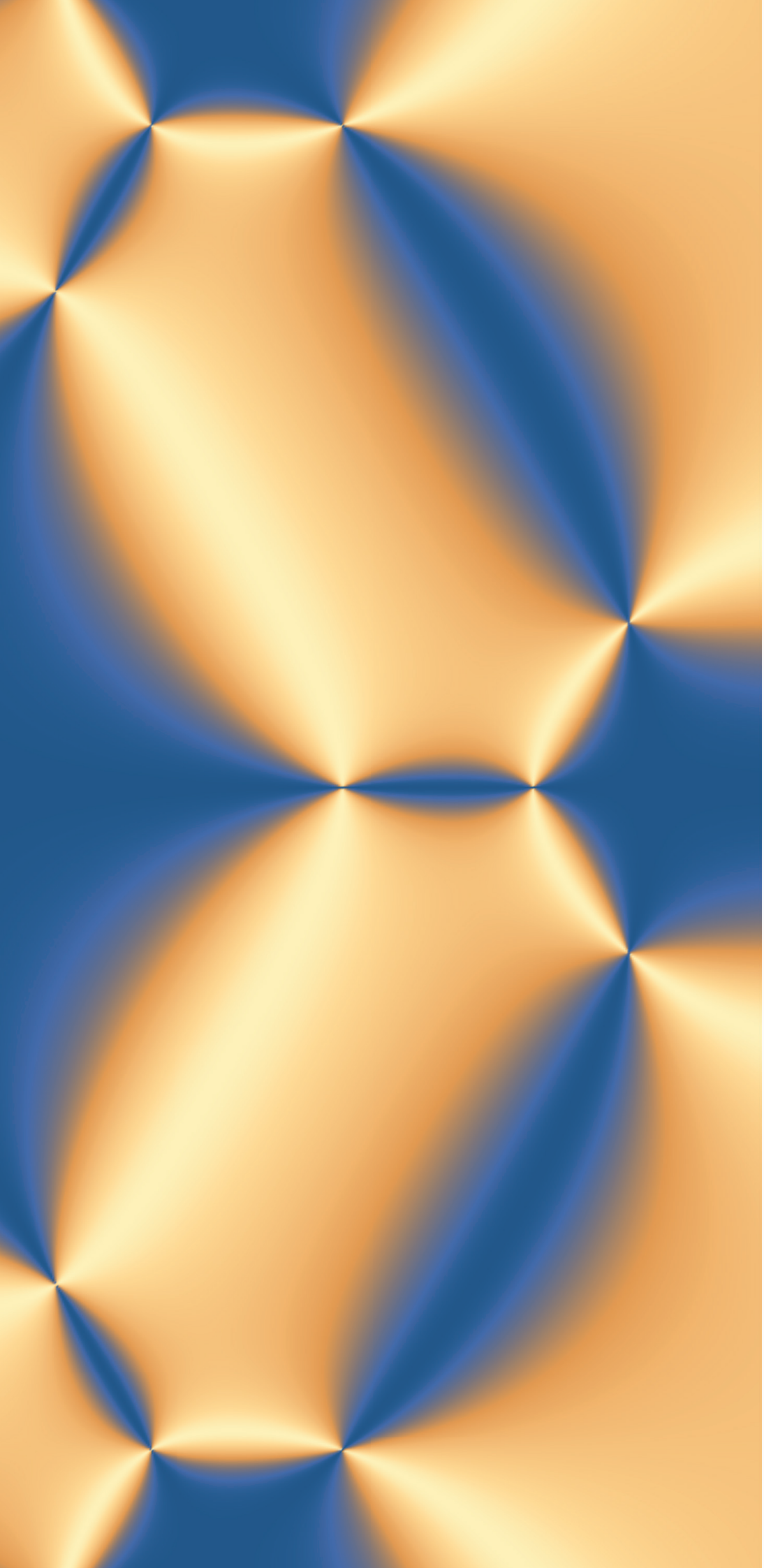

Max Planck Institute
for the Physics of
Complex Systems

Scientific Report

1/2019–9/2021

mpipks

Front cover
Dr. Owen Benton: Pinch points
in the correlations of a spin liquid
on the honeycomb lattice.

IMPRESSUM

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Contents

Chapter 1

Scientific Work and its Organization at the Institute – an Overview

1.1 History and Development of the Institute

1992-1994 • The Max Planck Institute for the Physics of Complex Systems (mpi**pks**) was founded by the Senate of the Max Planck Society in November 1992. The concept for the institute 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 mpi**pks** decided to broaden its research spectrum considerably by installing temporary Junior Research Groups: The group *Pattern Formation in Reaction-Diffusion-Systems* headed by *Dr. M. Bär* started its activities in 1995, the group *Quantum Chaos and Mesoscopic Systems* headed by *Dr. K. Richter* in January 1996, and the group *Quantum Chemistry* headed by *Dr. M. Dolg* soon after. At the same time, plans for the institute's building and guest houses took shape. The architects Brenner und Partner (Stuttgart) won the competitive bidding, and construction started in September 1995. After less than two years the institute moved into the new main building and took into service the three guest houses. In the meantime, the 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 mpi**pks** 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 mpi**pks**; *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 mpi**pks** 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 mpi**pks** 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 mpi**pks** to head the Junior Research Group *Dynamics of Biological Networks*, and *Dr. B. Lindner* set up the activities of the research group *Stochastic Processes in Biophysics*. In the same year, *Dr. S. Skupin* started his Junior Research Group *Computational Nonlinear and Relativistic Optics*, with close links to the 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 mpi**pks** 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 mpi**pks** to head the research group *Molecular Quantum Optics*. In the following year, *Prof. R. Ketzmerick* (TU Dresden) was appointed by the Max Planck Society as a *Max Planck Fellow* and started the activities of the Max Planck Fellow group *Quantum Chaos and Quantum Dynamics* at the mpi**pks**. In winter 2010, *Dr. E. Altmann* arrived to set up the Otto Hahn Group *Dynamical Systems and Social Dynamics*. The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* was 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 mpi**pks** and the MPI-CBG was intensified and institutionalized in the form of the newly founded *Center for Systems Biology Dresden* (CSBD).

2013-06.2015 • During this period, the research at the mpi**pks** has once more acquired new foci due to the installation of new 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.

07.2015-2018 • Several new research groups began their scientific work at mpi**pks**. 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 mpi**pks** 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 mpi**pks** since its foundation, retired in 2017, with *Mrs. K. Huppertz* taking over the responsibility as head of administration.

2019-09.2021 • A large part of this period was overshadowed by the global Covid 19 outbreak, which impeded the scientific life at the institute in both of its essential pillars - internal activities as well as the visitors program. In this period, a transition from exclusively in-person to virtual and hybrid meeting formats was commenced. Even in these difficult times, several groups have successfully concluded their work at the institute with the group leaders transitioning to faculty positions, while the in-house research activities were reinforced by new arrivals. Following the departure of Prof. Dr. Takashi Oka, the new joint research group *Correlations and Topology* between the mpi**pks** and the MPI-CPfS was founded and is headed by *Dr. A. Cook*. The Finite Systems division welcomes *Dr. M. Eiles* who heads the group *Correlations and Transport in Rydberg Matter*, while the arrival of *Dr. M. Popovic* strengthens the Biological Physics division with the foundation of the group *Order and Disorder in Driven Systems*. The new Max Planck research group *Self-organization of Multicellular Systems* at the Center for Systems Biology Dresden is headed by *Dr. P. A. Haas* and further intensifies the collaborations between the mpi**pks** and the MPI-CBG.

Present status of former group leaders

Research groups established 1995-2010

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 Chemnitz
Motor Systems	2006 - 2013	S. Grill	Director at the MPI-CBG
Dynamics of Biological Networks	2007 - 2011	T. Gross	Professor University of Oldenburg
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 EPFL Lausanne
Complex Dynamics in Cold Gases	2008 - 2017	T. Pohl	Professor Aarhus University
Molecular Quantum Optics	2009 - 2011	K. Hornberger	Prof. at U. 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	Prof. at Univ. of Geneva
Dynamical Systems and Social Dynamics	2010 - 2016	E. Altmann	Associate Professor University of Sydney

Research groups established since 2011

group	active	leader	current affiliation
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 Biology and Evolutionary Genomics	2011 - 2021	M. Hiller	Professor University of Frankfurt
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
Ultrafast Laser-Matter-Interactions	2014 - 2019	A. Landsman	Associate Professor Ohio State University
Nonequilibrium Quantum Matter	2015 - 2020	T. Oka	Professor University of Tokyo
Quantum Many-Body Systems	2016 - 2021	A. E. B. Nielsen	Associate Professor Aarhus University
Mesoscopic Physics of Life	2018 - 2021	C. A. Weber	Professor University of Augsburg

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 *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 the propagation of fluctuations in biological systems with an emphasis on using technologies from single-cell genomics.

- 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 *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 *Correlations and Topology* headed by *Dr. A. Cook* focuses on the search for novel phases of matter and exploration of mechanisms for experimental realization of exotic phases, and aims to accelerate the process of transitioning from the prediction of novel phases of matter in the literature to experimental realization.
- The research group *Correlations and Transport in Rydberg Matter* headed by *Dr. M. Eiles* aims to answer fundamental questions about atomic structure, low-energy collisions and scattering, and the behavior of ultracold gases via the study of Rydberg systems, while also raising new questions related to localization, transport, highly correlated systems, quantum chaos, semiclassical dynamics, and quantum simulation.
- The research group *Order and Disorder in Driven Systems* headed by *Dr. M. Popovic* studies mechanical and rheological properties of out-of-equilbrium systems, with an emphasis on development of biological tissues and the role of structural disorder.
- 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 *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 research group *Self-Organization in Multicellular Systems* headed by *Dr. P. A. Haas* studies the continuum theories that represent the rich mechanical behavior of tissues during development and thus allow understanding how robust development is compatible with mechanical constraints and biological variability.

1.3 Workshop and Visitors Program

Its large program for visiting scientists makes the mpi**pks** 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. 125), but also international workshops and seminars (p. 130). For these it offers 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.

Special programs include *Advanced Study Groups* (up to two per year) to foster the exchange between outstanding scientists and young researchers in residence (p. 48). 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 mpi**pks** annually awards the *Martin Gutzwiller Fellowship* to an internationally recognized and experienced scientist (p. 126), who spends up to one academic year at the institute.
Moreover, the mpi**pks** annually offers one *Distinguished PKS Postdoctoral Fellowship* to an excellent young postdoc (p. 128).

Given the internationality and the rich interactions of the workshop and visitors program, it has experienced a severe setback with the outbreak of the Covid 19 pandemic, as it impeded two essential aspects

of scientific life - the ability to travel and the ability to interact. While the usual number of visiting scientists (including workshop participants) per year typically ranges between 1.000 and 1.500, it has dropped during the years 2020 and 2021, especially for short-term guests (p. 125). In order to provide an alternative platform for scientific interactions during the lockdowns, mpi**pks** was among the first institutes to organize virtual workshops starting from April 2020 (p. 130). Moreover, the institute has started building up an infrastructure for the organization of hybrid workshops which allows to interface a virtual audience with participants on site, with the first events of this kind taking place in autumn 2021. In the long run beyond the pandemic, this kind of infrastructure will also enable us to conduct two-node workshops, by virtually merging two audiences on, say, two different continents. Such a format will be particularly suitable for short events with a considerable fraction of overseas participants, as it eliminates the necessity for long-distance flights for just a few days of attendance and thus positively contributes to reducing the environmental footprint and enhancing the sustainability of our workshop program.

1.4 Teaching and Training

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

Training • The mpi**pks** runs the IMPRS *Many Particle Systems in Structured Environments*, which offers a structured PhD training framework (p. 15). 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. 152).

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. 134). In addition, the institute organizes soft skill training events such as German courses or a presentation series on professional skills and career coaching (p. 154). 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. 153). The benefit is mutual: The lectures offered often cover latest developments, thus complementing the standard curriculum; at the same time, our young researchers gain valuable teaching experience.

Research Organization • The large Workshop and Seminar Program at the mpi**pks** also offers young scientists the opportunity to gain experience in the organization of meetings. Thus, they can influence a broader research agenda and grow in visibility. Between January 2019 and September 2021, non-tenured junior scientists were involved in the coordination of almost half of all the events taking place under the umbrella of the visitors program (p. 134).

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 mpi**pks** 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. Furthermore, about 4-5 female scientists in residence volunteer to be listed as contact persons on the institute homepage as contacts for first-hand information about life and work at mpi**pks**, in particular as a woman scientist. The percentage of female researchers is currently 18% among postdocs and 28% among doctoral students.

To accommodate the requirements of researchers with small children the institute provides a *parent & child office* in one of the guest houses. It can be used by members of the mpi**pks** or short-term guests who might need to bring their children during working hours. Furthermore, a number of slots are reserved at two daycares nearby for children (from toddlers to pre-school age) of institute members.

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. 157), and the lecture series *Science in the Theater* (p. 157). Unfortunately, in 2020 the *Long Night of the Sciences* was cancelled because of the pandemic, and had to be transferred to a virtual format in 2021. Our institute contributed by streaming an experimental show, short talks given by scientists in residence, and ScienceLab workshops for children.

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. 158): 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.

1.7 Research Networking

Local • The mpi**pks** finds itself in the midst of a rich research environment formed by the TU Dresden and the surrounding research institutes. The vivid scientific dialogue with the TU Dresden is mirrored in the Max Planck Fellow Group *Quantum Chaos and Quantum Dynamics* headed by *Prof. R. Ketzmerick* (until 2020), as well as in the mpi**pks** participation in two clusters of excellence: *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. 15), and the research training group *Itinerant Magnetism and Superconductivity in Intermetallic Compounds*. The mpi**pks** has particularly close contacts to the Institute of Theoretical Physics of the TU Dresden and is involved in a number of joint projects (p. 152). Further collaborations with the TU Dresden include the Biotechnology Center (BIOTEC), the Center for Regenerative Therapies (CRTD), the Center for Molecular and Cellular Bioengineering (CMCB) and the Center for Molecular Bioengineering (BCUBE).
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).

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) is jointly operated by the mpi**pks** and the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), in collaboration with the TU Dresden. The center was established in 2013 as an intersectional operation of the Max Planck Society. A new building, funded by the Free state of Saxony, was inaugurated in 2017, which hosts research groups conducting theoretical and computational research. The mpi**pks** 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 mpi**pks** and the ELBE PhD program

administered by MPI-CBG. The initial funding period of the CSBD is drawing to a close in 2023. The Dresden University of Technology (TUD) partly finances the professorship of Prof. Ivo Sbalzarini, who is also a group leader at MPI-CBG.

Research at the CSBD studies integrated biological systems and processes using computational and theoretical approaches in close collaboration with experiments. The center serves as a hub and intellectual incubator that brings physicists, computer scientists, engineers, mathematicians and biologists together to stimulate research activities aiming for a quantitative understanding of living systems. In tight cooperation with experimental groups at the nearby MPI-CBG, researchers at the CSBD develop a quantitative approach to biology based on theoretical physics, computational approaches, and state of the art microscopy techniques. The MPI-CBG has the research theme "How do cells form tissues?". Understanding the principles of cellular and tissue organization requires the study of collective effects and emergent phenomena. Molecules organize collectively in cells and cells organize collectively in tissues. Research at the center investigates the principles underlying system behaviors and spatiotemporal processes. For example the question how tens of thousands of cells coordinate their behavior in space and time to form tissues of a given form and function. 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 also engineers 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, which yields valuable insights that stimulate theory and approaches from physics. This combination of theoretical physics, computer science and experimental biology, with the goal to understand how cells form tissues, is the main mission of the Center.

Scientists at the CSBD work in a melting pot of the different scientific environments and speak the language of different disciplines. PhD students and postdoctoral researchers typically have a background in one discipline. A key mission of the CSBD is to train PhD students and postdoctoral researchers to conduct research projects that reach out to other fields. To this end, the ELBE postdoc program and the ELBE PhD track have been established. 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 mpi**pks** and administered by mpi**pks**. The ELBE postdoc program also stimulates 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 PhD students that carry out projects across disciplines.

Operations of the center are managed by a steering committee. It has representatives of both Max-Planck Institutes and it 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. Furthermore, a 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.

Members of the center are research groups affiliated with MPI-CBG and mpi**pks**. Groups that use office space in the CSBD building are

- Ricard Alert, (mpi**pks**): The physics of living matter (since 2021)
- Pierre Haas, (mpi**pks** and MPI-CBG): Self-organization of multicellular systems (since 2021)
- Michael Hiller, (mpi**pks**): Computational biology and evolutionary genomics (until 2020)
- Florian Jug, (MPI-CBG): Computer vision and machine learning for quantitative bioimage computation (until 2020)
- Frank Jülicher, (mpi**pks**): Theory of biological systems
- Carl Modes, (MPI-CBG): Network complexity and systems biophysics
- Eugene Myers (MPI-CBG): Exploring cells and 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 (until 2021)
- 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 research groups that are involved in the governance and research of the CSBD as members: Jan Brugués (**mpipks**), Stephan Grill (MPI-CBG), Suzanne Eaton† (MPI-CBG), Tony Hyman (MPI-CBG), Moritz Kreysing (MPI-CBG), Marko Popovic (**mpipks**), Steffen Rulands (**mpipks**), Pavel Tomancak (MPI-CBG), and Marino Zerial (MPI-CBG). The program is further strengthened by its close involvement with all the researchers of the MPI-CBG, **mpipks**, and the following additional CSBD affiliates: Björn Andres (TU Dresden), Stefan Diez (TU Dresden), Benjamin Friedrich (TU Dresden), Anna Pötsch (TU Dresden) 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, as well as with the cluster of excellence Physics of Life.

CSBD building. The Center for Systems Biology Dresden (CSBD) is jointly operated my **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 condensed matter physics, specifically at the intersection with materials physics. This was central to Peter Fulde's strongly correlated electron systems division, and it has continued seamlessly into the present through the condensed matter division.

At the same time, the institute benefits from the experimental research activities of the neighbouring Max Planck Institute for the Chemical Physics of Solids (MPI-CPfS). This institute is devoted to an interdisciplinary approach to materials physics, linking a broad spectrum of approaches from chemistry and physics, with directors Yuri Grin, Hao Tjeng, Claudia Felser and Andrew Mackenzie.

The two institutes collaborate in various ways, both on an ad-hoc basis as well as in a more structured fashion. The backbone of the latter is provided by a joint theory research group. Its purpose is to facilitate communication and collaborations between the two institutes. This enables members of both institutes to join forces in studying strongly correlated electron physics, superconductivity and magnetism. Its current head is Ashley Cook, who has succeeded Takashi Oka, who has moved to take up a professorship at the Institute for Solid State Physics at the University of Tokyo.

In addition, both institutes are involved in large-scale collaborative 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".

