scoring*. Dresden, 2018
- Mietke, A.: *Dynamics of active surfaces*. Dresden, 2018
- Pönisch, W.: *Dynamics of bacterial aggregates - theory guided by experiments*. Dresden, 2018
- Roy, S.: *Nonequilibrium and semiclassical dynamics in topological phases of quantum matter*. Chemnitz, 2018
- Sanz Mora, A.: *Interfacing mechanical resonators with excited atoms*. Dresden, 2018
- Scholich, A.: *Biaxial Nematic Order in Liver Tissue*. Dresden, 2018
- Xypakis, E.: *Quantum Transport in Three Dimensional Topological Insulator Nanowires*. Dresden, 2018
- Vorberg, D.: *Generalized Bose-Einstein Condensation in Driven-dissipative Quantum Gases*. Dresden, 2018
- Panpan Zhang, P.: *The hierarchy of pure states for calculating transport and optical properties of*

molecular aggregates. Dresden, 2018

Master

- Belohlavy, S.: *Competition between nucleosomes and transcriptional machinery determines the timing of genome activation in the zebrafish embryo*. Dresden, 2015
- Suarez, H.: *Improving pairwise genome alignment nets by removing random local alignments*. Dresden, 2015
- Oltsch, F.: *Shape stability of chemically active droplets*. Dresden, 2016
- Gemsheim, S.: *High Harmonic Generation with Twisted Electrons*. Dresden, 2018

Bachelor Thesis

- Ehmcke, T.: *Bose-Einstein-Kondensation in stationären Nichtgleichgewichtszuständen eines zwei-dimensionalen Tigh-Binding-Modells*. Dresden, 2016
- Kieler, M.: *Interbandübergänge in periodisch getriebenen optischen Gittern*. Dresden, 2016

Diploma

- Elsner, M.: *Development and characterization of a CRISPR/Cas9 labelling strategy for studying chromatin reorganization upon activation of gene expression in zebrafish embryos*. Dresden, 2015
- Fischer, R.: *Efficient Sampling of Networks with high Clustering*. Dresden, 2015
- Multrus, F.: *Calculation of the Electric Potential for a Neuronal Activity Model in the Brain*. Dresden, 2015
- Rosenberger, J.: *Development of Fluorescent Intensity Modulation Spectral Analysis FIMSA*. Gothenburg, 2015

3.6.4 Appointments and Awards

Appointments

- Prof. E. Altmann accepted the offer for an associate professorship at the *University of Sydney*.
- Prof. A. Barato accepted the offer for an assistant professorship at the *University of Houston*.
- Prof. J. H. Bardarson accepted the offer for a professorship at the *KTH Royal Institute of Technology, Stockholm*.
- Prof. S. Bhattacharjee accepted the offer for a professorship at the *TIFR-ICTS, Bangalore*.
- Prof. S. Bialonski accepted the offer for a professorship at the *FH Aachen*.
- Prof. O. Erten accepted the offer for an assistant professorship at the *Arizona State University, USA*.
- Prof. H. P. Goswami accepted the offer for an assistant professorship at the *Tezpur University, India*.
- Prof. J. Götte accepted the offer for a professorship at the *Nanjing University, China*.
- Prof. M. Haque accepted the offer for a professorship at the *Maynooth University, Ireland*.
- Prof. L. Hilbert accepted the offer for a junior professorship at the *Karlsruhe Institute of Technology*.
- Prof. A. E. B. Nielsen accepted the offer for an assistant professorship at the *Aarhus University*.
- Prof. T. Pohl accepted the offer for a professorship at the *Aarhus University*.
- Prof. F. Pollmann accepted the offer for a professorship at the *TU München*.
- Prof. B. Roy accepted the offer for an assistant professorship at the *Lehigh University, USA*.
- Prof. D. Roy accepted the offer for a professorship at the *RRI Bangalore, India*.
- Prof. K. Saha accepted the offer for an assistant professorship at the *NISER Jatni, India*.
- Prof. J. Viti accepted the offer for a professorship at the *Escola de ciencia e tecnologia, UFRN, Natal, Brazil*.
- Prof. J. Wu accepted the offer for an associate professorship at the *Shanghai Jiao Tong University, China*.
- Prof. S. Wüster accepted the offer for a professorship at the *Bilkent University, Ankara*.