In parallel, the ad-hoc collaborations exist on subjects such as electronic transport in ultraclean electronic systems. This includes electronic hydrodynamics, a topic extending existing efforts at the institute which reaches deep into the biophysical research carried out here.

1.7.3 International Max Planck Research School

International Max Planck Research Schools (IMPRS) are structured doctoral programs intended to attract talented students from around the world. There are 68 such graduate schools across a wide range of topics, they are all English language based and involve collaborations between research groups at Max Planck Institutes and universities.

The IMPRS headquartered at mpi**pks** was established in 2005 with a focus on Dynamical Processes in Atoms, Molecules and Solids. This school ran successfully for two six-year funding periods whereupon it was restructured to respond to various changes to the research landscape in Dresden – including the foundation of an IMPRS based at the neighboring MPI for Chemical Physics of Solids. It was subsequently renewed as the IMPRS for Many-Particle Systems in Structured Environments in 2017, with a focus on many-particle quantum systems, especially those out of equilibrium.

The structured environments from which the IMPRS takes its name include analogue and digital quantum simulators, solid state materials driven out of equilibrium, organic molecules in solution, metal-organic frameworks, nuclear matter at high temperatures and densities as well as engineered nano-scale devices. Recent developments of new quantum technologies present us with new platforms to address classic open problems in many-body physics. They also open up unexplored directions to concrete investigation. Each of these areas presents new questions and exciting opportunities for young researchers. Members of the IMPRS find themselves part of an active research community, both within the graduate school and, partly through events that the school organizes, they are exposed to the frontiers of all these topics, of course alongside carrying out original research for their PhD thesis.

The location of mpi**pks** in the immediate vicinity of Poland and the Czech Republic made it possible for the IMPRS to be established on the strength of international research collaborations in three different countries. In particular, the IMPRS for Many-Particle Systems in Structured Environments is a consortium of research groups at the follow institutions:

1. Max Planck Institute for the Physics of Complex Systems - mpi**pks**
2. Technische Universität Dresden - TUD
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
6. Institute of Organic Chemistry and Biochemistry - IOCB (Prague, Czech Republic)
7. University of Chemistry and Technology - UCT (Prague, Czech Republic)
8. Charles University (Prague, Czech Republic)

The school has 29 partners who make up the IMPRS board including one coordinator and 28 who act as PhD advisors for students of the graduate school. All matters concerning the large-scale operation of the graduate school are decided in the board meetings including the admission of new students, the allocation of IMPRS funds, the program of IMPRS events including the summer school and retreat.

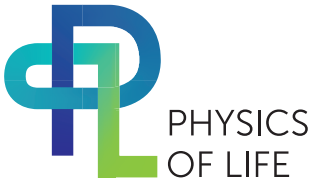
- Prof. A. Bäcker (TUD)
- Prof. D. Blaschke (University of Wrocław)
- Prof. J. Budich (TUD)
- Prof. B. Büchner* (IFW)
- Dr. A. Cook (mpi**pks**)
- Prof. G. Cuniberti* (TUD)
- Dr. A. Eckardt* (mpi**pks** → TU Berlin)
- Dr. M. Eiles (mpi**pks**)
- Dr. A. Eisfeld (mpi**pks**)
- Dr. F. Großmann (TUD)
- Prof. T. Heine (TUD)
- Dr. M. Heyl (mpi**pks**)
- Prof. P. Jungwirth* (IOCB)
- Prof. R. Ketzmerick (TUD)
- Dr. D. Luitz (mpi**pks**)
- Prof. O. Marsalek (Charles University)
- Dr. P. McClarty* (coordinator, mpi**pks**)
- Prof. R. Moessner* (chairman, mpi**pks**)
- Dr. F. Piazza (mpi**pks**)
- Prof. J.-M. Rost* (mpi**pks**)

- Prof. U. Saalmann (mpi**pks**)
- Prof. R. Schmidt (TUD)
- Prof. A. Sedrakian (University of Wrocław)
- Prof. P. Slavicek (UCT)
- Dr. I. Sodemann (mpi**pks**)
- Prof. W. Strunz* (TUD)
- Prof. J. Sznajd* (ILTSR)
- Prof. H.-H. Tu (TUD)
- Dr. hab. T. Zaleski (ILTSR)

There is a board composed of some subset of the partners (asterisked) that meets approximately once per year.

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

1.7.4 Cluster of Excellence: Physics of Life



The Cluster of Excellence Physics of Life (PoL, https://physics-of-life.tu-dresden.de) was established in 2019 at the Technical University Dresden. It was selected in the German Excellence Strategy, implemented by the Deutsche Forschungsgemeinschaft (DFG) and the German Council of Science and is funded for a period of 7 years. The concept of the cluster was developed with strong support from scientists at the mpi**pks** and at the Max-Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG). The cluster brings together 25 principal investigators from from TU Dresden and from several research institutions in Dresden to identify paradigms for understanding life and to deepen our knowledge of living biological matter. This is done by elucidating laws of physics that underlie the dynamic spatiotemporal organization of life into molecules, cells and tissues. A key aim is to bring fundamental physics to biology for the purpose of solving biological questions. It will also bring new experimental methods and technologies as well as computational approaches and systems microscopy to TU Dresden. The research of the cluster will merge theory and experiment, driven by a sparkling collaborative atmosphere in Dresden between University and non-University research institutions.

The cluster will recruit 4 full professorships (W3) and 6 tenure track assistant professorships (W2), as well as additional junior research groups. They will create a strong pillar of research on the physics of life at the Technical University Dresden with broad visibility. Two new full professors have been recruited in 2021. Prof. Otger Campas (formerly at UC Santa Barbara) works on the experimental physics of embryonic self-organization. Prof. Helmut Schiessel (formerly at Leiden University) holds a professorship on the theoretical physics of living matter. Three new appointments at the assistant professor level are Prof. Rita Matheus (formerly at University of Geneva) who works on biophysical principles of growth, Prof. Benjamin Friedrich pursuing research on Biological Algorithms and Prof. Ellen Adams (formerly at Ruhr-Universität Bochum) with a research profile on the physical chemistry of soft biological matter. The new groups will be accommodated in a new building that is currently being planned. The Cluster of Excellence provides a thriving research environment for scientists and postdocs from various disciplines, as well as a training ground for undergraduate and graduate students as well as for PhD students. A new master degree course "Physics of Life" is currently being developed. The Cluster of Excellence Physics of Life is closely integrated with the research program of the Biological Physics division at mpi**pks**.

1.7.5 Cluster of Excellence: Complexity and Topology in Quantum Matter

The cluster of excellence "Complexity and Topology in Quantum Matter" (ct.qmat) is a collaborative research structure based in Dresden and Würzburg. It is based on an integrated research strategy, in which researchers from the fields of physics, chemistry and materials science cooperate to understand, control and apply topological states of quantum matter.

The study of topological phenomena has been one of the central themes of modern condensed matter physics, ever since the groundbreaking discovery of the quantum Hall effect by von Klitzing forty years ago. Indeed, two locations from which important contributions to this field in Germany have originated are Würzburg (observation of quantum spin Hall effect) and Dresden (prediction of magnetic monopoles in spin ice). At present, both **mpipks** and the Max Planck Institute for the Chemical Physics of Solids have strong research programmes in the field. These range from detailed materials modelling to the transfer of field theoretic insights from high-energy physics.

The cluster of excellence is organised into four research areas: topological electrons, quantum magnetism, topological photonics, and tailoring topological functionality. Functioning as a platform for exchange (including teaching) and collaborations, it provides funding for student and postdoctoral researchers as well as experimental projects. It also aims to strengthen the research efforts in Dresden and Würzburg in the long term, with the appointment of four new professorships in the field. As one of three clusters of excellence in Dresden, it underpins the 'official' excellence status of the Technical University of Dresden.

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 focus of our work is the extension of the reach of equilibrium statistical mechanics, in particular into the topological realm. The aim is to identify qualitatively new phenomena, to develop their theoretical description, and to link them with experiment. Magnetic systems, specifically spin liquids, have been particularly productive here, in their dual role as simple model systems as well as their manifold realisations in materials physics.

The behaviour of many-body systems out of equilibrium is presenting a particularly exciting research frontier. The controlled accessibility of a wide variety of ingredients, such as quantum coherence, driving protocols, or various forms of quenched disorder has led to a plethora of interesting phenomena, and the resulting identification of new regimes and organising principles.

Our research programme is enhanced by copious interlinking between the different research strands. While it is hard to document these in the necessarily rather barebones list below, we would like to mention the following connection as an example. We have constructed and classified a new class of classical spin liquids, the effective description of which is in terms of a higher-rank 'fractonic' gauge theories, a specific realisation of which we have in turn identified in the familiar phenomenon of the absence of curvature in the folds of paper underpinning, for example, the construction of paper airplanes.

Spin liquids and their descendants: This field has continued to broaden and mature, especially as far as connections between theory and experiment are concerned. A central aspect of our research are the collective properties of the topological excitations found in these systems. Results include a determination of the fine-structure constant of the emergent quantum electrodynamics in quantum spin ice, which for the canonical model is determined to be about an order of magnitude larger than that of conventional QED, thereby opening a window on a regime of strong interactions. Another are collective states of the Majorana fermions emerging in Kitaev spin liquids, which are found to be reminiscent of quantum Hall states but with unconventional symmetry properties. Further, we have devoted much effort to developing reliable microscopic models for the detailed descriptions of spin liquid experiments. Finally, particularly noteworthy are results from previously unattainable regimes, such as the ground state of a frustrated three-dimensional quantum magnet of about 100 spins using DMRG, or a high-order high-temperature expansion allowing extrapolation to low temperatures.

Intermediate energy dynamics: While low-energy excitations are in large part determined by hydrodynamical considerations, little is known about generic properties outside this asymptotic regime. In our work, a new regime of applicability of spin wave theory in disordered magnets at intermediate energies was identified. Separately, it was shown that *strong* interactions between quasiparticles can lead to their survival even in regimes where their decay is kinematically permitted.

Quantum computing: Flowing from previous work on Floquet systems, we propose to use noisy intermediate scale quantum computing platforms specifically to study these periodically driven systems, as the structure of their time evolution is ideally matched to the architecture of the unitary quantum gates of these machines. A specific target phenomenon is discrete time crystallinity.

Non-equilibrium dynamics: This field has proven to be exquisitely rich, varied and fast-moving. Telegraphically, our proposal of a disorder-free Stark many-body localisation has been realised in a number of experimental platforms. We have identified the folding of paper as perhaps the most accessible realisation of fractonic physics. We have developed a theory for prethermalisation in the absence of temperature. We have identified several novel driving protocols with characteristic properties, such as random multipolar driving, and a particular strong driving regime. In addition, we have investigated extensions of Kibble-Zurek physics, both to a non-hermitian regime, and to include coarsening in the 'inert' regime near the gap closing. Finally, we have identified a lattice spin system exhibiting a form of jamming.

New electronic transport regimes: While the properties of Fermi liquids are well understood, new settings exhibiting novel phenomena continue to be discovered. This is in good part driven by materials discoveries, such as metals with very long mean-free paths. Besides continuing our strand of work on electronic hydrodynamics, a collaboration with an experimental group at MPI-CPfS and EPF Lausanne has uncovered an Aharanov-Bohm effect in a bulk material. The interference loop in question is extremely anisotropic: it is almost macroscopic – the sample size – in one direction, and microscopic – the lattice constant – in the other.

Perspectives. The development of the condensed matter division of mpi**pks** has continued to be dynamic. Members of the division have been very successful in the national and international job markets, with group leaders Markus Heyl, David Luitz, Anne Nielsen, Takashi Oka, Inti Sodemann leaving, or about to leave, to take up professorships. Several other group members have also obtained faculty positions, e.g. Falko Pientka and Piotr Surowka nearby in Frankfurt and Wroclaw, respectively.

The long-standing collaboration with MPI-CPfS continues, with Ashley Cook arriving to take over leadership of the joint group after Takashi Oka's departure. At the same time, the past few years have seen many inter-divisional research activities, on the topic of hydrodynamics with the biological physics division, and plentiful and manifold interactions, down to the joint supervision of summer research interns, with the finite systems division.

The research foci of the division will continue to be broadly divided between (mainly topological) condensed matter and materials physics, and many-body dynamics in and out of equilibrium, with the development of these fields continuing to present high levels of discovery and innovation.

Embedding in local research landscape. The condensed matter division is actively involved in two large-scale cooperative grants. One is the collaborative research center SFB 1143 at TU Dresden, entitled "Correlated magnetism: from frustration to topology", for which the renewal proposal for a final funding period is currently in preparation. The other is the cluster of excellence ct.qmat — "complexity and

topology in quantum matter", which is localised in Würzburg and Dresden.

Selected cooperations with theory groups internationally

- France: University of Bordeaux (Ludovic Jaubert); CEA Grenoble (Mike Zhitomirsky); École Normale Supérieure Lyon (Peter Holdsworth); Université Paris (Benoît Douçot), Cergy-Pontoise (Dima Kovrizhin)
- Great Britain: University of Cambridge (Claudio Castelnovo); Loughborough University (Achilleas Lazarides); Oxford University (John Chalker)
- Hungary: Budapest University of Technology and Economics (Balazs Dora)
- India: IACS Kolkata (Arnab Das, Arnab Sen); Indian Institute of Science (Vijay Shenoy); Tata Institute for Fundamental Research (Kedar Damle, Subhro Bhattacharjee)
- Italy: ICTP Trieste (Antonello Scardicchio)
- Japan: Gakushuin University (Masafumi Udagawa)
- United States: Boston University (Chris Laumann); Stanford University (Vedika Khemani); University of Minnesota (Natalia Perkins); Princeton University (Shivaji Sondhi); UC Riverside (Kirill Shtengel); Rice University (Andriy Nevidomskyy)

Selected cooperations with experimental groups

- Argentina: UNLP-Conicet La Plata – Santiago Grigera (non-equilibrium behaviour in spin ice)
- Canada: McMaster University – Bruce Gaulin (quantum spin liquids)
- China: Beijing Computational Science Research Center – Peng Xue (photonics)
- Germany: MPI-CPfS – Andy Mackenzie (electron transport); High magnetic field laboratory, Helmholtz Zentrum Dresden-Rossendorf – Jochen Wosnitza (frustrated magnets)
- Japan: ISSP Tokyo – Satoru Nakatsuji (quantum spin liquids)
- United States: google AI – Pedram Roushan (noisy intermediate scale quantum computing); Oak Ridge National Laboratory – Steve Nagler, Alan Tennant (magnetic materials)

Research Group: Dynamics in Correlated Quantum Matter
(Head: Dr. Markus Heyl)

The research group Dynamics in correlated quantum matter started at the mpi**pks** in September 2016. It currently consists of four postdocs (Chun Chen, Clement Delcamp, Reyhaneh Khasseh, Tiago Mendes Santos) and five PhD students (Roberto Verdel Aranda, Heiko Burau, Nilotpal Chakraborty, Luca Leone, and Vighnesh Naik). 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 interacting 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 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. During the past years, the group has focused particularly onto the following main lines of research:

Dynamics in nonergodic and constrained quantum many-body systems
It is a central property of realistic thermodynamic systems to exhibit relaxation towards thermal equilibrium independent of initial conditions. However, it has been realized in recent years that new types of quantum states can be generated when constraints inherent to equilibrium states can be lifted. Targeting such states, in turn, requires to break ergodicity. We have mainly explored two mechanisms leading to such absence of thermalization and some resulting quantum states with new properties. On the one hand, we have studied many-body localized systems, where nonergodicity originates from imposing strong disorder. In this context we have (i) introduced a method to efficiently solve many-body localized systems

of fermions and bosons at weak interactions and strong disorder, which we have also applied for the description of many-body localized systems coupled to thermal environments, (ii) formulated a theoretical description for the spatiotemporal growth of many-body localized spin-glass order, and (iii) revealed anomalous diffusion in many-body localized systems with particle-hole symmetry. On the other hand, we have investigated the breakdown of ergodicity in lattice gauge theories: (i) we have shown that lattice gauge theories can generically exhibit nonergodic behavior without imposing disorder but rather caused by local constraints imposed solely by gauge invariance, which has been termed disorder-free localization; (ii) we have further explored the potential to realize genuinely nonequilibrium quantum phases such as a gauge time crystal or the emergence of critical correlations and subdiffusive dynamics in two-dimensional lattice gauge theories.

Machine learning quantum dynamics

While during the last two decades powerful numerical approaches have been developed for the solution of the dynamics in one-dimensional interacting quantum matter, it has remained a central challenge to access the regime of two spatial dimensions. This is not only of central importance for their theoretical understanding but also in the experimental context of so-called programmable quantum simulators such as Rydberg atoms, which are just now starting to target quantum matter in this regime. In our group we are aiming to contribute at this frontier using a crossdisciplinary approach at the interface between quantum many-body theory and machine learning, which has been remarkably successful in the computer science context. Concretely, this is achieved by encoding the quantum many-body state in artificial neural networks. In this context we have (i) demonstrated that this machine learning approach for quantum many-body dynamics in two spatial dimensions can be made competitive or even superior to state-of-the-art high-performance computational approaches upon introducing a set of crucial algorithmic improvements, (ii) developed a technique utilizing ideas from both quantum renormalization groups and artificial neural networks to numerically compute the long-time dynamics of quantum models with strong disorder, which has allowed us to describe the yet unexplored buildup of long-range many-body localized spin-glass order, (iii) to explore the paradigmatic quantum Kibble-Zurek mechanism of defect production upon dynamically sweeping through a quantum critical point of a two-dimensional quantum Ising model. Moreover, we have also been exploring further promising intersections of the two fields of quantum many-body physics and machine learning. In this context we have (i) developed an experimentally feasible scheme to detect quantum entanglement, which is a key but challenging to measure property of quantum matter, by adapting powerful techniques of image recognition to data resulting from measurements in quantum simulators and (ii) used the technique of reinforcement learning, a powerful machine learning approach to develop complex strategies, to optimize certain quantum algorithms, where we have achieved reductions of the required resources by one order of magnitude as compared to those used recently in quantum computers.

Collaborations with theory groups

- Prof. Peter Zoller (IQOQI Innsbruck, Austria): Quantum information
- Prof. Wojciech Zurek (Los Alamos, US): Quantum Kibble-Zurek mechanism
- Prof. Marcello Dalmonte (ICTP Trieste, Italy): Dynamics in lattice gauge theories
- Prof. Frank Pollmann (TU Munich, Germany): Quantum dynamics and many-body localization
- Prof. Alexey Gorshkov (University of Maryland, US) : Quantum dynamics of spin chains featuring confinement
- Prof. Nathan Goldman (University of Brussels, Belgium): Quantum metrology
- Prof. Rosario Fazio (ICTP Trieste, Italy): Dynamics in quantum matter
- Prof. Marcos Rigol (PennState, US): Quantum quenches and quantum phase transitions
- Prof. Philipp Hauke (University of Trento, Italy): Quantum dynamics and quantum information
- Prof. Jacek Dziamarga (Jagiellonian University, Poland): Quantum Kibble-Zurek mechanism
- Prof. Marek Rams (Jagiellonian University, Poland): Quantum Kibble-Zurek mechanism
- Prof. Michal Heller (University of Ghent, Belgium): Dynamics of particle collisions in spin models.
- Prof. Balazs Dora (Budapest University of Technology and Economics, Hungary): Quantum dynamics
- Prof. Arnab Das (IACS Kolkata, India): Quantum quenches and quantum phase transitions
- Prof. Soumya Bera (Indian Institute of Technology Bombay, India): Many-body localization
- Prof. Jan Carl Budich (TU Dresden, Germany): Quantum entanglement

Collaborations with experimental groups

- Prof. David Weld (University of California, Santa Barbara, USA): Floquet prethermalization
- Jianming Cai (, China): Quantum metrology with nitrogen-vacancy centers in diamond
- Wei Yi (, China): Quantum Kibble-Zurek mechanism in non-Hermitian systems
- Prof. Guang-Can Guo (University of Science and Technology of China, Hefei, China): Quantum walks

Research Group: Computational Quantum Many-body Physics
(Head: Dr. David Luitz)

The research group "*Computational Quantum Many-Body Physics*" was established at **mpipks** in April 2018. It currently consists of four PhD students (Luis Andres Colmenarez Gomez, Robin Schäfer, Maurits Tepaske and Dominik Hahn) and two postdocs (Dr. Manuel Weber and Dr. Zhenjiu Wang). We have also hosted four summer interns (Owen Howell, Kevin Wang, Oscar Emil Sommer and Ziwei Wang). Three previous postdocs have moved on to continue their careers (Dr. Laura Baez, now at Deutsche Bank; Dr. Harshini Tekur, now at Uni Freiburg; Dr. Imre Hagymasi, now at FU Berlin).

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, many-body localization and digital quantum simulation. 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.

Open quantum systems. Quantum systems in reality are rarely completely isolated from their environment. We are interested in new quantum many-body phenomena due to dissipation and try to understand the behavior of generic open systems from the perspective of dissipative quantum chaos. Interestingly, it turns out that the locality of dissipative interactions alone can for example give rise to a hierarchy of dissipative timescales which are relevant in present day quantum computers. Open quantum systems can exhibit entirely new phenomena due to the nonhermitian nature of the Liouvillian or effective Hamiltonian, such as the emergence of exceptional points, which give rise to a peculiar topology of quantum many-body spectra.

Digital quantum simulation. We live in an era of the beginnings of universal quantum computers. While there is still a long way to go before we will have truly universal and error corrected quantum computers, we are now reaching a regime in which we can simulate quantum many-body physics on existing quantum computer prototypes. We have contributed pioneering studies of open quantum systems on the IBM platform and are continuing our efforts in this direction.

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 phase as well as the avalanche mechanism driving the transition.

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. We consider periodically driven systems on two levels: As generic models for quantum many-body physics with to some extent simpler properties due to a homogeneous density of states, but also as interesting classes of models which can exhibit interesting prethermal states (protected by a conservation law) before relaxing to the equilibrium "infinite temperature" state at a much longer timescale.

Frustrated quantum magnets. As part of a collaboration in the SFB1143, our group studies model systems for frustrated quantum magnets, in particular the physics of the Heisenberg antiferromagnet on the pyrochlore lattice which is strongly frustrated due to omnipresent tetrahedral motifs. We have shown that such three dimensional systems can be efficiently studied using the density renormalization group. By careful finite size scaling, we showed that the ground state is not a spin liquid but a state which spontaneously breaks the inversion symmetry of the lattice.

Collaborations

- Princeton University, USA: Collaboration with David Huse on many-body localization, and with Shivaji Sondhi on prethermal time crystals.
- Stanford University, USA: Collaboration with Vedika Khemani on prethermal time crystals.
- Oxford University, UK: Collaboration with John Chalker on information spreading and thermalization.
- Nottingham University, UK: Collaboration with Juan Garrahan on metastable states in open quantum systems.
- TU Dresden, DE: Collaboration with Jan Budich on nonhermitian quantum many-body systems.
- Helmholtz Zentrum Dresden Rossendorf, DE: Collaboration with Joachim Wosnitza and Hannes Kühne on Kosterlitz Thouless Transitions in quantum magnets.

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). Secondly, light from intense pulses or in microcavities provides another, quite universal kind of environment. Thirdly, noise creates an important class of environment, also studied at **mpipks** outside the *Finite Systems* department in various contexts, from cavities over chaotic dynamics to biological systems.

The research group *Finite Systems* within the department has presently two foci: The first one concerns fundamental time-dependent mechanisms in light-matter coupling. Here, we concentrate on short pulses relating the fields of attosecond and time-dependent X-ray science and in general strong field physics (project leader *Ulf Saalmann*). Furthermore, we investigate time-dependent phenomena in ultracold systems which are slow on an absolute timescale but ultrafast relative to the system scale (project leader *Panos Giannakeas*). The second focus lies on ultracold Rydberg excitations in structured environments (project leader *Matthew Eiles*, now group leader in the *Finite Systems* department). Fruitful synergy emerges here from the relation between exciton dynamics in traditional quantum aggregates and their counterpart in the context of ultracold Rydberg complexes. This connection is pursued in collaboration with *Alexander Eisfeld* and his research group *Quantum Aggregates*. The affiliated research group *Strongly Correlated Light-Matter Systems*, headed by *Francesco Piazza* who is interested in systems coupled to structured environments formed by cavities and whose group, furthermore, provides a fruitful bridge to the condensed matter department.

Research topics

Rydberg assemblies. In an ultracold (e.g. BEC) environment, one can form *Rydberg Composites*, where a Rydberg excited electron is bound to many ground state atoms from the environment. The latter can act as a "frozen gas" of atoms at random positions, or as "solid" if the atoms are arranged regularly, e.g. through an optical array. With Rydberg Composites we have developed a systematic approach which can interpolate between both limits with the same description opening the possibility to uncover topological and localization phenomena in this context originating from geometry and randomness. Our research regarding *Rydberg Aggregates* has advanced to explicitly include atomic motion for coherent Rydberg excitation transport.

Non-adiabatic light driven dynamics. In dynamics involving laser driven ionization/fragmentation or the opposite, association of particles, there is often a mismatch of time scales between the laser driving and the natural time scale of the relevant motion of the particles. We aim at identifying these time scales and at revealing their mismatch as the origin of intriguing phenomena. This refers to such disparate situations as the ionization of bound electrons of different orbital character by circularly polarized light fields (by recognizing that the dynamics is adiabatic in the body-fixed rotating frame but non-adiabatic in the lab-fixed frame) or photo association of ultracold atoms in a pulsed magnetic field which changes slowly on ab absolute scale but fast relative to the slow ultracold dynamics.

Light induced dynamics with delocalized electrons. In a condensed matter context, electrons are delocalized. As we have seen this enables coherent electron backscattering in systems with broken translational symmetry implying more efficient high harmonic generation. Gapless or weakly-gapped 2D materials couple almost exclusively at the Dirac points to light pulses which suggests relatively simple pulses polarized linearly along the line of the Dirac points in reciprocal space in order to maximize valley polarization.

Extracting information from dynamics triggered by noisy pulses through machine learning. The idea behind this project is that the response to a noisy pulse reveals in a single laser shot much more information about the system than a standard Fourier-limited almost monochromatic pulse, *if* one is able to extract the relevant information from the necessarily noisy response. For this purpose we develop machine learning concepts and have demonstrated that through a suitably trained deep neural network one can "purify" noisy measurements as they are typical, e.g., for SASE generated XFEL pulses. We can also a posteriori extract from measurements the time-delay of double pulses which occurs randomly up to a maximal time span in such experiments.

Long-time non-stationary dynamics in open systems. In this project, we develop a semiclassical concept to understand the prerequisites for long-time non-stationary dynamics, that is the existence of diffusion-free subspaces. This allows us to make use of powerful results from classical mechanics such as the KAM theorem to extend the conditions for non-stationary long-term dynamics from integrable systems also to the much wider class of near-integrable systems.

Perspectives for the future

In the ultrafast domain, we will concentrate on phenomena involving light driven delocalized electrons.

Our efforts to develop new concepts will progress along two lines:

(i) Using advanced classical mechanics in a quantum context.
We will systematically exploit the high density of Rydberg states to elucidate the relation of localization and semiclassical scarring phenomena. Our concept of Rydberg Composites will allow us to formulate this relation also in the context of condensed matter systems. This topic will be pursued together with *Matt Eiles'* group.
We have just started to describe long-term non-stationary quantum dynamics in open systems with the underlying classical dynamics through the semiclassical link which is a very promising route for future deeper understanding with the perspective to propose environments and coupling to it tailored for specific desired properties of the quantum system.

(ii) Synthetic Hamilton Matrices.
In the context of purifying noisy spectra with neural networks we have developed "Synthetic Hamilton Matrices", that is, a matrix representation of artificial systems which could exist but do not necessarily exist but are used by the neural network to identify the "real" system by interpolation from measured spectra. We will pursue the concept of these synthetic matrices to eventually develop a novel kind of spectroscopy to identify the relevant Hamilton matrix from spectroscopic data and use it to predict other observables of the underlying system.

Collaborations

- Prof. B. von Issendorf (Uni Freiburg) regarding photo ionization of clusters,
- Prof. C. H. Greene (Purdue University, USA) on ultracold non-adiabatic effects,
- Prof. F. Robicheaux (Purdue University, USA) on ultracold few-body Rydberg dynamics,
- Prof. L. di Mauro, (Ohio State Univ., USA) on long-wavelength light illuminating clusters,
- Prof. T. Pfeifer (MPI for Nuclear Physics, Heidelberg) regarding ionization in XUV pulses,
- Prof. K. Singh (IISER, Mohali, India) on attosecond ionization,

- Prof. S. Wüster (IISER Bhopal, India) on electron transport in Rydberg aggregates.
- Through the two Priority Programs 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 the fields of ultrafast and ultracold dynamics, respectively.

Local cooperations

With Prof. Großmann from the TU Dresden we collaborate on *semiclassical propagation techniques*.

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

The group was established in October 2012. Since 2019 I am funded via a Heisenberg fellowship of the German research foundation (DFG). Currently the group consists of four PhD students (Ghassan Abumwis, Sidharta Nayak, Juan Moreno and Aritra Mishra) and three postdoctoral guest scientists (Lipeng Chen, Christopher Wächtler and Carlos Benavides). During the evaluation period the group hosted two more postdoctoral guest scientists (Fulu Zheng and Farhad Ghahramani).

The main focus of our research is the emergence of collective quantum effects in mesoscopic assemblies of atoms and molecules (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. Exemplary topics we are currently investigating can be found below.

Molecular aggregates on dielectric surfaces: We consider various situations in collaboration with experimental groups: molecules are deposited either under ultra-high vacuum (group of Prof. Sokolowski, Bonn), in solution (groups of Prof. Hauer, TUM, and Dr. Mertens, Lancaster) or on rare earth clusters (group of Prof. Stienkemeier, Freiburg). On the rare earth clusters, we are in particular interested in the influence of the cluster material on the lifetime and quantum yield of acene molecules, from which we draw conclusions about non-radiative channels such as singlet fission. For regular monolayers we have indications that electronic excitation is coherently shared by hundreds of molecules. To see this directly, we investigate the use of metallic tip based near-field spectroscopy to gain access to all eigenstates and their corresponding wavefunctions. Using neural networks, we can even reconstruct the delocalized eigenstates of the aggregate. At the moment we investigate the information that pump-probe spectroscopy can provide about dephasing and relaxation pathways to gain more insight into the interaction of the molecules with the surface. Recently, we became interested in topological properties of regular molecular aggregates on surfaces, where individual molecules have degenerate transitions.

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. In collaboration with Prof. Strunz from the TU Dresden we have succeeded to derive an exact hierarchy of coupled stochastic equations (HOPS) for the propagation of pure states. This hierarchy 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 two years we have made important conceptual steps forward that put us now in the position to investigate for example large photosynthetic complexes with realistic couplings to internal vibrations and the surroundings. Our main results are: (i) formulation of HOPS in terms of matrix product states; (ii) demonstration that the stochastic leads to localization of the trajectories, which allows one to use adaptive grids; (iii) non-perturbative stochastic formulation of correlation functions, for non-linear spectroscopy. We are now applying our formalism to photosynthetic light harvesting systems and molecules on surfaces.

Quantum simulators for open quantum systems: Quantum simulators are well controlled quantum systems that can be used to simulate quantum Hamiltonians. Such an approach will be particularly fruitful, if the corresponding numerical simulation on a classical computer is intractable. We focus on finite dimensional systems interacting with a structured environment. In collaboration with Dr. Wüster and the experimental group of Dr. Whitlock (U. Heidelberg) we have recently shown that ultra-cold Rydberg aggregates embedded in a laser driven background gas are 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. We now have also demonstrated theoretically, that one can simulate femtosecond experiments within this framework by using short microwave pulses and a phase-cycling scheme. Beside this analog quantum simulator we also work on digital quantum simulators; in collaboration with Dr. Mostame (IBM) we recently implemented the vibronic Hamiltonian of a small aggregate on the IBM quantum computer.

Transport at critical parameters: Critical phenomena describe the drastic change of a system upon modification of a parameter and appear in various areas of physics. We study such critical phenomena in classical and quantum systems under nonequilibrium conditions, in particular self-induced nonlinear dynamics and exceptional points. The former can be observed in the electron shuttle, a paradigmatic nanoelectromechanical system (NEMS) that integrates electrical and mechanical functionality at the nanoscale. We focus on shuttles without an intrinsic frequency, which exhibit rich dynamics and are capable of performing a broad range of objectives (e.g. rectification of currents). In the context of optical waveguides we investigate the effect of exceptional points, for example for the amplification of signals.

Collaborations:

- Dr. Croy (TU Dresden): Nano-electro mechanical devices; quantum rotors.
- Dr. Eiles (mpi**pks**): Rydberg atoms.
- Prof. El-Ganainy (Michigan Tech, USA): Non-linear photonics.
- Prof. Hauer (TUM): Spectroscopy of organic dye aggregates.
- Prof. Mertens (Lancaster,UK): Molecules on surfaces.
- Dr. Mostame (IBM, New York): Digital quantum simulator.
- Prof. Rost (mpi**pks**): Rydberg composites.
- Prof. Sokolowski (Uni Bonn, Germany): PTCDA monolayers on dielectric surfaces, superradiance.
- Prof. Stienkemeier (Uni Freiburg, Germany): Phase-modulated spectroscopy, molecules on clusters.
- Prof. Strunz (TU Dresden, Germany): Stochastic Schrödinger equations.
- Prof. Whitlock (Strassburg, France): Dynamics of driven Rydberg assemblies.
- Prof. Wüster (IISER Bhopal): Rydberg aggregates in Bose Einstein condensates.

Research Group: Correlations and Transport in Rydberg Matter
(since January 2021, Head: Dr. Matthew Eiles)

The group was established in January 2021 and consists of one PhD student (Aileen Durst) and two postdocs (Viktor Ivady and Črt Lozej). Our research focuses on Rydberg atoms and the phenomena which emerge as a result of their exaggerated sizes, energy scales, and interaction strengths. We use Rydberg systems to bridge the gap between the microscopic world of atoms and electrons and the mesoscopic world of condensed matter physics.

Our research has two primary motivations. On the one hand, we want to understand and interrogate dynamical processes in and fundamental properties of ultracold gases. Rydberg states probe their local environment through their interactions with it, and are thus a valuable tool for this purpose. On the other hand, we want to explore emergent physics which become apparent or can be created by interfacing excited Rydberg atoms with an environment such as other Rydberg atoms, interacting strongly at large distances, or ground state atoms, exploiting the vast size and degeneracy of Rydberg states.

Below is an overview of our research activities.

Long-range Rydberg molecules. Several varieties of long-range Rydberg molecules have been observed in ultracold gases. They are characterized by remarkably large bond lengths, ranging from tens of nanometers to a few microns. Their properties depend on the particle bound to the Rydberg atom, which can be another Rydberg atom, an ion, a dipolar molecule, or a neutral ground state atom. The binding mechanism of the latter relies on the overlap between the Rydberg electron and the ground state atom rather than the long-range electrostatic interactions present in the others. We have developed analytical and numerical methods to study these molecules, for example:

A semi-analytical method built around the *generalized local frame transformation* and the core concepts of multichannel quantum defect theory. We used this to extract more accurate electron-atom scattering

phase shifts from a comparison between theoretical and experimental vibrational spectra. We also used this method to calculate photoionization cross sections when an atom is ionized in a dilute frozen gas.

A *Green's function method* incorporating the electronic and nuclear spin degrees of freedom of both Rydberg and ground state atoms, which become relevant at the accuracy of recent experiments.

Physically motivated models of *non-adiabatic processes* in Rydberg molecules, whose unusually oscillatory potential energy curves occasionally vary dramatically due to the disparate energy scales present. We have predicted prominent signatures of non-adiabatic effects in angular momentum changing collisions and begun a systematic study of beyond-Born-Oppenheimer physics enhanced by external field control.

We have started to adapt these methods to other types of long-range Rydberg molecules, particularly the Rydberg-ion molecules which have recently provoked both experimental and theoretical interest.

Rydberg composites and quantum simulation. A Rydberg atom can be interfaced with an array of ground state atoms. These in turn structure the otherwise highly degenerate spectrum of the Rydberg atom and sculpt its electronic wave function. We have recast the *Rydberg composite* Hamiltonian into a tight-binding form, highlighting a deep connection between the excited states of atomic spectra and foundational solid-state models. With this reformulation we demonstrate how the hydrogenic properties inherited by a Rydberg atom enable a thermodynamic limit, and studied Anderson localization of the Rydberg electron. Recently, our attention has turned to the subject of symmetry-protected topological order. Using the connection between the Rydberg composite's spectrum and a lattice system we have studied how to design a Rydberg composite such that the Rydberg electron exists in a topological edge state protected by a chiral or inversion symmetry.

Quantum scarring, localization, and chaos. The same properties which make Rydberg atoms in an impurity environment fascinating can be found in many other systems, for example in quantum dots, electrons moving in magnetic fields, and semiconductor excitons. By adapting our Rydberg toolkit to these systems, we investigate the underlying connections between quantum scarring induced by disorder, quantum chaos and semiclassical dynamics, and Anderson localization. Building on the intuition developed here, we will study many-particle counterparts of these phenomena, such as the many-body scar states recently observed in constrained Rydberg lattices or Rydberg polarons in ultracold gases.