- Prof. X. Zhang accepted the offer for an assistant professorship at the *Chongqing University, China*.
- Prof. Y. Zhou accepted the offer for a professorship at the *The Chinese University of Hong Kong*.
- Prof. V. Zaburdaev accepted the offer for a professorship at the *Friedrich-Alexander-University of Erlangen-Nürnberg*.

Awards

- Bardarson, J.H.: *APS Outstanding Referee 2015*
- Bardarson, J.H.: *ERC Starting Grant 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*
- Bennet, B.: *Azubipreis 2016 of the MPG*
- Fulde, P.: *Honorary citizen of the city Pohang, Korea*
- Bardarson, J.H.: *IOP Outstanding reviewer 2017*
- Grassberger, P.: *EPS Statistical and Nonlinear Prize 2017*
- Jülicher, F.: *Gottfried Wilhelm Leibniz-Preis 2017*
- Roldan, E.: *EPS Statistical and Nonlinear Physics Prize 2017*
- Rost, J.-M.: *Appointment to the Science Council*
- Bruges, J.: *VW Foundation, Life 2018*
- Heyl, M.: *Dozentur Professor Bernhard Hess, University of Regensburg*
- Nielsen, A.E.B.: *Sapere Aude: DFF-Starting Grant 2018*
- Hänggi, P.: *Marian-Smoluchowski-Emil-Warburg-Preis 2019*

3.7 Public Relations

3.7.1 Long Night of the Sciences

Over the last four 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 2800 visitors counted at each event.



Impressions of the Long Night of the Sciences

3.7.2 Max Planck Day

The year 2018 brought several round anniversaries for the Max Planck Society: the 160th birthday of Max Planck, the 100th anniversary of the award of the Nobel Prize to Max Planck, and the 70th anniversary of the Society itself. On this occasion, the Max Planck Society launched a major public outreach event throughout Germany under the participation of all institutes: the Max Planck Day on September 14th. A large variety of programs for the broad public were organized in 32 cities, Dresden being one of them. The local program took place in the City Hall in the heart of Dresden as a joint effort of the three Max Planck Institutes and featured a number of formats for the public to get an insight into the research performed at the institutes:

- An exhibition with hands-on experiments, information booths and cinema,
- Talks on various research topics pursued at the three institutes, delivered by scientists from the institutes in a fashion accessible for the broad public (contributions from **mpipks** by Dr. M. Heyl, Dr. F. Piazza, Dr. C. Weber and Prof. H. Kantz),
- A podium discussion on the role of fundamental research for the society, with Dr. Eva-Maria Stange (Saxonian Minister for Science and Arts), Dr. Peter Plaßmeyer (Staatliche Kunstsammlungen Dresden, director of the Mathematisch-Physikalischer Salon), Ulrich Bahnsen (scientific portfolio editor of DIE ZEIT), Prof. W. Huttner (director MPI-CBG), Prof. J. Grin (director MPI-CPfS), Prof J. M. Rost (director **mpipks**),
- A Science Café, providing the visitors and residents of Dresden with the opportunity to talk to researchers of the institutes face-to-face.



Impressions from the Max Planck Day

3.7.3 Science in the Theatre

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 the three annual lectures have taken place in the "Kleines Haus" of Dresden's State Theater.