Strongly interacting atoms. Rydberg atoms interact over large distances through resonant dipole-dipole interactions when they are prepared in different quantum states. In collaboration with Dr. Eisfeld's Quantum Aggregates group, we pursued a numerical investigation of eigenstate delocalization in interacting Rydberg gases. We found that, although some eigenstates fragment into strongly-interacting clusters, the remaining eigenstates remain delocalized and have the structure of an approximately homogenous network. The fraction of delocalized states grows with the system size.

Collaborations:

- Prof. Schmelcher (University of Hamburg): Non-adiabatic effects and dynamics.
- Prof. Rost (mpi**pks**): Rydberg composites and long-range Rydberg molecules.
- Prof. Robicheaux (Purdue University): Photoionization in ultracold gases.
- Dr. Eisfeld (mpi**pks**): Rydberg aggregates.
- Prof. Greene (Purdue University): Green's function methods for few-body systems.

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

Living matter is an inherently dynamic and highly organized form of condensed matter that is maintained away from thermodynamic equilibrium. The division *Biological Physics* develops theoretical approaches to study the spatiotemporal organization of living matter at scales ranging from molecules to cells and tissues. This research is done in tight interaction with quantitative experiments and in interdisciplinary collaborations at the Center for Systems Biology Dresden. The study of living matter from a physics approach is based on an integration of statistical physics, soft matter physics and nonlinear dynamics. A key goal is to identify fundamental principles that underlie the self-organization of complex cellular processes such as cell division, intracellular transport, the spatial and temporal organization of organelles as well as the collective behaviors of many cells. A key example is to study how complex morphologies

and patterns emerge when an organism develops from a fertilized egg. Living matter is fundamentally active and driven far from thermodynamic equilibrium by a supply of free energy via metabolic processes. It exhibits significant stochasticity while operating robustly even when perturbed. Living matter poses many challenges related to its enormous complexity and the nonequilibrium character. However important breakthroughs have been made in recent years. A key example is the insight that biological structures often emerge from the self-organization of active mechano-chemical processes.

We study specific biological processes in close collaboration with experiments to reveal underlying physical interactions and organizational principles. We also develop general theoretical approaches to the complex dynamics of soft active matter.

Our research focusses on several themes including:

Physics of biological condensates. Many organelles of cells are membraneless condensates of macromolecules that phase separate from the cell cytoplasm. Such condensates often behave as liquid droplets that can confine cellular biochemistry. We study the material properties of such condensates and have revealed that they can exhibit viscoelastic behaviors and glass-like ageing. A focus of our research is to study how such condensates organize molecular processes in the cell. In addition to condensates in the cell cytoplasm, we are also studying the physics of protein condensation on DNA and the role of protein condensates in the organization of chromatin, which holds the genetic information in the cell nucleus.

Theory of chemically active emulsions. Liquid mixtures can undergo phase separation and demixing. Such mixtures are also host to many different chemical processes. We investigate the physics of phase separating systems that undergo chemical reactions. Such reactions can govern the dynamics of droplet growth and disassembly. Furthermore, droplet phases can organize chemical reactions in space. We develop theoretical approaches to investigate the rich physics of such systems which exhibit novel and unconventional regimes and behaviors, in particular when maintained away from thermodynamic equilibrium.

Emergence of tissue shape and size. During the development of an organism, tissues form patterns and complex morphologies and they grow to a specific size. Size and shape arise from the collective interplay of cell populations in a tissue. Such tissue patterning involves signaling molecules called morphogens that are secreted locally and form graded concentration profiles. We are investigating the transport and the kinetics of morphogen signaling and we develop theoretical approaches to understand how scalable tissue patterns emerge in growing tissues and how tissue growth is controled.

Liquid crystal organization of tissues. Tissues are soft active and dynamic materials which often appear amorphous, but which can exhibit structural order. We have developed tensor-based approaches to characterize anisotropies in liver tissue at different scales. This revealed large scale biaxial nematic order of tissue organization. This reveals that tissues can exhibit structural order similar to liquid crystal phases.

Electrohydraulics and flexoelectricity of tissues. Tissues are not only mechano-chemical systems but also generate fluid flows and electric fields and currents. In particular ion pumps drive currents which in turn lead to fluid flows via osmosis. We are extending hydrodynamic theories of active matter to include electric fields and fluid flows. Such approaches reveal that active processes can provide tissues with flexoelectric properties, i.e. electric fields can lead to tissue bending or conversely, tissue bending can alter electric fields and currents. This shows that tissues are in fact electrohydraulic devices.

Shaping active surfaces. Active surfaces are thin sheets of fluid or elastic materials that are driven by a supply of chemical free energy away from thermal equilibrium. They provide models for the cell cortex or cell sheets that play a key role for the generation of shape in biology. We are studying the self-organization of mechano-chemical processes on such active surfaces, which can lead to the generation of shapes via the self-organization of chemical processes on surfaces.

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 of time-delayed coupling developed for biological systems to engineering, where we study how the self-organization of phase-locked loops can provide time references in distributed electronic networks. For high clock rate at tens of GHz, centimeter distances imply communication delays that can govern synchronisation.

Integration in the Dresden scientific environment

Dresden provides a rapidly developing and flourishing scientific environment at the interface of physics and biology. Most important for our research is a tight and longstanding collaboration with the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG). We are closely collaborating with several groups at MPI-CBG to bring physical approaches to biology for the study of living matter. Our department is also linked to 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.

We are integrated in the Center for Systems Biology Dresden (CSBD), which is jointly operated by the MPI-CBG and the **mpipks** in partnership with the Technical University Dresden (TUD). The CSBD provides a hub that facilitates the interaction of theoretical physics and computer science with cell and developmental biology and stimulates collaborations and new research directions. It also brings us in proximity to the experiments next door to the new CSBD building. Research in biological physics has in recent years been flourishing at the TUD in particular with the recruitment of new research groups at the Biotechnology Center (BIOTEC) and at the Center for Molecular Bioengineering (BCUBE). A new milestone was reached in 2019 with the establishment of the Cluster of Excellence Physics of Life (PoL) at TU Dresden. The cluster of excellence brings strong new research groups with a focus on the physics of living matter to Dresden. It connects different institutions and provides a broad platform connecting experimental biophysics with theoretical physics and with quantitative biology. These activities pursue a common vision to identify physical principles that underlie the organization of living matter. Our department was closely involved in the development of the PoL concept and is tightly integrated in its research program. The cluster of excellence PoL will attract and train students and prepare them to enter research in biological physics. Overall, Dresden now features an attractive, very competitive and internationally visible research environment focussing on key challenges in the physics of living matter.

Collaborations

- Max Planck Institute of Molecular Cell Biology and Genetics, Dresden
  - Collaborations with Jan Brugues, Stephan Grill, Anthony Hyman, Ivo Sbalzarini and Christoph Zechner on cell physics.
  - Collaborations with Anne Grapin-Botton, Nathalie Dye, Stephan Grill, Carl Modes and Marino Zerial on the dynamic organization of tissues.
- TU Dresden
  - Collaboration with Elisabeth Friedrich-Fischer on the material properties of biological condensates.
  - Collaboration with Benjamin Friedrich on tissue organization.
- Institut Curie, Paris
  - Collaboration with Jacques Prost on cell and tissue physics.
  - Collaboration with Pascal Martin on active cellular processes.
- Collège de France, Paris
  - Collaboration with Jean-Francois Joanny on the self organization of active matter.
- École Polytechnique Fédérale de Lausanne
  - Collaboration with Andy Oates on genetic oscillations and waves.
- University of Geneva
  - Collaboration with Marcos González-Gaitán on tissue scaling and growth control.
  - Collaboration with Guillaume Salbreux on active surfaces.

Research Group: Statistical Physics of Living Systems
(Head: Dr. Steffen Rulands)

The self-organisation of cells into complex tissues is one of the most intriguing non-equilibrium processes in nature, relying on tightly regulated molecular and cellular programs. Understanding the mechanisms underlying the regulation of cell behaviour is pivotal not only for understanding the processes responsible

for development, regeneration and ageing, but also for the diseases that occur upon dysregulation, such as cancer. On the molecular level, different kinds of processes are involved in regulating cellular fate: besides the expression of genes it has, in recent years, become clear that there are additional, epigenetic, layers of regulation: dynamic changes in the way the DNA is folded, modifications to the protein complexes which the DNA is wrapped around or chemical modifications of the DNA itself.

Recent technological breakthroughs in single-cell biology now allow probing all of these processes with unprecedented microscopic detail in living organisms (in vivo) and even in human 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 spatial organisation of chromatin of thousands of single cells from living organisms. Single-cell multi-omics technologies allow profiling of several layers of regulation in the same cell. These technological developments have led to detailed descriptions of the molecular processes underlying cellular behaviour. Biological function, such as cell differentiation, proliferation or death, however, is determined by emergent (collective) states on the cellular and tissue scale which arise from interactions between processes occurring at many different loci on the molecular scale. But how can detailed quantitative information on the microscopic scale inform on emergent processes that determine biological function at the cellular and tissue scale?

As an example, in the realm of 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 rules that govern on the microscopic scale (emergence). Therefore, the collective dynamics underlying biological function cannot be straightforwardly inferred from detailed molecular measurements. Hence, despite the excitement that novel developments in single-cell genomics are causing and that is reflected in large-scale research endeavours like the Human Cell Atlas and the declaration of these methods as the "2018 breakthrough of the year" by Science, insights from these technologies remain descriptive until matched with methods to identify collective degrees of freedom. Concepts from (non-equilibrium) statistical physics such as field theory and renormalisation provide a powerful framework to begin to understand the collective processes underlying cellular behaviour *in vivo*.

The Statistical Physics of Living Systems group pursues an interdisciplinary approach and combines novel technologies in single-cell biology with tools from non-equilibrium statistical physics to understand collective processes underlying the behaviour of active biosystems.

The group follows four broad research directions:

Understanding collective molecular processes using single-cell genomics (ERC funded) In several collaborations with experimental groups we use methods from non-equilibrium statistical physics overcome conceptual limitations in the emerging field of single-cell genomics. Together with our experimental collaborators we apply these theories to understand the collective 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 studied collective processes underlying the formation of the embryonic epigenec landscape, and showed how this landscape changes during ageing.

Propagation of fluctuations in cellular decision making Biological systems are organised in a hierarchy of non-equilibrium processes on vastly different spatial scales. We investigate how active biosystems manipulate how fluctuations propagate across spatial scales in order to perform specific biological functions, such as sensing molecular signals and triggering the response of cells to such signals. Together with experimental collaborators, we apply these ideas to understand the decisions of cells to commit suicide, to respond to viral attacks and the self-organisation principles underlying insect societies.

Self-organisation of cells into complex tissues To build and maintain complex tissues relies on a tight regulation of the behaviour of many cells. Based on experiments conducted by our collaborators we aim to understand the self-organisation of cells gives rise to complex structures such as the skull or the brain. In a more clinical context we ask how the dysregulation of these processes gives rise to tumours and develop theories of treatment strategies using tumour organoids.

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

novel contexts.

Collaborations

- 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
- Meritxell Huch, MPI-CBG on liver regeneration
- Michaela Fre, Institut Curie, Paris (UK) on pancreas development
- Maria Pilar Alcolea, Wellcome Trust Gurdon Institute, Cambridge (UK) on regeneration and tumour initiation
- Attika Toth, TU Dresden on spatio-temporal control of meiotic recombination

Research Group: Mesoscopic Physics of Life
(until August 2021, 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. Throughout the last years, a strong focus is 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 physicochemical 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.

Chemically 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 emulsion 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 could also show that phase separation leads to prolonged life-time of thermodynamically unstable chemical species. 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.

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. Currently, we work on the theory where these droplets in turn affect the concentration gradients. Moreover, we scrutinize our theoretical model with experimental studies in living cells to understand whether position-dependent ripening can also explain the positioning of intra-cellular drops. An other study is concerned with the question whether positioning of droplets in flux-driven concentration gradients is a non-equilibrium phase transition.

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 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.

Selection of molecules via cycles of phase separation. Living cells and pre-biotic systems are complex aqueous mixtures composed of thousands of different heteropolymers. In such multicomponent mixtures, enrichment and selection of a small set of components are important to achieve biological function. However, when the number of components increases, each of them becomes more diluted impeding a significant enrichment of selected components. We have developed a theory to study a selection mechanism relevant for prebiotic mixtures. The mechanism is based on cycles of phase separation combined with material exchange of the dense phase with a reservoir. One of our key findings is the selective enrichment of components up to two orders of magnitude coinciding with a growth of the dense phase up to the system volume. Such enrichment of specific components is robust also in mixtures composed of a large number of components. For a prebiotic soup, our findings indicate that cycles of phase separation and material exchange with a reservoir, e.g. the accumulation DNA gel in rock pores periodically filled with DNA rich aqueous solution, could provide a mechanism for the selection and enrichment of specific heteropolymers sequences in a multi-component mixture at the origin of life.

Collaborations:

Theoretical Collaborations:

- Thomas C.T.Michaels (Harvard University, Cambridge, USA) on aggregation kinetics in with co-existing phases.
- Christoph Zechner (Max Planck Institute of Molecular Cell Biology and Genetics and Center for Systems Biology, Dresden) on optimal control of biochemical reaction via phase coexistence.
- 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 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 Biology and Genetics, Dresden) on the formation of the tight junctions.
- Dora Tang (Max Planck Institute of Molecular Biology and Genetics, Dresden) on enzymatic reaction in coacervates.

Research Group: Order and Disorder in Driven Systems
(since January 2021, Head: Dr. Marko Popovic)

Our research group "Order and Disorder in Driven Systems" was established in January 2021. We are interested in understanding mechanical and rheological properties of developing biological tissues. While a significant part of our research interest involves fundamental problems in physics of non-equilibrium mechanical systems we also closely collaborate with several biological research groups. Here we outline our ongoing research projects.

Rheology of proliferating tissues In absence of mechanical or thermal noise, cellular materials are yield stress materials, as we have recently shown on the example of the vertex model of epithelial tissues [1]. However, such description does not account for the activity present in the living systems whereby active cellular processes, such as cell divisions, introduce fluctuations in mechanical stress. Interestingly, such mechanical fluctuations are fundamentally different from thermal fluctuations as they are driven by biological processes in cells. In this project we use vertex model simulations and mesoscopic elasto-plastic models that were originally developed to study the yielding transition in amorphous solids. Our current results show that fluidisation of the yield stress state by cell divisions is significantly stronger in comparison to the exponentially suppressed fluidisation by thermal fluctuations in amorphous solids which we recently described [2]. This could account for the fluid-like behaviour of proliferating tissues on developmental time-scales. Finally, we aim to extend the relationship between statistics of epithelial tissue geometry and mechanical state we established in [1] to active tissues, which will provide a non-invasive method to distinguish plastic and fluid regimes of tissue flow.

Random yielding transition Yielding transition is a dynamical phase transition observed in athermal amorphous solids that plastically flow beyond a critical value of imposed shear stress Σ_c. Recently it was pointed out that the classical yielding transition can be generalised by introducing a finite correlation length of the imposed driving stresses, where the homogeneous shear driving corresponds to an infinite correlation length. In this project we use the vertex model of epithelial tissues to study the opposite limit, denoted random yielding transition, in which each cell in the tissue is driven by an independent randomly oriented force. The random yielding transition setting can be easily generalised to curved manifolds, such as spheres, which are relevant in biological context. Furthermore, this will allow us to study the influence of curvature and topology on critical exponents of the transition. Finally, motivated by cell polarity systems in biological tissues, we aim to introduce a short range alignment coupling between the orientations of driving forces. The resulting competition between the cell polarity coupling and random driving will produce a self-organised polarity correlation-length. Investigation of the corresponding tissue states ranging from uniform translation or rotation to a disorderly flowing phase should allow us to elucidate experimental observations of complex dynamics of multicellular spheroids performed by our collaborators in the group of Anne Grapin-Botton at MPI-CBG.

Mechanics of cell divisions in growing tissues Cell divisions are essential to growth and maintenance of biological tissues. As mentioned above, cell divisions are involved in fluidising tissues, thus allowing them to flow in response to an applied shear stress. In this project, on the other hand, we are interested in the interplay between cell divisions and mechanics of the surrounding epithelial tissue. Cell growth and anisotropic splitting during a division produce spatio-temporal fluctuations of isotropic stress. By charaterising theoretically the spectrum of this noise and relating it to fluctuations of cell size, our first aim is to establish a relationship between the state of tissue growth and the statistics of cell sizes. This

would allow us to distinguish growing from homeostatic tissues by simply imaging an epithelial tissue. Furthermore, biochemical regulation of cellular processes can respond to mechanical stresses, as we have shown recently in the fruit fly wing epithelium where it is responsible for generation of spatial patterns of cell shape and size [3]. Here, our second aim is to account for mechanosensitive response in regulation of cell division cycle and identify the resulting morphological and proliferation patterns that can be tested in experimental data.

Emergence of hexatic order in sheared 2d cellular systems Cellular configurations in biological tissues are typically disordered during development, which greatly facilitates significant shape changes they undergo. However, in collaboration with experimental group of Suzanne Eaton and Natalie Dye at MPI-CBG, we have found that in the developing fruit fly wing epithelium cells suddenly reorganise into a highly ordered state with a pronounced increase in the hexatic order parameter ψ_6 of cells in the tissue. Interestingly, this transition occurs by the end of the large scale shear flows that reshape the wing tissue. In this project we aim to understand how an imposed shear deformation of a cellular system leads to a transition from a disordered to an ordered state. Our current results indicate that in sheared cellular systems in absence of mechanical fluctuations the transition to the ordered state might be unavoidable. This suggests that a disordered state in biological tissues needs to be actively maintained. Therefore, it will be important to understand how the balance of active biological fluctuations and mechanical driving allows developing tissues to control the onset of the ordered state.

Collaborations:

Theoretical collaborations:

- Matthieu Wyart (EPFL, Lausanne, Switzerland) on activated flow of amorphous solids
- Frank Jülicher (MPI-PKS, Dresden, Germany) on mechanics and patterning of developing fruit fly wing and active rotations of cellular spheroids
- Guillaume Salbreux (Universtié de Genéve, Genéve, Switzerland) on active rotations of nematics

Experimental collaborations:

- Natalie Dye (Physics of life, TU Dresden, Germany) on mechanics and patterning of developing fruit fly wing
- Andrew Oates (EPFL, Lausanne, Switzerland) on robustness of symmetric somite formation in zebrafish embryo
- Anne Grapin-Botton (MPI-CBG, Dresden, Germany) on active rotations of cellular spheroids

[1] Popović M., Druelle V., Dye N. A., Jülicher F., Wyart M. New J. Phys. **23.3** (2021) 033004
[2] Popović M., de Geus T. W., Ji W., Wyart M. Phys. Rev. E, **104(2)** (2021) 025010
[3] Dye N. A., Popović M., Iyer K. V., Fuhrmann J. F., Piscitello-Gómez R., Eaton S., Jülicher F. Elife **10** (2021), e57964

1.9 Groups

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

The group Self-organization of biological structures started in September 2013 and aims to uncover the principles of how cellular compartments emerge from the collective behavior of individual molecules. Current research in my group is centered around two general questions, both aiming at understanding the emergence of cellular compartmentalization. First, we are studying how the size and shape of spindles arise from the interplay of mechanics, microtubule nucleation, and motor activities, and how these properties are regulated during early development and determine cytoplasmic compartmentalization. Second, we want to understand the principles that govern active chromatin organization in the nucleus, a question that has been largely ignored from the physical point of view. My group has shown key aspects of microtubule nucleation, spindle shape and mechanics, and scaling in embryos and artificial cell-like compartments. We have provided the first direct proof of DNA loop extrusion in a cellular context by reconstituting

and visualizing this process on single DNA molecules in cell extracts using single molecule microscopy. We also have shown that capillary forces driven by transcription factors lead to the emergence of DNA condensates, providing a new physical principle that could explain how distant DNA sequences meet to initiate and regulate transcription in the nucleus. Both research directions synergize and benefit from our strong expertise in theory, quantitative microscopy, biophysical approaches, and reconstitution. Below I provide a description of the most relevant research areas we currently investigate

Mechanisms of spindle scaling and orientation. Reductions in cell size during early animal development require that intracellular structures adjust their size accordingly. The mitotic spindle is a microtubule-based structure that robustly segregates chromosomes over a large range of cellular volumes. However, we still lack a mechanistic understanding of the microtubule-based processes regulating spindle relative to cell size. We developed a high-resolution microscopy-based assay to systematically quantify, for the first time, microtubule dynamics, nucleation and 3D organization in spindles over a large range of sizes in early zebrafish embryos. We discovered a hierarchical regulation of spindle scaling with cell size. In large cells, microtubule nucleation exclusively scales spindle size relative to cell size by changing microtubule number. In small cells, microtubule-dynamics additionally fine-tune spindle size by modulating microtubule length, though not sufficiently to account for spindle scaling alone. Our data, in combination with theory, support a model in which component limitation of microtubule nucleators and membrane partitioning of a nucleation inhibitor quantitatively explains both the exact scaling of spindles with cell size, and also the hierarchical regulation of microtubule nucleation and dynamics. In the future, we want to use the methods we developed to reconstitute the early embryo reduction divisions using encapsulated cycling egg extracts in physiological membranes. These extracts self-organize into 'cell-like' compartments that partition the cytoplasm and autonomously go through the cell cycle forming large scale mitotic waves that lead to surprisingly uniform partitioning. This experiments in combination with theory will allow us to dissect the physical principles that mediate spindle scaling, how orientation of spindles and centering depends on geometrical cues, and what self-organization principles determine the patterns of actin and microtubules in the cell boundary.

Theory and simulations of spindle morphology. The combination of theory and experiments allowed us to show that microtubule nucleation is autocatalytic and spatially regulated. 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). For example, this phenomena leads to self-organized patterns of microtubule growth in autonomously cycling extracts, with wavelengths similar to an embryo, suggesting a limit of how spatial information can be transmitted and synchronized in embryos. Similarly, we have shown that material properties in spindles are key to understanding microtubule flows in Xenopus egg extract spindles. In particular, we have shown that spindles undergo a sol-gel transition that is essential to drive polarity-independent flows and propagate stresses throughout the structure. Our work starts to provide a unified view of how self-organized flows are generated in the spindle. In the future, we will incorporate motor activities and autocatalytic microtubule growth into a continuum theory and a microscopic simulation that recapitulates not only the assembly of the entire spindle and scaling but also explores the phase space of the interplay between motor activities and autocatalytic growth in determining spatial compartmentalization driven by mitotic waves.

The role of transcription factor-mediated capillary forces in organizing chromatin. Proximity of enhancer regions and gene promoters drive transcription in cells and embryos. However, how transcription factors, co-factors, and general transcriptional machinery work in concert to physically cluster DNA remains unclear. We have developed a new assay that combines quantitative microscopy and in vitro reconstitution to visualize the interactions between single DNA molecules and the pioneering transcription factor FoxA1. Using this assay we have shown that FoxA1 binds DNA and can mediate the nucleation of DNA condensates via a first-order phase transition. Surprisingly, after formation, DNA condensates exert capillary forces on the remaining non-condensed strand. These findings could represent a possible mechanism to facilitate enhancer–promoter contacts, and play a more general role in DNA compaction and chromatin rigidity. However, the physics of protein-DNA condensation in the chromatin fiber are completely unexplored. In the future, we aim to investigate protein-DNA co-condensation in the context of single molecule chromatin: how chromatin influences capillary forces, size and nucleation of condensates; how condensation affects the specificity of transcription factors; and how different types of

condensates compete for available chromatin.

Physical mechanisms of DNA loop extrusion reconstituted in single DNA molecules. Loop extrusion by structural maintenance of chromosomes complexes (SMCs) has been proposed as a mechanism to organize chromatin during the cell cycle. However, the requirements for chromatin organization in these cell phases are very different, and it was unknown whether loop extrusion dynamics and the complexes that extrude them also differ. We used Xenopus egg extracts to reconstitute and image for the first time loop extrusion of single DNA molecules in a cellular context during the cell cycle. Our work showed that loop extrusion is a general mechanism for the organization of DNA, with dynamic and structural properties that are molecularly regulated during the cell cycle. However, in light of our discovery of transcription factor-mediated DNA condensation—that generate similar forces—these two mechanisms may self-organize in the nucleus. For example, protein-mediated DNA condensation may act as a roadblock and interfere with loop extrusion. Alternatively, loops formed may be further stabilized by capillary forces within the loop. We will use our assays to investigate the interplay between these two processes, and extend our theory of protein-DNA co-condensation to include activity driven by loop extrusion. The synergy between transcription factor-mediated DNA co-condensation and loop formation may be a general mechanism to organize transcription in the nucleus. Because cell extracts are transcriptionally active upon titration of nucleosomes, these experiments will allow to increase the complexity of our experimental system to reconstitute chromatin domains, and to correlate loop formation with gene expression.

Characterizing emergent properties of chromatin reconstituted in synthetic nuclei. We have developed an assay to reconstitute functional nuclei in encapsulated extracts (synthetic nuclei). We aim to use this assay in combination with quantitative imaging and mechanical measurements, to understand how molecular activities give rise to the emergent physical properties of chromatin. Our assay allows to precisely control the amount of genetic material per synthetic nucleus, titrations of components, and size of synthetic nuclei. Tuning the length of DNA will allow to investigate whether the viscoelastic behaviors of synthetic nuclei scale with polymer length as expected from equilibrium polymer physics and how those behaviors deviate in the presence of active chromatin processes. To study emergent physical properties of chromatin from molecular activities, we aim to combine passive two-point microrheology and active rheology measurements in chromatin. However, combining this type of measurements in cells is challenging, and has not been performed in chromatin. We will exploit mechanical accessibility of extracts to disentangle active and passive contributions to the physical properties of chromatin by combining two-point microrheology with active rheology. As an ultimate goal to this research line, we will investigate the impact of chromatin material properties and DNA-condensation on transcription by reconstituting it in synthetic nuclei.

Collaborations

- Nadine Vastenhouw (University of Lausanne, Switzerland)
- Christoph Zechner (CSBD Dresden)
- Tony Hyman (MPI-CBG Dresden)
- Stephan Grill (MPI-CBG Dresden)
- Frank Jülicher (mpi**pks** Dresden)

Research Group: Correlations and Topology
(since September 2020, Head: Dr. Ashley Cook)

The Correlations and Topology research group focuses on the interplay between correlation effects in electronic systems and their relation to topologically-nontrivial phases of matter, or those phases of matter unaffected by sufficiently small perturbations. In particular, the group has two main directions. First, the group specializes in introducing novel topological phases of matter into the literature. While topological phases of matter were first studied in the early 1980's in earnest with discovery of the integer quantum Hall effect, the group has made significant advances by returning to the foundations of this area of research. We have introduced a variety of novel topological phases, including the topological skyrmion phases and multiplicative phases (the latter of which is summarized in the report). Second, the group focuses on experimental realization of correlated and topological phases of matter, and is the only hard condensed matter group at mpi**pks** with the explicit goal of supporting experimentalists at MPI CPfS.

More specifically, recent work includes (i) characterizing two kinds of bulk-boundary correspondence for topological skyrmion phases of matter, confirming that a key assumption of many foundational works on topological condensed matter known as the flat-band limit assumption, that effectively non-interacting topological phase transitions always occur with closing of a direct band gap, does not hold, (ii) introducing multiplicative topological phases of matter, which may be characterized by Hamiltonians with a symmetry-protected tensor product structure and can combine topology of disparate topological phases, (iii) providing evidence in support of transport studies of AgCrSe2 that the material displays a near-quantized quantum anomalous Hall response due to effects of Rashba spin-orbit coupling, and (iv) characterizing previously-overlooked topological phases due to additional effects of open-boundary conditions on bulk-boundary correspondence, which also shows the flat-band limit assumption does not hold even for non-interacting systems and applies to virtually all known topological phases of matter.

Max Planck Research Group: Self-Organisation of Multicellular Systems
(since January 2021, Head: Dr. Pierre Haas)

The Max Planck research group "Self-Organisation of Multicellular Systems" was established at mpi**pks** in January 2021, and is jointly affiliated with MPI-CBG and based at the Center for Systems Biology Dresden. The theoretical research of the group focuses, often in close collaboration with experimental groups in Dresden and farther afield, on the biomechanics of cell sheets and their regulation in development. This research programme divides into two strands:

(Continuum) Mechanics of Biological Tissues. Biological tissues do not obey the constitutive equations of classical continuum mechanics, not only because living systems are active and out of thermodynamic equilibrium, but also because of (i) large geometric deformations specific to biological tissues, and (ii) constitutive peculiarities resulting from the underlying cell-level mechanics. Our continuum models for these effects, which we discuss in more detail below, thus answer fundamental physical questions, in particular by revealing how tissue-scale rheology emerges from cell-scale mechanics. This bridging of scales—which is not possible within discrete cell-based models that obfuscate the physical principles at the tissue level by their very definition—complements recent efforts by other groups, both at the CSBD and elsewhere, at learning physical equations from experimental data by providing mechanistic understanding of such equations. Moreover, understanding these equilibrium effects is necessary for moving beyond a mere qualitative comparison of biological experiment and physical theory to the more quantitative understanding that is enabled, on the experimental side, by ever increasing amounts of biological data at ever increasing temporal and spatial resolutions.

(i) *Large geometric deformations* specific to biological tissues break underlying assumptions of classical continuum theories. Examples of such deformations include apical constriction and internal rearrangements from cell intercalations. On the latter, we collaborate with the group of Pavel Tomancak at MPI-CBG in the context of *Tribolium* epiboly. The former is associated with "large bending deformations" in which a radius of curvature of a cell sheet becomes comparable to its thickness. We have recently derived an elastic shell theory for this new, biological scaling limit: its predictions differ even qualitatively from those of a classical shell theory, which stresses the importance of these geometric effects.

(ii) The *constitutive equations* of biological tissues are taken from a family of nonlinear constitutive relations wider than those of classical continuum mechanics. Indeed, we have shown that the one-dimensional continuum limit of a simple discrete model of a cell sheet involves nonelastic, nonlocal terms. We are now exploring how such nonclassical behaviour arises in more biologically relevant models, too. In particular, two-dimensional continuum limits will include a tensorial coupling of in-plane deformations associated with cell neighbour exchanges, which we will seek to elucidate in the longer term.

We also contribute more widely to developing a physical framework for the poorly understood triple interplay of mechanics, hydraulics, and biochemistry that underlies morphogenesis. Such a framework must balance representing the tissue-scale contributions of complex subcellular structures necessary for morphogenesis with the simplicity that allows physical understanding. In this context, we collaborate with the group of Marino Zerial at MPI-CBG on the mechanical role of recently discovered subcellular apical structures termed "bulkheads" in the formation of the bile canaliculi during liver morphogenesis.

Robustness and Variability of Development. How is robust development compatible with the huge variability of biological systems? This is a fundamental biological problem, and the mechanisms underlying the exquisite precision of morphogen signalling have indeed been analysed in detail, but the role and importance of mechanics for robustness have remained unexplored: what are the mechanical limits of cell sheet folding during development? How does the actual variability of such morphogenetic processes compare to that which is allowed mechanically? We have previously provided proof-of-principle of extracting physical information from this experimental variability, but answering these questions requires an even more quantitative framework of experiments, mechanical models, and inference. Building on our recent developments of biological continuum mechanics, we are now developing such a framework for the inversion of the green alga *Volvox* within our long-standing collaboration on *Volvox* mechanobiology with Stephanie Höhn and Ray Goldstein (University of Cambridge).

The group also has wider interests in theoretical ecology and more abstract problems related to the physics of complex systems:

Theoretical Ecology of Phenotypic Variation. Forty years ago, May argued that random ecological communities are overwhelmingly likely to be unstable. Ever since, theoretical ecology has been seeking to identify those structures that allow actual ecological communities to overcome this statistical constraint. We have recently shown, as have others independently, that the subpopulations resulting from phenotypic variation are one such structure, and we have since been analysing the dynamics of phenotypic switching in more detail: for example, in very recent work, we have revealed that phenotypic switching in response to competitors adds novel dynamics even to simple two-species models.

Complex Systems: Turing Instabilities and Beyond. Models of complex physical systems, be they biological tissues or ecological communities, are inherently and implicitly low-dimensional averages of very high-dimensional systems. From this abstract point of view, our results on phenotypic variation show, however, that subpopulation dynamics cannot in general be averaged out. This observation led us to start thinking about this averaging more generally. In this context, we have recently shown how the usual simplification of neglecting slow diffusers in reaction-diffusion systems generically leads to incorrect predictions of their Turing instabilities.

Experimental collaborations

- Pavel Tomancak (MPI-CBG), on the mechanics of cell intercalation during epiboly in *Tribolium*;
- Marino Zerial (MPI-CBG), on the mechanics of bile canaliculi formation during liver development;
- Stephanie Höhn and Ray Goldstein (University of Cambridge), on the inversion of the alga *Volvox*;
- Nuno Oliveira (University of Cambridge), on the ecology of bacterial persistence.

Research Group: Computational Biology and Evolutionary Genomics
(until February 2021, Head: Dr. Michael Hiller)

Since Oct 2011, our research group is jointly affiliated with the mpi**pks** and the MPI-CBG as part of the Center for Systems Biology Dresden (CSBD), which is a joint initiative of both Max Planck Institutes. The 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. Thus, we aim at contributing to our understanding how nature's incredible diversity has evolved at the molecular level.

In order to discover the genomic changes that underlie phenotypic changes between species, my group has developed several new computational methods that accurately detect functionally-relevant changes in genes or in regulatory elements. Application of these methods to genomes of mammals led to a number of insights into the genomic basis of trait differences. Since the last advisory board meeting in 2019, we published new studies showing that key immune-related genes such as the major bacterial flagellin sensor TLR5 are repeatedly lost in mammals (Sharma et al. MBE, 2020), highlighting an unexpected variability in genes that are thought to fulfill essential roles. Similarly, we discovered mammalian losses of genes that are cause disease phenotypes when mutated in humans, yet the mammals that naturally lost these genes show no disease-like symptoms (Sharma & Hiller, NAR Genomics and Bioinformatics, 2019).

In the last years, my lab also became an important contributor to the international Bat1K project that aims at sequencing the genomes of all bats and understanding the molecular basis of their unique traits. As detailed in Research Report 1, my lab generated highly-complete gene annotations of the first six genomes that were generated in this project. Furthermore, using the methods repertoire that we developed and established during the last years, we performed comprehensive comparative analysis that generated insights into the genomic changes that could be involved in the unique immune system of bats and the evolution of echolocation. These results were published in Nature 2020. We continue to work closely with the growing Bat1K community in utilizing our expertise in genome annotation and analysis in uncovering the molecular secrets in this interesting group of mammals.

Another major achievement was the development of TOGA (Tool to infer Orthologs from Genome Alignments), the first method that integrates gene annotation and ortholog inference. TOGA implements a novel methodology to infer orthologous genes that does not rely on coding sequences. Instead TOGA uses machine learning to distinguish orthologs from paralogs or processed pseudogenes based on alignments of intronic and intergenic regions, achieving a higher accuracy than state-of-the-art methods. TOGA scales to hundreds of genomes, which we demonstrated by applying it to >450 mammals and >400 birds, creating the largest comparative dataset so far. TOGA also integrates the detection of gene losses and generates accurate codon alignments for positive selection screens. These properties make TOGA a powerful and scalable method to annotate and compare genes in the genomic era. While we are just finishing the publication, the method is already used by dozens of groups world-wide.

Michael Hiller received two offers for W3 professorships and joined in Sep 2020 the LOEWE Center for Translational Biodiversity Genomics in Frankfurt with a joined appointment at the Senckenberg Research Institute and the Goethe University.

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. A good example is the weather, which is subject to clear and easily understandable seasonality, but which poses severe challenges when we want to predict the irregular deviations from 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 the characterization, modelling, understanding, and prediction of fluctuations in open classical systems, and using this methodology to study specific systems and phenomena.

This comprises research in non-equilibrium statistical mechanics, low- and high-dimensional dynamical systems, nonlinear stochastic processes driven by Gaussian and non-Gaussian noises. A particular field of application is our atmosphere and climate, a very complex driven dynamical system where predictions of short and long time spans are of the utmost general interest. An issue of continual interest in the context of climate change is the suspected 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 We have continued our work on the statistical verification of long range temporal correlations (LRC) in data and in model processes. One key area in which progress has been made has been on understanding how typical time scales, (which are generally related to exponential relaxation or to periodic oscillations), influence the signatures of statistics which are designed to quantify LRC. While many of the model processes have Gaussian distributions, the observed data generally does not. One such example is precipitation data, where there are no negative values, there is a huge peak at zero, and there are outliers with large values. We have designed a data model for such data which relies on the transformation of a Gaussian LRC process onto the non-Gaussian distribution, under control of the correlation structure. Details can be found in Sec.2.24.

Models with anomalous statistical properties - violations of the central limit theorem Anomalous diffusion can have several root causes, among them the aforementioned LRC, and therefore there is also a multitude of stochastic models which give rise to anomalous scaling. We continue our efforts to understand the properties and quantify such phenomena in different models. If in an experiment one observes anomalous scaling of the mean squared displacement, it is relevant to identify which of the different models is most appropriate to describe the phenomenon. In a recent study of oceanic tracers, we were able to identify

that fractional Brownian motion is a good model for oceanic transport, since it also reproduces the observed first passage time distribution. We also participated in the AnDi-challenge, which had the goal to design a set of criteria in order to distinguish between quite different model classes for anomalous diffusion.