Science in the Theatre

2015 - 2018

- *Die Evolution des Denkens*
Prof. Onur Güntürkün, (about 250 participants)
- *Die Augen der Insekten: Ein Vorbild für Miniaturisierte optische Systeme*
Prof. Norbert Kaiser, (about 200 participants)
- *24 Bilder und Geschichten aus der Mathematik - ein Adventskalender*
Prof. Günter Ziegler, (about 340 participants)
- *Quantenphysik: Seltsam wirksam*
Prof. Markus Arndt, (about 345 participants)
- *Gentechnik bei Pflanzen: Müssen wir uns 30 Jahre nach ihrer Entdeckung immer noch fürchten?*
Prof. Hans-Jörg Jacobsen, (about 200 participants)
- *Einsteins Gravitationswellen: Wir hören Töne aus dem dunklen Universum!*
Prof. Karsten Danzmann, (about 340 participants)
- *Der humanoide Roboter Myon: Von der Bleistiftskizze zum lernfähigen Individuum*
Prof. Manfred Hild, (about 240 participants)
- *Die Hintergründe der Selbstheilung*
Prof. Karin Kraft, (about 350 participants)
- *Integration als Chance und Notwendigkeit*
Prof. Marina Münkler, (about 200 participants)
- *Bienen treffen Blumen: Eine elektrisierende Beziehung*
Prof. Daniel Robert, (about 280 participants)

3.7.4 mpipks School Contact Program



JUNIOR DOKTOR



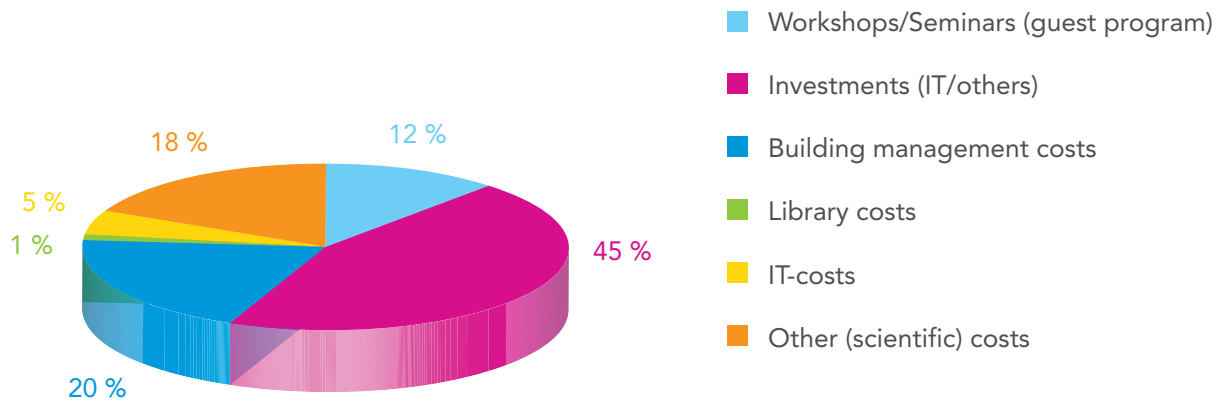
Public lecture for Junior Doctors

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 science, pursuing a PhD, etc.

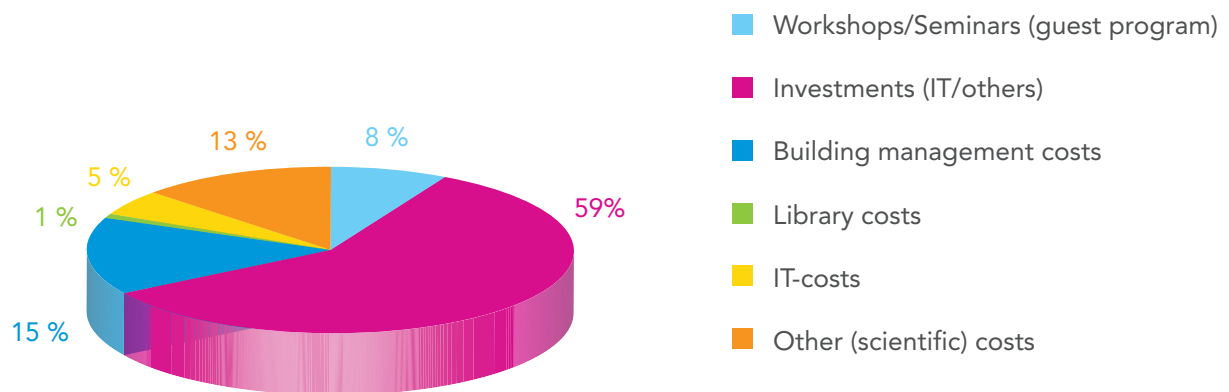
In addition, the institute participates in the program *Junior Doctor* organized by the network *Dresden - Stadt der Wissenschaft*. The participating research institutes offer a variety of lectures for children, who are awarded a "Junior Doctor degree" when attending a stated number of talks. Each school year, the **mpipks** contributes to the curriculum with four lectures for students from the 3rd grade onwards.