ENSO, heat waves, flood risk, the growing season, and the first frost in autumn: Within the European ITN CAFE *Climate advanced forecasting of sub-seasonal extremes* we study the predictability of the El Niño Southern Oscillation (ENSO) phenomenon as well as related flood risk in South America and in Africa. We have introduced a new type of surrogate data for the assessment of ENSO forecasts, in collaboration with scientists from the Munich Re re-insurance company. A second topic which has been studied in co-supervision with colleagues of the European Centre for Medium Range Weather Forecasts (ECMWF) in Reading, UK, is about European heat waves. Similar in spirit are our investigations of flood risk in China, and a forecast scheme of the beginning of the growing season in Germany. Still ongoing is a PhD thesis on the prediction of the first frost in autumn. All these projects have in common that they combine long data records from observed meteorological quantities with statistical modelling and forecasting, i.e., they are in the field of big data and statistical learning. For the analysis of flood risk and heavy precipitation, Extreme Value Theory plays a relevant role: Due to the rareness of really extreme events ("the century flood") one needs sophisticated extrapolation methods to determine reliable values for the probabilities of outliers which are larger than the largest observed event in the data set. In the PhD thesis of Katja Polotzek we made exciting progress in the robust estimation of these return levels.

Network analysis of the evolution of astrophysical knowledge Colleagues from the MPI for the history of science have compiled a corpus of students' textbooks of early modern times. We perform a network analysis which is designed to reveal the process of the evolution of knowledge, more precisely the diversification of knowledge, its spreading across Europe, and its consolidation. We report on this work in more detail in Sec.2.25.

Machine learning Following the recent hype in machine learning, we have begun an attempt to understand the performance of reservoir computing. This denotes a recurrent neural network where the random weights in the internal layers are fixed and where the training phase exclusively optimizes the output weights. Being recurrent, the system has a time dependent internal state and hence is not an instantaneous input-output model. It is reported to be a very powerful forecasting scheme. We intend to understand the relevance of the internal state, and we want to drive it to the limits of modelling: We use it to forecast an electrocardiogram (ECG) signal. Such a signal consists of a sequence of very sharp peaks which represent the contractions of the ventricles, and has much smoother waves which reflect the re-polarization of the heart muscle. This separation of time scales and in particular the sharpness of the peak make it hard to set up a dynamical, oscillator-like model for the heart.

Collaborations

- Eli Barkai (Bar Ilan, Israel), Aleksei Chechkin (Charkov, Ukraine), Ralf Metzler (Potsdam), Trifce Sandev (Skopje), Alexander Iomin (Haifa), Erez Aghion (Boston), Kevin Bassler (Houston): Projects related to anomalous diffusion.
- CAFE project: A European ITN on medium range prediction on extreme weather events, coordinated by Alvaro Corral in Barcelona with colleagues from Spain, France, UK, Uruguay, and Germany, including Munich Re as a company. Co-supervising a PhD student at the European Centre for Medium Range Weather Forecast ECMWF in Reading, UK.
- Fluctuations in the electric power grid: Marc Timme (TU Dresden), Dirk Witthaut (University Cologne), Mernaz Anvari (PIK Potsdam), Benjamin Schäfer (NMBU Oslo), Christian Beck (QMUL London).
- Meagan Carney (Brisbane, Australia) and Matthew Nicols (Houston): Hurricane model and storm tracking.
- Imre Janosi (Budapest, Hungary) and Jason Gallas (Paraíba, Brasil): collaboration on oceanic transport.
- Roland Ketzmerick, Physics Department, Technical University of Dresden: Chaos and intermittency in Hamiltonian systems.

Research Group: Ultrafast Laser-Matter Interaction
(until November 2019, Head: Dr. Alexandra Landsman)

Overview 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 involved 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).

The group was funded for 5 years, and after the end of this period, the group leader moved on to the Associate Professor position at the Ohio State University in the USA. There, she is currently leading a group of two graduate students and a postdoctoral fellow.

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 activities, each with a representative publication cited.

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 momenta distributions or HHG spectra can be used to reconstruct the interaction between strong ultrafast laser pulses and atoms, molecules and condensed matter systems [2].

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 Schrodinger 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 [2].

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 [3].

[1] S. Han, et al, Nature Communications **10** (2019) 1-6.
[2] S. Biswas, et al, Nature Physics **16** (2020) 778.
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Max Planck Research Group: Quantum Many-Body Systems
(until February 2021, Head: Dr. Anne Nielsen)

The independent Max Planck Research Group "Quantum Many-Body Systems" was established in January 2016 and was active until February 2021. The group studies the collective behavior of strongly-correlated quantum many-body systems. We are particularly interested in topological properties, non-thermal behaviors, and non-periodic 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 exchange properties. The size is important, e.g., because the anyons

need to be well-separated, when they are exchanged, to obtain robust results. 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 exist in dimensions between one and two and on quasicrystals. We have also shown how one can use an optimized potential to reduce the size of an anyon, which makes it easier to meet the requirement of well-separated anyons during exchange processes. As another example, we have shown that the creation of anyons in a system can be a helpful tool do detect topological phase transitions.

Nonthermal systems: Statistical physics describes how physical systems approach thermal equilibrium, and closed quantum systems typically thermalize through a mechanism explained by the eigenstate thermalization hypothesis. There are, however, examples of quantum systems that do not thermalize, and these are interesting, e.g., due to their ability to store quantum information. Many-body localization is an example of a strong violation of the eigenstate thermalization hypothesis, in which all states in the spectrum are nonthermal, and quantum many-body scars is an example of a weak violation, in which only a few states are nonthermal. We construct and analyze different types of quantum many-body scars, including some with topological order. We have found many-body localization on fractal lattices with a transition point that is in between the transition points for one and two dimensions. We have also proposed a different type of nonthermal system, which realizes a weak violation of many-body localization by embedding a critical state into a spectrum of many-body localized states.

Nonperiodic systems: We investigate how the properties of quantum many-body systems are affected by modifying the space on which the models are defined. In particular, we study quantum many-body systems on lattices in fractal dimensions, quasicrystals, and disordered systems. We have, e.g., studied different topological models on fractal lattices. An important difference compared to periodic lattices is that the fractal lattices have additional edges, which affect the physics. By studying the integer quantum Hall effect on quasicrystals, we have discovered an interesting type of topological transport states that live in the bulk, and we have shown that a significant fraction of all the states are of this type. This opens interesting perspectives for controlled transport in the bulk.

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 makes it easier to analyze the properties of the models accurately. The states are similar to matrix product states, but the matrices are infinite-dimensional. Using a similar approach, we have also analyzed interfaces between different fractional quantum Hall systems and constructed and analyzed interesting models in 1D and on ladders. We have also introduced a new type of tensor network states that we call field tensor network states, and we have provided evidence that they can describe chiral topological phases.

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.

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. We have, e.g., shown how one can use a continuous, weak measurement to detect phase transitions in strongly interacting quantum systems.

Research Group: Nonequilibrium Quantum Matter
(until September 2020, Head: Prof. Dr. Takashi Oka)

Overview The Joint Research Group *Nonequilibrium Quantum Matter* co-sponsored by the mpi**pks** and the MPI-CPfS was established in August 2015. As the group was a joint research group of two institutes, efforts were made to integrate the groups in both institutes. The goal of the group was to understand the nonequilibrium properties of correlated quantum systems as well as topological systems based on analytical and numerical methods, and to uncover and characterize new quantum states emerging in these systems. Problems ranging from topological band theory, quantum magnetism, and Mott insulators were studied.

The group was funded for 5 years until September 2020. In January 2020, the group leader became a Professor at the Institute of Solid State Physics at the University of Tokyo in Japan. During the report period, it hosted two postdocs (Shintaro Takayoshi (2018 to 2020), and Francesco Peronaci (2019 to 2020)), who have already moved out.

Quantum Coherent Transport and Correlation Effect in 2D Delafossite Materials As a bridging group between mpi**pks** and MPI-CPfS, we have made considerable effort to assist the experimental groups in MPI-CPfS. In the department of Andrew Mackenzie at MPI-CPfS, one group of materials under active research is the two-dimensional layered delafossites. In addition to writing several theoretical papers on these materials, we have worked on experiment-theory collaborative projects.

First, we have constructed a model that explains the formation of a replica band in the Mott layer discovered by angle resolved photoemission. Using the Kondo lattice Hamiltonian, we showed that the replicas arise because a hole created in the Mott layer moves to and propagates in the metallic layer while retaining the memory of the Mott layer's magnetism. This finding opened a new route to use the non-magnetic probe of photoemission to gain insights into the spin-susceptibility of correlated electron systems. In fact, this led to a theoretical proposal of a way to use STM to detect a single Majorana in Kitaev's chiral spin liquid. Second, with MPI-CPfS as well as Philip Moll at IMX-EPFL, we reported a new phase-coherent oscillation of out-of-plane magnetoresistance in the layered delafossites PdCoO2 and PtCoO2. The oscillation period is equivalent to that determined by the magnetic flux quantum, h/e, threading an area defined by the atomic interlayer separation and the sample width. We explained this result as a consequence of the in-plane quantum coherence of the electrons that leads to multi-channel interference when they tunnel to the inter-plane direction.

Floquet Engineering and Strong Field Physics Floquet engineering is a theoretical framework for the control of quantum systems using periodic driving. Recently, it has attracted interest in solid-state physics due to the rapid developments in laser and ultrafast spectroscopy techniques as well as application to various "quantum materials" hosting interesting exotic quantum properties. Using Floquet engineering, we studied the control of topological properties (anomalous Hall effect, etc.) in Dirac and Weyl semimetals, memory switching in strongly correlated materials, as well as collective effects (magnetism and superconductivity). We reported a new classification scheme of Floquet topological states using the Wilson loop formalism. In 2020, we reported a novel nonperturbative phenomenon induced by strong laser fields that we named the "twisted Schwinger effect". It occurs in the pair production of particles induced by rotating electric fields. We demonstrated that, surprisingly, the excitations become chirality dependent due to nonadiabatic geometric effects. We made two predictions based on this mechanism. One is the field-induced valley polarization in 2D Dirac materials. The second is the generation of a nonlinear spin current in 3D Dirac and Weyl materials, taking place in the nonperturbative regime of the electric fields. In collaboration with Zhe Wang, an experimentalist at HZDR Dresden (now a professor at TU Dortmund), we demonstrated the high harmonic generation in a 3D Dirac semimetal. We explained the nonlinearity in the THz regime as a consequence of the semiclassical carrier dynamics.

External collaborations

Theory

- Antoine Georges, College de France, France
- Kazuhiko Kuroki, Osaka Univ., Japan
- Masaya Nakagawa, Univ. of Tokyo, Japan
- Jianda Wu, Tsung-Dao Lee Institute, Shanghai Jiao Tong University, China
- Masafumi Udagawa, Gakushuin Univ. Japan

Experiment

- Philip Moll, IMX-EPFL, Switzerland
- Zhe Wang, HZDR Dresden, Germany
- Philip D. C. King, St. Andrews, UK

Max Planck Research Group: Strongly Correlated Light-Matter Systems
(Head: Dr. Francesco Piazza)

The research group "Strongly-Correlated Light-Matter Systems" was established in March 2017. It currently consists of two PhD students: Christian Johansen (since September 2018) and Mariano Bonifacio (since September 2020), and two postdocs: Tomasz Wasak (since June 2018) and Johannes Lang (since January 2019). Two postdocs just left: Ahana Chakraborty (moved to Rutgers in October 2021) and Peter Karpov (moved to LMU in November 2021).

General topic.— Our research area lies at the boundary between condensed matter physics 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 which implement variations of Quantum Electrodynamics (QED) in the strong-coupling regime. So far the focus has been mainly on ultracold atoms coupled to light in nanophotonics structures like optical waveguides or cavities. More recently, the scope has extended to include correlated electrons in solid state.

Approach.— We develop non-equilibrium field-theoretical methods, 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 applications in the control of material's properties as well as quantum nonlinear optics and metrology.

Controlling photon-mediated electron pairing by engineering the quantum state of light. Recently, it has become possible to couple electrons in materials to the quantum electromagnetic field of optical cavities. This realises a yet unexplored regime of QED, which is non-relativistic, non-vacuum, and strongly coupled. This new playground for quantum many-body physics is at the same time exciting and theoretically challenging to describe, requiring us to develop new approaches merging quantum optics, condensed matter, and quantum-field-theory. One main direction is to extend the light-based control of materials from classical to quantum electromagnetic fields.

The so far mostly investigated case is the one of superconductivity, where cavity photons mediate pairing between electrons. Photons are potentially a more interesting mediator with respect to the phonons of the standard Bardeen-Cooper-Schrieffer paradigm: We have recently discovered that cavity-photons mediate a novel type of non-BCS pairing which can be directly manipulated by injecting selected states of the electromagnetic field. This yet unexplored type of pairing is possible due to the very long range of photon-mediated interactions between electrons.

Many-body dynamics of polaron-polaritons. The above implementation of cavity QED within materials is also very exciting within the context of quantum optics and photonics. Indeed, the correlations in the material together with the strong coupling with light can be used to implement novel types of optical nonlinearities for single photons, with direct promise for light-source engineering and light-based quantum information processing. In this context, we have developed a systematic field-theoretical approach to the description the nonlinear driven-dissipative dynamics of exciton-polaron-polaritons in monolayer semiconductors, following recent experimental progress, especially with charge-tuneable transition metal dichalcogenides (TMDs). Our theory offers the first microscopic explanation of several features of the nonlinear dynamics which were recently observed experimentally in Atac Imamoglu's group at ETH.

Our formalism also recently allowed us to predict and characterize a novel type of coherent light source from 2D semiconductors: a Fermi-polaron laser, characterized by a low-threshold and a reduction of the emitted linewidth even below the exciton non-radiative decay scale, which is possible due to the many-body dressing with electrons and holes.

Superradiant Floquet polaritons. The creation of interacting polaritons having access to a macroscopic number of modes is essential for the study of thermodynamic phases of photons and complex types of order. The strong-coupling between matter and light, required to implement photon interactions, can be realized by reducing the electromagnetic-mode volume using optical cavities or evanescent fields. This task becomes more challenging if it needs to be achieved for a whole set of electromagnetic modes, which are in general separated in frequency. One solution is to shape the geometry such that a set of quasidegenerate electromagnetic modes is formed.

An alternative idea is to use a periodic modulation of the light-matter coupling with a frequency matching the mode spacing. We recently studied this Floquet protocol to generate multimode Floquet polaritons mixing a cavity-photon with a density excitation in a gas of ultracold atoms. The mutual interactions between those induce avoided crossings. Eventually, a low-lying polariton can be red-shifted to zero frequency and subsequently become undamped, corresponding to an instability towards a multimode superradiant phase with macroscopic occupation of the polariton. Interestingly, we found that this superradiant phase can show persistent oscillations, stabilized by the balance between the periodic modulation and the photon loss.

Light-induced quantum droplets of ultracold atoms The implementation of cavity QED in synthetic materials made of ultracold atoms offers the interesting possibility to engineer the gauge coupling between matter and light, thanks to the high degree of control over both photonic and atomic degrees of freedom. This allowed to explore several new scenarios for the many-body physics of open systems, that we recently summarized in a review article.

Among the different exotic types of light-induced macroscopic order that our group and others have studied, the formation of self-bound quantum droplets of atoms is currently in our focus. It is induced by the finite-range interactions mediated by cavity photons. Quantum droplets are currently intensively studied in other experimental platforms with ultracold dipolar gases and mixtures, and we are the first to predict and study these in the context of QED. The tunability of the range of the cavity-mediated interactions allows to access two different regimes. In the strongly glued regime, the interaction range exceeds the droplet size and the physics resembles the one of the standard Bose gas in an self-consistent external potential. In the opposite weakly glued regime, the energy depends much more strongly on the droplet density profile and pronounced metastability is found.

External collaborations

Theory

- Darrick Chang, ICFO Barcelona, Spain
- Sebastian Diehl, University of Cologne, Germany
- Dieter Jaksch, University of Hamburg, Germany
- Giovanna Morigi, University of Saarland, Germany
- Alessio Recati, University of Trento, Italy
- Helmut Ritsch, University of Innsbruck, Austria
- Richard Schmidt, MPQ Garching, Germany
- Michael Sentef, MPSD Hamburg, Germany

Experiment

- Jean-Philippe Brantut, EPFL Lausanne, Switzerland
- Tobias Donner, ETH Zurich, Switzerland
- Andreas Hemmerich, University of Hamburg, Germany
- Atac Imamoglu, ETH Zurich, Switzerland

Max Planck Research Group: Fractionalization and Topology in Quantum Matter
(Head: Dr. Inti Sodemann)

The research group Fractionalization and Topology in Quantum Matter was established at the mpi**pks** in September 2017. It currently consists of four PhD students (Oles Matsyshyn, Sebastian Mantilla, Peng

Rao, and Nikolaos Stefanidis) and two postdoctoral researchers (Li-kun Shi and Zhenjiu Wang - Zhenjiu is co-supervised with the group of Dr. David Luitz).

Our work deals with the interplay of strong interactions and topology in quantum matter. Our studies fall within three broad categories: (a) quantum transport, dynamical and optical phenomena involving Berry's phase, (b) fractionalized and topological phases of matter, particularly spin liquids and quantum Hall systems, and (c) non-perturbative approaches to strongly interacting phases of gapless fermions. We summarise below some of the recent research projects and findings over the last few years which are new relative to the previous scientific report :

Symmetry and Quantum Kinetics of the Non-linear Hall Effect. My work on the Non-linear Hall effect with Liang Fu (PRL 115, 216806 (2015)) triggered considerable theoretical and experimental activities to discover and further study this effect. Our original theory focused on the "intrinsic" contributions arising from the Berry curvature. In this project, together with visiting student Snehasish Nandy, we developed a quantum kinetic theory of "extrinsic" contributions, predicting and quantifying the contributions of the counterparts to the side-jump and skew-scattering effects to the non-linear Hall effect.

Cyclotron resonance inside the Mott gap: a fingerprint of emergent neutral fermions. The Spinon Fermi Surface is a fascinating state of matter featuring spin-charge separation in two dimensions and higher, and the emergence of a Fermi sea of spinons gauge-coupled to an emergent photon. The conclusive observation of this state in real materials has remained controversial to this date. Together with my student Peng Rao, we showed that in spite of behaving as an electrical insulator to charge transport, this state can display cyclotron resonance peaks reminiscent of a metal when it is subjected to a magnetic field. The observation of this phenomenon would provide a strong evidence for the presence of this state via relatively simple optical measurements in correlated materials.

Nonlinear Hall Acceleration and the Quantum Rectification Sum Rule. The intrinsic Non-linear Hall conductivity is proportional to a dipole moment of the Berry curvature of occupied states, but also to the scattering time, and, therefore, changes depending on sample quality. Together with my student Oles Matsyshyn, in this work, we elucidated a sum rule that allows to obtain the intrinsic Berry curvature dipole in a way that bypasses knowledge of the scattering rate. We showed that the integral over frequency of the Drude-like pole of the rectification conductivity is identical to the Berry curvature dipole and independent of the scattering rate. We also showed that the inter-band contributions to this sum-rule integrate to another purely geometric tensor entirely determined by the Berry phases of the bands, dubbed the Berry Phase Rectification Tensor.

Excitonic Laughlin States in Topological Insulator Flat Bands and Moiré Superlattice Materials. The recent discovery of a zoo of correlated insulators and superconductors in magic angle twisted bilayer graphene has triggered a race to understand and realize novel states of matter in these amazing systems. It has become clear that a key ingredient of the physics is the presence of topological flat bands with opposite Chern numbers. In this work we investigated an ideal model motivated by these systems, to study the competition of integer Chern magnets and analogues of fractional quantum Hall states. We showed that there is an interesting class of Laughlin states made from excitons which compete energetically with the integer Chern magnet even at total filling one and investigated the physical properties of these Excitonic Laughlin states.

Infinite Berry Curvature of Weyl Fermi Arcs. "Hot-spots" in momentum space where the Berry curvature diverges, such as Weyl and Dirac nodes, are of great interest because they lead to a variety of amusing and enhanced Berry phase effects in measurable quantities. In this work, together with Dennis Wawrzik, Jhih-Shih You, Jorge Facio, Jeroen van den Brink, we discovered a divergence of the Berry curvature over an entire line, dubbed the "hot-line", that occurs generically in the surface Brillouin zone of Weyl semimetals. These surfaces feature open Fermi surfaces, known as Fermi arcs. The hot-line is distinct from the Fermi arc itself but they are connected at the end of the Fermi arc. We studied the impact of these hot-lines on the non-linear Hall effect on Weyl semimetal slabs.

Theory of weak symmetry breaking of translations in Z2 topologically ordered states. Unlike short ranged entangled phases (trivial phases), fractionalized phases of matter can display much richer symmetry implementations such as "weak symmetry breaking". Phases with weak symmetry breaking have ground states that are perfectly symmetric under a symmetry group of the Hamiltonian, but whose quasiparticles break the symmetry. In this work we developed a theory of this phenomenon for the case of the lattice translational symmetry in Z_2 spin liquids. We utilized a recently developed exact lattice charge-flux attachment construction to provide exactly solvable models for this phenomenon and explained its

connection to the formation of states analogous to weak topological superconductors of spinons in the spin liquid.

The universal shear conductivity of electrons and spinons and its detection with NV centers. In this work we showed that the transverse conductivity of metals in the clean quasi-static limit is controlled entirely by the geometric shape of the Fermi surface and fundamental constants of nature. We also showed that a related behavior is also present in the spinon Fermi surface spin liquid state. This conductivity controls also the magnetic field noise generated by thermal and quantum fluctuations above 2D samples which can be measured with NV center spin qubits. We showed that in the right regime the decay rate of the spin qubit becomes universal and controlled by the geometric shape of the Fermi surface giving rise to the magnetic noise.

Rabi Regime of Current Rectification in Solids. We addressed here the question of the ultimate limit of current rectification in Bloch bands lacking inversion and time reversal symmetries in response to applied oscillating electric fields in the case when the lifetime of electron-hole recombination becomes very large. We showed that even in this "clean limit" there is a finite rectified rectified current, but which scales non-perturbatively with the amplitude of the driving electric field. This regime can be understood as one in which the electrons in the Bloch band become synchronized Rabi oscillators and provided a connection between this regime and the periodic Gibbs ensemble utilizing the Schwinger-Keldysh formalism.

Pseudoscalar U(1) spin liquids in α-$RuCl_3$. A recent experiment has reported the existence of oscillations of the thermal conductivity of the insulating magnet α-$RuCl_3$ under applied in plane field which are reminiscent of the quantum oscillations in metal. However the experiment also reported that these quantum oscillations can appear even when there is a symmetry that forbids the thermal Hall effect. To explain this we proposed the existence of an amusing variant of the traditional spinon Fermi surface state, where the emergent magnetic field is scalar and not pseudo-scalar. This field is allowed even in the presence of mirror symmetries that would forbid the Hall effect and could be behind the observed quantum oscillations in this material.

Collaborations

- Liang Fu, Department of Physics, Massachusetts Institute of Technology, USA.
- T. Senthil, Department of Physics, Massachusetts Institute of Technology, USA.
- Patrick Lee, Department of Physics, Massachusetts Institute of Technology, USA.
- Falko Pientka, Goethe-Universität Frankfurt, Germany.
- Jun Yong Khoo, Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore.
- Joseph Falson, Department of Applied Physics and Materials Science, Caltech, USA.
- Brian Skinner, Ohio State University, USA.
- Yan Sun, Max-Planck Institute for the Physical Chemistry of Solids, Germany.
- Roderich Moessner, Max-Planck Institute for the Physics of Complex Systems, Germany.
- Francesco Piazza, Max-Planck Institute for the Physics of Complex Systems, Germany.
- David Luitz, Max-Planck Institute for the Physics of Complex Systems, Germany.
- Jeroen van den Brink, Leibniz Institute for Solid State Physics, IFW Dresden, Germany.
- Dennis Wawrzik, Leibniz Institute for Solid State Physics, IFW Dresden, Germany.
- Jorge I. Facio, Leibniz Institute for Solid State Physics, IFW Dresden, Germany.
- Jhih-Shih You, National Taiwan Normal University, Taiwan.
- Po-Yao Chang, National Tsing Hua University, Taiwan.
- Zheng Zhu, Department of Physics, Massachusetts Institute of Technology, USA.
- Debanjan Chowdhury, Department of Physics, Cornell University, USA.
- Donna Sheng, Department of Physics and Astronomy, California State 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 active from 2010 to 2020 on the basis of the Max Planck Fellowship of Prof. Roland Ketzmerick (Technische Universität Dresden) for the purpose of strengthening the collaboration between TU Dresden and the mpi**pks**. The group was co-headed by Dr. André Eckardt, who was appointed to a W3 professorship at TU Berlin in 2020. The group was further supported by Prof. Arnd Bäcker from TU Dresden.

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. For scattering systems with partial escape we found an approximate classical description of their average phase-space distribution based on conditionally invariant measures of the classical dynamics. The fluctuations of individual resonance states around the multifractal average is found to be universal. 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 non-equilibrium properties of open quantum systems. On the one hand, we are interested in non-equilbrium steady states of driven-dissipative systems, such as open Floquet (i.e. time-periodically driven) systems, systems coupled to several baths of different temperatures, or pumped lossy photonic systems. Here, an important theme of our work is ordering and phase transitions in non-equilibrium steady states. We worked on the theoretical description of generalized forms of Bose condensation under non-equilibrium conditions. On the other hand, we are also interested in the transient relaxation dynamics of open quantum systems. For instance, we studied the impact of many-body localization (of the system alone) on the bath-induced relaxation to thermal equilibrium. Or, we showed that under certain conditions quantum systems coupled to a thermal bath can effectively forget their initial state long before having reached thermal equilibrium.

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 implement 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). A second major theme is the development of novel measurement schemes, where the far-from equilibrium dynamics of a system is monitored after a sudden quench (an abrupt change in the Hamiltonian). In a recent collaboration with the experimental group led by Monika Aidelsburger and Immanuel Bloch in Munich, we realized and probed so-called

anomalous Floquet topological band insulators, which are characterized by spatio-temporal winding numbers (without counterpart in static systems).

Collaborations

- 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.

- 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.
  - Prof. Monika Aidelsburger and Prof. Immanuel Bloch (LMU Munich) on probing anomalous Floquet topological insulators (within the DFG Research Unit FOR 2414).

- and with the theory groups of
  - Prof. Gediminas Juzeliunas and Prof. Egidijus Anisimovas (Vilnius University) on Floquet topological quantum systems.
  - Prof. Sergey Denisov (Oslo Metropolitan University) on Floquet engineering in open quantum systems.
  - Prof. Nathan Goldman (Unversité libre de Bruxelles) on probing anomalous Floquet topological insulators.
  - 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.
  - Prof. Haris Skokos (University of Cape Town, South Africa) on geometry of complex instability in galactic potentials.
  - Prof. Peter Schlagheck (University of Liege, Belgium) on the generation of highly entangled triple-NOON states in a driven Bose-Hubbard model.
  - Prof. Eduardo Altmann (University of Sydney, Australia) on classical and quantum aspects of open dynamical systems.

1.11 Advanced Study Groups

Advanced Study Group 2018/2019: Forecasting with Lyapunov Vectors
(Convenor: Prof. Marcus W Beims)

Nowadays, forecasting is undoubtedly one of the most required research directions in distinct areas, such as climate change, stock markets, critical transitions, extreme and rare events, including giant ocean

waves, extreme weather, and laser peaks, among others. Such realistic systems are complex systems making the forecasting task a challenging problem. The main scientific goal of the ASG was to study the applicability of the alignment of Lyapunov vectors for the prediction of large peaks and/or extreme events in general complex systems. It is known that for some systems, the alignment of the Lyapunov vectors may occur instants before the appearance of large peaks in chaotic time series [1]. Nevertheless, even if the time interval between the alignment and the peaks can be short, the alignment can still be used to predict the peaks. Significant improvements in such predictions were obtained in the ASG combining the alignment of Lyapunov vectors, bred vectors, machine learning procedures and classification techniques [7, 8].

Furthermore, a distinct but related line of research is the decomposition of nonlinear time series. A bottom-to-top procedure for the decomposition of time series was proposed [6] by smoothness-controlled cubic splines. We have successfully validated the procedure on a series of synthetically constructed composite signals. We illustrated the method's capability by reconstructing a synthetic signal composed of a chirp, a strong nonlinear background, and a large-amplitude additive noise, where all empirical mode decomposition-based algorithms fail spectacularly. Specifically, we demonstrated the efficiency of the method on two real signals: daily sea ice extent over the Arctic and over the Antarctic as determined by satellite image processing. In this way, we uncover distinct freezing-melting dynamics between the Arctic and the Antarctic.

The ASG brought together experts from relatively distinct areas to explore our proposal in a more general perspective, emphasising time series analysis and the alignment of Lyapunov vectors. Its convener was Marcus Werner (UFPR, Brazil) and the invited long-term members were Imre Jánosi (University of Public Service, Hungary) and Jason Gallas (UFPB, Brazil). A mini-workshop on Jan 22-23th provided an opportunity to present several ideas and have a brainstorming session among participants and members of the mpi**pks**. The ASG has also benefited from the visits of other scientists, which typically resulted in new collaborations and/or the invigorating/extension of existing ones: G. M. Ramírez-Ávila (UMSA, Bolivia), P. Lind (OMU, Norway), B. Hunt (UM, USA), T. Tel (LEU, Hungary), D.Weingaertner (UFPR, Brazil), H. Varela (USP, Brazil), J-C Garreau (UL, France) and PhD student E. L. Brugnago (UFPR, Brazil).

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Advanced Study Group 2019/2022: Open Quantum Systems Far From Equilibrium

(Convenor: Prof. Dr. Dr. h.c. mult. Peter Hänggi, University of Augsburg, Germany)

The idea of this Advanced Study Group consists in exploring the realm of open many-body quantum systems taken far out of equilibrium. As objects of studies, these systems are located on the interface of several, currently very active, research fields such as the physics of open quantum systems, many-body quantum physics, the role of heat and work in quantum thermodynamics, and, last but not least, computational quantum physics.

The group work was organized in three consecutive stages: December 2019 - January 2020 (first stage), June-August 2021 (second stage), and November 2021-January 2022 (third and final stage). The core members of the group are Peter Hänggi (University of Augsburg, Germany), Sergey Denisov (Oslo Metropolitan University, Norway), and Dario Poletti (Singapore University for Technology and Design).

Despite the problems caused by the COVID-19 pandemic, the group benefited from visits by other researchers and collaborators. Main visitors include Prof. Darius Chruściński (Nicolas Copernicus University, Torun), Prof. Karol Życzkowski and Dr. Wojciech Tarnowski (Jagellonian University, Cracow), Dr. Juzar Thingna (Center for Theoretical Physics of Complex Systems, Institute for Basic Science, South Korea), Prof. Dr. Mikhail Ivanchenko and Dr. Tetyana Laptyeva (Lobachevsky University of Nizhny Novgorod, Russia), and Dr. Alexander Schnell (TU Berlin). In addition, several mpi**pks** members engaged into the group's work, including David Luitz (leader of the group "Computational Quantum Many-body Physics") and Francesco Piazza (leader of the group "Strongly Correlated Light-Matter System").

The main objective of the ASG was to investigate manifestations of Dissipative Quantum Chaos, i.e., phenomena emerging for the dynamics of many-body open quantum when shifted far out of equilibrium.

The existing well-developed theory of Quantum Chaos addresses exclusively Hamiltonian systems; i.e., those are fully isolated from the influence of their environments. The corresponding theoretical predictions have been validated, by using, e.g., microwave billiards, ultracold atoms, and stylized quantum electronic circuits. However, with the emergence of new types of real-life quantum systems, such as optomechanical systems, microwave superconductive circuits, and polaritonic devices, the Hamiltonian idealization lost much of its appeal. Particularly, dissipation in these systems acts as a full-fledged generator of time-evolution, no less complex and diverse than the unitary evolution generated by quantum Hamiltonians. It therefore becomes necessary to understand the underlying physics of this very specific quantum evolution.

The ASG addressed the following challenges:

- What are the spectral signatures of Dissipative Quantum Chaos?
- Open periodically-modulated (Floquet) systems: do there exist effective time-independent Lindbladians?
- Quantum thermodynamics: How to measure transport of mass and charge in open many-body systems far from equilibrium? How to quantify physical quantities such as quantum "work" and "heat" which formally cannot be encoded in terms of quantum observables (but rather constitute quantum processes)?

Chapter 2

Selection of Research Results

2.1 Topological Magnons and Spin-Space Groups

A. Corticelli, P. A. McClarty, and R. Moessner

Since the discovery of topological insulators protected by time reversal symmetry around 15 years ago, symmetry has been central to the search for new types of topological materials. This search has been handsomely rewarded. To date, a bewildering variety of topological materials have been found or proposed protected by combinations of lattice symmetries and internal symmetries. The most complete classification scheme known to date is grounded in the theory of magnetic space groups that themselves classify all crystalline symmetries with or without time reversal symmetry. This implications of this classification scheme has been most explored in the context of electronic band structures but there is intense activity exploring topological band structures in other contexts.

Until recently the intersection between the study of spin waves in magnetically ordered materials and band topology was largely restricted to the realization of so-called Chern numbers in magnon bands. These arise rather naturally in magnetic systems in the total absence of symmetries. Yet, in the 1960's, long before the discovery of topology in band structures, Brinkman and Elliot recognized that magnons often have higher symmetry than even the magnetic space groups allow [1]. This is because spin rotation symmetries can act nontrivially in conjunction with crystalline and time reversal symmetries. The relevant groups are known as spin-space groups. In our recent work, we explored how spin-space groups can enrich band topology [2].

The simplest type of spin-space group arises in Heisenberg models that have a global spin rotation symmetry coming from $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ terms in the Hamiltonian. The magnetic Hamiltonian has some set of lattice symmetries whose elements are denoted $\{g|\boldsymbol{t}\}$ where g is a point group element acting both on space and spin degrees of freedom and $\boldsymbol{t}$ is a translation. This notation handles both pure point group elements as well as nonsymmorphic elements such as screw symmetries that involve a point group element combined with a non-Bravais translation. Spin-space elements are denoted $[R||\{g|\boldsymbol{t}\}]$ where, in addition to the space group element, there is a rotation element R that acts only on the spins. Finally, we include an anti-unitary time reversal symmetry element $\mathcal{T}$.

Now suppose the magnetic moments are long-range ordered. In other words, there is some non-vanishing expectation value for the local moments. For Heisenberg couplings and collinear structures, for example, all of the point group symmetries in the paramagnetic phase remain symmetries in the ordered phase because spin rotations can restore the ground state magnetic structure. In particular, this means that, while physical time reversal is broken by the magnetic order, time reversal times a spin rotation survives. This is an effective time reversal symmetry $\mathcal{T}^*$. This has important consequences for magnon band topology [2]. For example, in systems with an inversion symmetry $\mathcal{P}$, the resulting $\mathcal{PT}^*$ symmetry protects Dirac points and nodal lines and forces the Berry curvature to zero.

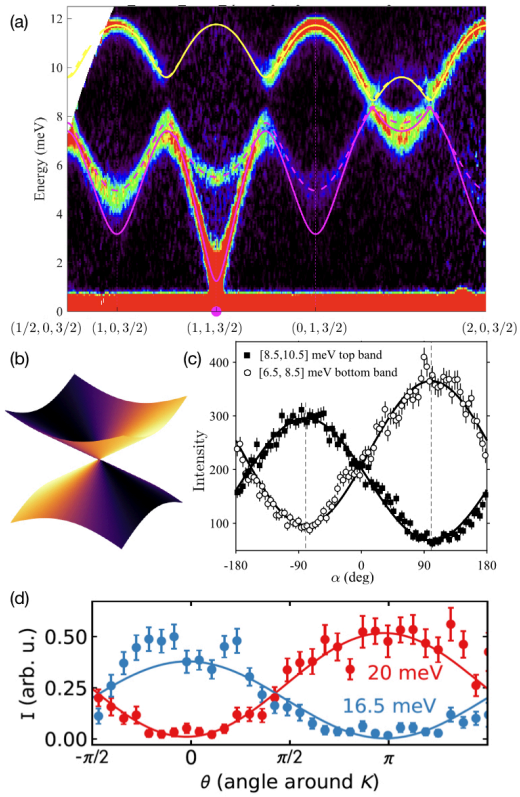

Figure 1: (a) Inelastic neutron scattering data on $CoTiO_3$ showing dispersing magnons and linear spin wave theory fit. The wavenumber cut passes through the nodal lines twice (arrows). (b) Characteristic pattern of intensity in the vicinity of the nodal lines. The intensity varies sinusoidally when encircling the nodal line and the winding is in antiphase in the upper and lower magnon bands. Data showing this intensity feature in $CoTiO_3$ (c) and in gadolinium (d).

Spin-space symmetries are crucial to the understanding of (magnon) band topology in a very wide range of materials. We give two examples from our recent work. The first is the material $CoTiO_3$. This is an ABC stacked honeycomb antiferromagnet. Spin-orbit coupling and trigonal local distortions of oxygen octahedra force the moments to lie in the plane and the dominant exchange is isotropic in the plane. There is then a spin-space symmetry. There is also effective time reversal. The crystal also has inversion symmetry and C_3. Altogether these force the presence of Dirac nodal lines running through

the zone corners in the $(0, 0, \ell)$ direction [3, 4]. Inelastic neutron scattering on this material resolves the dispersive spin wave excitations including the nodal lines (Fig. 1(a)).