3.8 Budget of the Institute

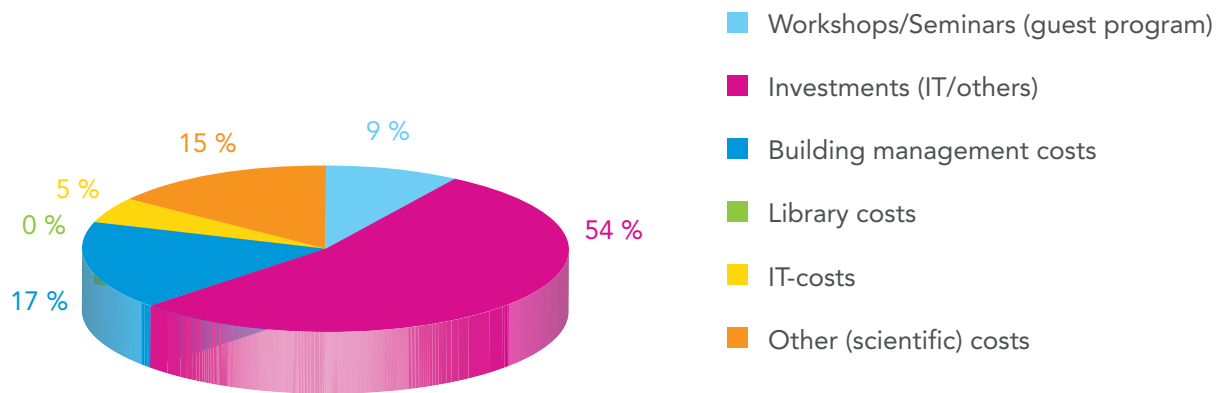
Research Budget 2015



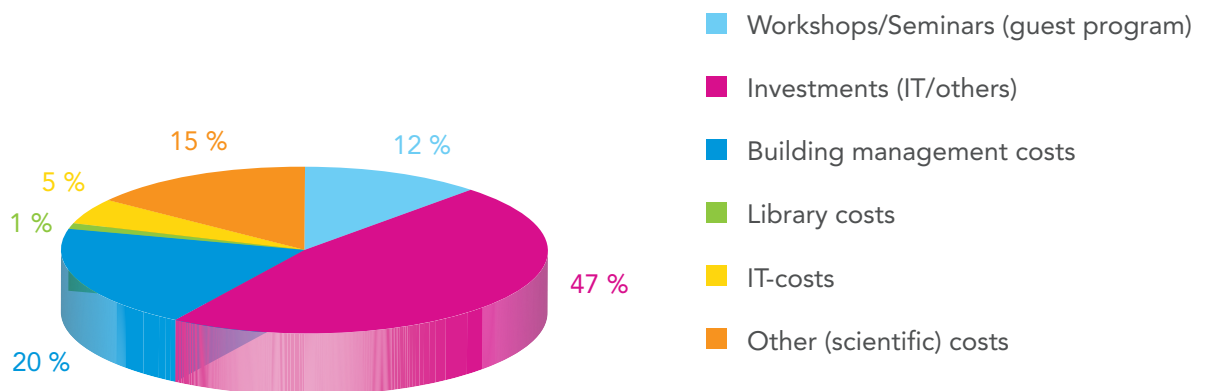
Research Budget 2016



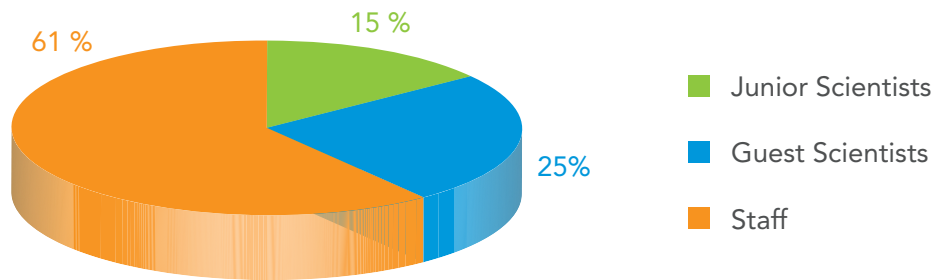
Research Budget 2017



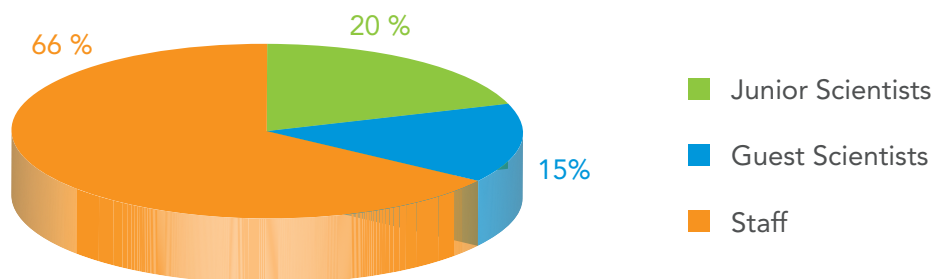
Research Budget 2018



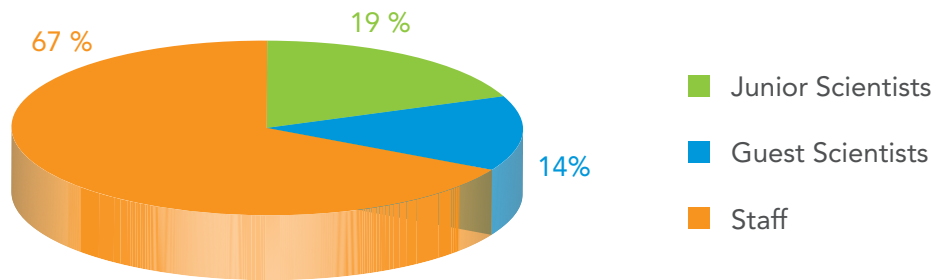
Personnel Budget 2015



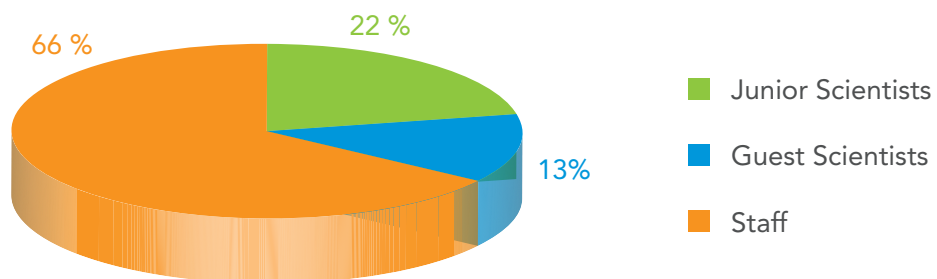
Personnel Budget 2016



Personnel Budget 2017



Personnel Budget 2018



3.9 Equipment and Premises

3.9.1 Computing Facilities

Due to the relatively wide field of theoretical physics covered by our scientists there is a very broad spectrum of requirements that our IT facilities have to cope with. This implies in particular that compute nodes of very different size have to be available on site for numerical calculations. The complexity is luckily reduced by the fact that nowadays most big applications are running on a Linux operating system, such that presently our computing facilities are homogeneous in the sense that both the hardware architecture (x86) and the operating system 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 department but also driven by the fact that visualization of results has become more important.

All of our offices are equipped with workstations in order to provide our scientists with a device that can run small applications and produce graphical output. For more elaborate calculations the institute hosts approximately 600 servers with a total of approximately 25,000 CPU cores on site. Furthermore we share a cluster located at the MPCDF in Garching together with the Fritz Haber Institute and the MPI for the Structure and Dynamics of Matter (Hamburg). This cluster is best suited for applications that are highly parallelized. In November 2015 it was number 264 in the ranking of the world's fastest computers.

Our compute nodes have up to 80 CPU cores and a maximum of 3 Terabytes of main memory and a maximum of fifty 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 PC's 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 with the possibility to continue their work while they are travelling or at home. Cloud services, VPN access, Wifi, including Eduroam and other services are also available for our scientists. For numerical and analytical calculations we offer various software packages. 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 350 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 four employees with their respective main tasks being Unix/Linux, Mac OS and cloud services, hardware and web, network and Windows. In addition to those four people we employ four trainees. 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. Still the highly specialized GPUs are not well accepted by our scientists since the effort for adapting programs to this architecture is relatively high. Nevertheless the overall speedup in some cases is significant. There are tendencies that programming GPUs might become easier, meaning that GPUs might play a bigger role in the future.

Starting early 2019 we will host some of our computers at the Lehmann Zentrum of the TU Dresden which is located just a few hundred meters away from our institute. This relatively new building has a perfect infrastructure for running large clusters, in particular it provides very efficient cooling. Due to the short distance we will be able to include the computers there into our cluster in such a way that our users will not notice any difference compared to those located inside our own building.

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. This cluster was shared with the Fritz Haber Institute (Berlin). In autumn 2015 this cluster was replaced by a new one and is now shared with with the Fritz Haber Institute and the MPI for the Structure and Dynamics of Matter, Hamburg. By the end of 2013 the era of Intel's IA64 based systems at our institute ended 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
2018	600	420	2000

3.9.2 Library

The library of the **mpipks** is a service unit with a wide range of duties. It is accommodated in guest house 4 on three floors 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.

Most evidently, the library provides a large stock of scientific books and journals for the use of all members of the **mpipks** including workshop 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 library atmosphere inspiring for their work or who simply need a desk for their literature search find quiet workplaces on the second floor

of the library building. The library is also open to 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 5,500 monographs, about 17,300 bound journal volumes and 15 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. Actually, the number of journal subscriptions in print has been drastically reduced in recent years, since most of our scientists nowadays prefer to use electronic access from their own computers.



Our library in guest house 4

Indeed, via the library homepage, **mpipks** users, identified through the IP address of their computer, have access to about 150,000 online journals and 690,000 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 resources 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. Since negotiations with the publishing company Elsevier failed in 2018, we will not have electronic access to issues of Elsevier journals published after the end of 2018, but fortunately the

contracts ensure access to the back-issues. Hence, more recent articles will, as long as there is no positive outcome of new negotiations, be ordered through the document delivery service on demand.

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.

The open access policy of the Max Planck Society is fostered by a centralised payment scheme for the article processing charges (APC) for selected journals/publishers, and the information about these is supplied through the library's web-page. For most participating journals this means that if the corresponding author is employed by a Max Planck Institute, then the APCs will be directly covered by the Max Planck Digital Library without involvement of the MPI where the scientist is employed.

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.

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.

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 accessible housing. 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 equipped similarly to those in guest house 2. On the ground floor, two apartments have been

converted into offices, which are used by short term guest scientists or scientists with children. An additional apartment is available for workshop participants who need to arrange for childcare during the workshop.

Since November 2012, the newly built guest house 4 offers 14 single and eight double rooms (with two separate bedrooms). All rooms are equipped with TV connection ports and telephones. Furthermore, the building has a multi-purpose room with kitchen appliances, a large terrace and a light garden for the common use and enjoyment. Guest house 4 also accommodates 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.

3.10 Committees

3.10.1 Scientific Advisory Board

According to the rules of the Max Planck Society, the **mpipks** has a Scientific Advisory Board. The members of the Board advise the board of directors concerning the research at the institute. The Board assesses the research direction of the institute, the scientific relevance and 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:

Brabec, T.
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CANADA

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3.10.2 Board of Trustees

In accord with the rules of the Max Planck Society the **mpipks** has formed a Board of Trustees. The board members discuss and consult the proposed budget, the annual report, and the budget of the last year of **mpipks** together with the directors. The Board of Trustees advises the institute on important issues and promotes the connection of the institute to research oriented circles in the society. The Board of Trustees had the following members during the period of this report (current membership is until December 31, 2018):

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Milbradt, G. Prof. Dr.	Ministerpräsident des Freistaates Sachsen a.D. Stiller Winkel 4 01328 Dresden
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Weber, S.

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3.11 Members of the mpipks

(as of December 2018)

1. mpipks positions	49
• Scientific personnel	18
<i>Scientific members</i>	3
<i>Research staff (including four junior research groups)</i>	15
• Technical staff	10
• Administration and infrastructure staff	21
2. Externally funded research staff	4
3. PhD students	80
• PhD students with internal supervision	63
<i>German PhD students</i>	19
<i>Foreign PhD students</i>	44
• PhD students with external supervision	17
<i>PhD students with external funding</i>	0
<i>IMPRS PhD students with external supervision</i>	17
4. Guest scientists	67
• German guest scientists	16
• Foreign guest scientists	51

Chapter 4

Publications

4.1 Atomic and Molecular Structure

2015

Bramanti, A. P., A. Santana-Bonilla, R. Rinaldi: Quantum-dot Cellular Automata: Computation with Real-world Molecules. *International Journal of Unconventional Computing* **11**, 63-82 (2015)

Cioslowski, J.: One-electron reduced density matrices of strongly correlated harmonium atoms. *The Journal of Chemical Physics* **142**, 114104 (2015)

Cioslowski, J.: The Coulomb, exchange, and correlation components of the electron-electron repulsion in harmonium atoms. *The Journal of Chemical Physics* **142**, 114105 (2015)

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Kraus, D., J. Vorberger, J. Helfrich, D. O. Gericke, B. Bachmann, V. Bagnoud, B. Barbrel, A. Blazevic, D. C. Carroll, W. Cayzac, T. Doepfner, L. B. Fletcher, A. Frank, S. Frydrych, E. J. Gamboa, M. Gauthier, S. Goede, E. Granados, G. Gregori, N. J. Hartley, B. Kettle, H. J. Lee, B. Nagler, P. Neumayer, M. M. Notley, A. Ortner, A. Otten, A. Ravasio, D. Riley, F. Roth, G. Schaumann, D. Schumacher, W. Schumaker, K. Siegenthaler, C. Spindloe, F. Wagner, K. Wuensch, S. H. Glenzer, M. Roth, R. W. Falcone: The complex ion structure of warm dense carbon measured by spectrally resolved x-ray scattering. *Physics of Plasmas* **22**, 056307 (2015)

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Zoubi, H.: Dark bogolon-excitons in a linear atomic super-lattice. *New Journal of Physics* **17**, 023053 (2015)

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Dyugaev, A. M., E. V. Lebedeva: Rules of Correspondence in Atomic Physics. *JETP Letters* **103**, 57-61 (2016)

Heuser, S., A. J. Galan, C. Cirelli, C. Marante, M. Sabbar, R. Boge, M. Lucchini, L. Gallmann, I. Ivanov, A. S. Kheifets, J. M. Dahlström, E. Lindroth, L. Argenti, F. Martin, U. Keller: Angular dependence of photoemission time delay in helium. *Physical Review A* **94**, 063409 (2016)

Leonhardt, K., S. Wüster, J. M. Rost: Orthogonal flexible Rydberg aggregates. *Physical Review A* **93**, 022708 (2016)

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Nguyen, H., N. T. T. Nguyen, V. L. Nguyen: The transfer matrix approach to circular graphene quantum dots. *Journal of Physics: Condensed Matter* **28**, 275301 (2016)

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2018

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4.3 Dynamics on Nanoscale Systems

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- Si, T.*: One-dimensional chain of quantum molecule motors as a mathematical physics model for muscle fibers. *Chinese Physics B* **24**, 128708 (2015)
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