The nodal lines are associated with a π winding number of the Berry phase around closed loops encircling the lines. This physics originates from an effective Hamiltonian in the vicinity of the nodal lines looking like $k_x\sigma_x + k_y\sigma_y$ where the pseudospins originate from the sublattice structure. In this Hamiltonian, spin and momentum are locked and this leads directly to a further observable signature, namely a universal winding of the neutron scattering intensity around the Dirac cones depicted in Fig. 1(b) [6]. This winding was clearly resolved in the experiment (Fig. 1(c)) [4].

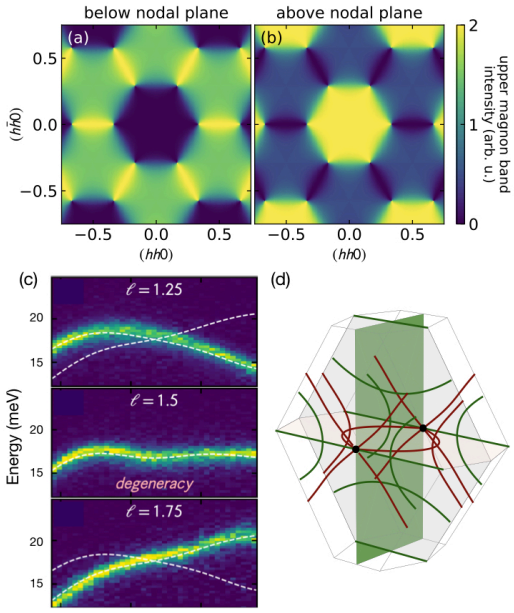

Figure 2: (a,b) Characteristic neutron intensity above and below the nodal surface in gadolinium. (c) Energy-momentum cuts at $\ell = 1.25, 1.75$ showing intersection of magnon bands at zone corner − cutting through a nodal line − and a nodal plane on the hexagonal Brillouin zone surface at $\ell = 1.5$. (d) Schematic of degeneracies in the four band magnon band structure of the hyperhoneycomb Kitaev-Heisenberg model in the Neel phase showing a nodal plane (dark green) with multiple nodal lines (red).

A second example is elemental gadolinium which, at low temperatures, is a collinear ferromagnet. Although this is a heavy element, the magnetic couplings are nearly isotropic because the orbital angular moment is quenched. Once again the spin-space symmetries ensure that there are nodal lines running along the hexagonal zone corners and these were recently observed experimentally by a group at Oakridge together with the predicted winding of the intensity (Fig. 1(d)) [5].

The experiment also revealed the presence of a nodal plane on the top and bottom surfaces of the zone where the two magnon bands become degenerate (Fig. 2(c)). This arises in this nearly Heisenberg system as a consequence of an effective time reversal symmetry times a two-fold screw with axis perpendicular to the triangular planes $[C_{2z}||\{C_{2z}|(0, 0, 1/2)\}]$ where the spin rotation is chosen to restore the moment direction. Breaking the spin-space symmetries lifts this degeneracy in general. Similarly to the nodal lines, the nodal plane has a characteristic intensity signature in inelastic neutron scattering. In particular, the intensity flips from high to low and vice versa in a given band on passing through the degenerate plane (Fig. 2(a,b)). This intensity flip comes from a discontinuous change in a nontrivial phase of the magnon wavefunctions when passing through the plane.

In the concrete examples we have given there is continuous spin rotation symmetry in the underlying magnetic Hamiltonian to a good approximation. One is led to ask whether spin-space groups can appear with discrete spin rotation symmetry. We recently showed that there are indeed such cases: in Heisenberg-Kitaev models where the spin part of the group is discrete rather than continuous and in certain models with anti-symmetric exchange [2]. To illustrate the relevance of these new kinds of spin-space symmetries we systematically explored such models on honeycomb and hyperhoneycomb lattices. Because the models are anisotropic, tuning the moment direction leads to a rich topological phase diagram based on a hierarchy of spin-space groups. An example is given in Fig. 2(d) for a Neel state on the hyperhoneycomb where the magnetic space group corresponding to the structure fails to capture features in the magnon spectrum. Instead, the discrete non-symmorphic spin-space group correctly gives the nodal plane degeneracy and allows for the presence of nodal lines.

An important future direction is to classify and tabulate all space-space groups with continuous and discrete symmetry. A significant step in this direction can be found in our paper where we directly compute for the spin-space groups under discussion the irreducible representations and character tables for all high symmetry points, lines and surfaces [2]. The methods exemplified there can be generalized to all spin-space groups.

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2.2 Non-Hermitian Kibble-Zurek mechanism with tunable complexity

BALAZS DORA, MARKUS HEYL, RODERICH MOESSNER, AND PENG XUE

Exceptional points (EPs) are ubiquitous in non-hermitian systems, and represent the complex counterpart of critical points. Driving a system through a critical point at finite rate induces defects, described by the Kibble-Zurek mechanism, which finds applications in diverse fields of physics. Here we generalize this to a ramp across an EP [1]. We find that adiabatic time evolution brings the system into an eigenstate of the final non-hermitian Hamiltonian and demonstrate that for a variety of drives through an EP, the defect density scales as $\tau^{-(d+z)\nu/(z\nu+1)}$ in terms of the usual critical exponents and $1/\tau$, the speed of the drive. Defect production is suppressed compared to the conventional hermitian case as the defect state can decay back to the ground state close to the EP.

We then use single-photon interferometry to realise this distinct scaling behaviour by simulating the defect production upon performing slow parameter ramps [2]. Importantly, we are able to provide access also to higher-order exceptional points. This work represents progress in extending Kibble-Zurek ideas to non-Hermitian settings, as well as in increasing the experimental complexity of non-Hermitian quantum time-evolution towards the many-body realm.

Background The Kibble-Zurek mechanism in quantum many-body systems applies to unitary real-time evolution. However, recent developments suggest rich features appearing for non-hermitian Hamiltonians describing intrinsically non-unitary dynamics, as recently realized also in experiments. While the eigenvalues of a non-hermitian Hamiltonian can still be interpreted in terms of energy bands, already the meaning of its eigenvectors cannot be treated conventionally as they are not orthogonal, and therefore possess finite overlap already in the absence of any additional perturbation. Particularly important in this context are EPs, where the complex spectrum becomes gapless. These can be regarded as the non-hermitian counterpart of conventional quantum critical points. At EPs, two (or more) complex eigenvalues and *eigenstates* coalesce, which then no longer form a complete basis.

Model, observables and realisations We consider Hamiltonians of the form

$$H = \sum_p H_p, \quad H_p = p\sigma_x + \Delta\sigma_y + i\Gamma\sigma_z \qquad (1)$$

which can be decomposed into different momentum sectors labeled by p. For $i\Gamma \in \mathbb{R}$ the problem is Hermitian. For $\Gamma \in \mathbb{R}$ instead, the above Hamiltonian becomes non-hermitian with a spectrum given by $E_\pm(p) = \pm\sqrt{p^2+\Delta^2-\Gamma^2}$. When $\Delta > \Gamma$, H_p has real eigenvalues for each p. For $\Gamma > \Delta$ on the other hand H_p, has, in general, complex eigenvalues. At sufficiently large $p > \sqrt{\Gamma^2-\Delta^2}$, however, the spectrum becomes real again. A Hamiltonian is $\mathcal{PT}$-symmetric if it commutes with the combined parity and time reversal operators. Consequently, the spectrum is $\mathcal{PT}$-symmetric and real for $\Delta > \Gamma$, while for $\Gamma > \Delta$, $\mathcal{PT}$-symmetry gets broken and the eigenvalues occur in complex pairs.

Non-Hermitian Hamiltonians of this kind can be emulated by optical waveguides, distributed-feedback structures, microcavities or electric circuits. Eq. (1) also accounts for the low energy dynamics of the quantum Ising chain in an imaginary transverse field or an imaginary mass fermion (i.e. tachyon) system. The last term in Eq. (1) assumes balanced gain and loss without loss of generality: one can shift the diagonal term in the Hamiltonian by any complex value without affecting the results.

Results We have studied the defect density – in theory and photonic experiment (Fig. 1) – generated by a ramp through an exceptional point, specifically for $\mathcal{PT}$-symmetric ramps, the fully non-Hermitian case, as well as the more complex higher-order exceptional points. Here, we present the results for $\mathcal{PT}$-symmetric case both in theory and experiment, where the instantaneous spectrum is always real. We choose $\Delta = \Delta_0$, $\Gamma = \Delta_0 t/\tau$ such that the time evolution ends exactly at an EP. We analyze the corresponding non-Hermitian Schrödinger equation with Eq. (1) both numerically and using scaling ideas and obtain the expectation value of the operator, which couples to the external drive, as

$$\langle\sigma_z(\tau)\rangle \sim \tau^{-2/3}, \qquad (2)$$

as shown in Fig. 2. The wavefunction for $t = \tau \to \infty$ agrees with the non-normalized right eigenfunction of the final non-Hermitian Hamiltonian.

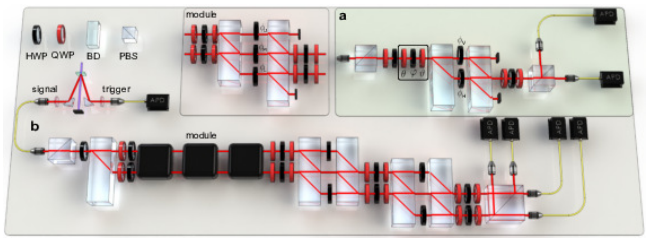

Figure 1: **Single-photon interferometer** for the nonunitary dynamics of (a) a single-qubit $\mathcal{PT}$-symmetric system and (b) a four-state qudit (consisting of spatial and polarisational degrees of freedom) for realising a higher-order exceptional point.

The gap in the instantaneous spectrum reads $\tilde{\Delta} = \Delta_0\sqrt{1-t^2/\tau^2} \approx \Delta_0\sqrt{2}\sqrt{(\tau-t)/\tau}$ for $t \sim \tau$. The distance from the critical point is $\hat{t} = \tau - t$, which is used to obtain the critical exponents $z\nu = 1/2$ from the scaling of the gap, $\tilde{\Delta} \sim |\hat{t}|^{z\nu}$. Then, the transition time separating a/diabatic dynamics is determined from $\tilde{\Delta}^2 \sim d\tilde{\Delta}/d\hat{t}$, which gives the transition time $\hat{t}_{\rm tr} \sim \tau^{1/3}$, in agreement with Kibble-Zurek scaling $t_{\rm tr} \sim \tau^{z\nu/(z\nu+1)}$.

Since the spectrum $\pm|p|$ is linearly gapless at the critical point, this defines $z = 1$, leaving us with $\nu = 1/2$ for the exponent of the correlation length. Therefore, the Kibble-Zurek scaling of the defect density in one dimension predicts $\sim \tau^{-d\nu/(z\nu+1)} = \tau^{-1/3}$ scaling, at odds with Eq. (2). We demonstrate that the correct exponent is indeed $-2/3$ and present a generalized Kibble-Zurek scaling to account for that.

Our numerical data indicates the following scaling of the momentum resolved defect density, $\sigma_z(p,\tau)$:

$$\sigma_z(p,\tau) = \frac{1}{(\tau\Delta_0)^{1/3}} f_{\rm PT}\left(\frac{p}{\Delta_0}(\tau\Delta_0)^{1/3}\right) \qquad (3)$$

with $f_{\rm PT}(x)$ a universal scaling function. Upon integrating this with respect to p the scaling of the defect density follows. In Eq. (3), the τ exponent $1/3$ originates from the $z\nu/(z\nu+1)$ combination of critical exponents and the p stems from the $z = 1$ dynamical critical exponents. Therefore, this expression is generalized to an arbitrary critical point for the momentum resolved defect density as

$$n(p,\tau) = \frac{1}{\tau^{z\nu/(z\nu+1)}} \tilde{f}_{\rm PT}\left(p^z \tau^{z\nu/(z\nu+1)}\right), \qquad (4)$$

which, after performing a d-dimensional momentum integral, gives $n \sim \tau^{-(d+z)\nu/(z\nu+1)}$. Notice the appearance of a τ dependent prefactor of the scaling functions in Eqs. (3) and (4). This is in contrast to the Hermitian case, where such non-trivial prefactors are absent.

We next provide two complementary explanations for this modified scaling. In an a/diabatic picture, excitations are created by populating the excited state similarly to Hermitian dynamics, but only its component perpendicular to the ground state represents defect production. As we approach the EP with increasing time, we enter into the diabatic regime at the transition time $\hat{t}_{\rm tr}$, where adiabatic time evolution breaks down, the dynamics gets frozen and defect production kicks in. The component of the excited state perpendicular to the ground state at this instance has an amplitude, parametrised as $\sin(\theta_p)$, as the ground and excited states are not orthogonal in general. The small momentum states close to the EP are the most sensitive to diabatic time evolution, as $\sin(\theta_{p\approx 0}) = \sqrt{\Delta^2-\Gamma^2}/\Delta \sim 1/\hat{t}_{\rm tr}$ at the adiabatic-diabatic transition: namely the angle becomes proportional to the energy gap. This results in a $\tau^{-z\nu/(z\nu+1)}$ suppression factor for the defect density. For the hermitian case, orthogonality ensures that $\sin(\theta) = 1$.

In a more dynamical picture, defects are created directly in the state perpendicular to the ground state, which decays to the ground state with a rate $1/\hat{t}_{\rm tr}$ reducing the Hermitian Kibble-Zurek scaling by the probability to remain in the perpendicular state, $1/\hat{t}_{\rm tr}$. At an EP, there is only a single eigenstate and any perpendicular component decays. Close to an EP, the state perpendicular to the ground state initially decays towards the ground state, which is followed by revival and periodic oscillation with frequency $E_+(p)$. Only for those p where the driving rate dominates the revival frequency, the decay is not compensated, and it is only those which yield the defect production.

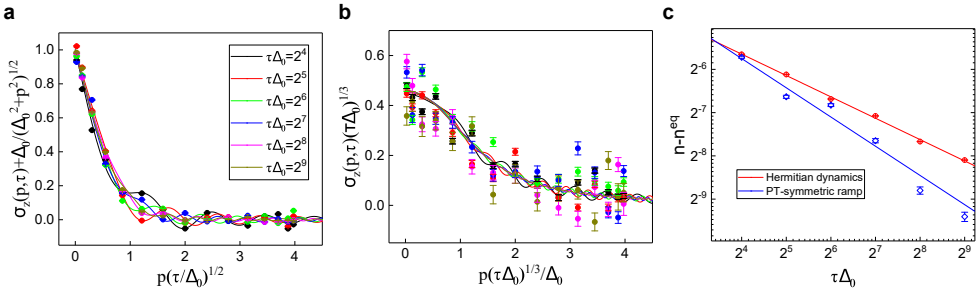

Figure 2: **Kibble-Zurek scaling of defect production for parametric ramps in Hermitian and $\mathcal{PT}$-symmetric non-Hermitian systems.** Data collapse for the momentum-resolved defect density for the Hermitian case **a** and the $\mathcal{PT}$-symmetric ramp **b**. Dots with error bars display the experimental measurements and solid lines refer to theory. **c** Total defect density n relative to the adiabatic values $n_{\rm eq}$ for the two considered cases as a function of the ramp time τ. Solid lines show the results for the best power-law fit $n - n_{\rm eq} \sim \tau^{-\alpha}$ to the experimental data. The fitted exponents $\alpha = 0.49$ for the Hermitian scaling (red), and $\alpha = 0.68$ for the $\mathcal{PT}$-symmetric ramp (blue).

Analogous results for different drives as well as higher-order exceptional points are also available, at a correspondingly more complex experimental setup, Fig. 1, presented together with a theoretical analysis in Ref. [2].

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2.3 Machine learning quantum dynamics

TIAGO MENDES SANTOS AND MARKUS HEYL

Introduction Understanding the collective dynamics of strongly interacting quantum particles is a task that is at the core of different areas of modern physics. In recent years the field has experienced rapid development driven, in particular, by the tremendous experimental progress in manipulating synthetic quantum systems, which can provide controllable access also to its dynamics [1]. Topics that have been motivated by such advances include dynamical quantum phase transitions, quantum many-body scars, the Kibble-Zurek mechanism, to mention a few. At the theoretical and numerical level, the exponential complexity typical of quantum many-body systems is still the main barrier to understand such topics. For instance, the rapid entanglement growth typical of high-dimensional systems hinders efficient simulations of real-time dynamics by state-of-the-art approaches such as tensor networks.

Recently, machine-learning (ML) techniques have been put forward to overcome the exponential complexity in describing quantum many-body systems. In part, this is motivated by the tremendous success that Artificial Neural Networks (ANNs) have achieved in recent years in many fields of science and technology in representing high-dimensional functions. The key idea has been to represent a quantum state as an ANN known also as Neural Quantum State (NQS) [2].

Since its proposal, a series of benchmark studies have already demonstrated the potential of the NQS approach as a numerical tool to explore open questions in quantum many-body physics. Here, we describe some recent advances achieved by our group in simulating the dynamics of many-body systems with NQS. These advances have gone along two fronts. First, we emphasize some algorithmic challenges of the NQS in describing real-time dynamics and, most important, discuss some improvements that are of essential importance to push the frontier of the NQS approach [3] to otherwise inaccessible system-size and time-scale regimes. Second, as an example of the power of the NQS approach, we consider its application to the quantum Kibble-Zurek mechanism in two-dimensional quantum matter, which is a challenge for other computational techniques.

Neural quantum states In a nutshell, the implementation of the NQS approach follows two steps. First, a quantum state of a many-body system, e.g.,

$$|\psi\rangle = \sum_s \psi_{\vec{\eta}}(s)|s\rangle, \tag{1}$$

is represented by an ANN; the set of parameters $\vec{\eta} = (\eta_1, \eta_2, ..., \eta_{N_p})$ are the so-called weights and biases of an ANN, and $|s\rangle = |s_1 s_2 ... s_{N_s}\rangle$ denotes the states of a computational basis such as the spin configurations for a system of spins with each $s_i = \uparrow, \downarrow$ for all $i = 1, \ldots, N_s$. Second, variational Monte Carlo (VMC) [or the time-dependent variational Monte Carlo (tVMC)] techniques are employed to compute the set of ANN parameters, or, as is dubbed in the Machine Learning, to *train* the ANN parameters. In practice, the wave function $\psi_{\vec{\eta}}(s)$ serves as a generative model, from which physical observables can be computed using VMC. In this way, the VMC+ANN approach (or simply, NQS) can be used to simulate quantum states of lattice models (e.g., ground or time-evolved states).

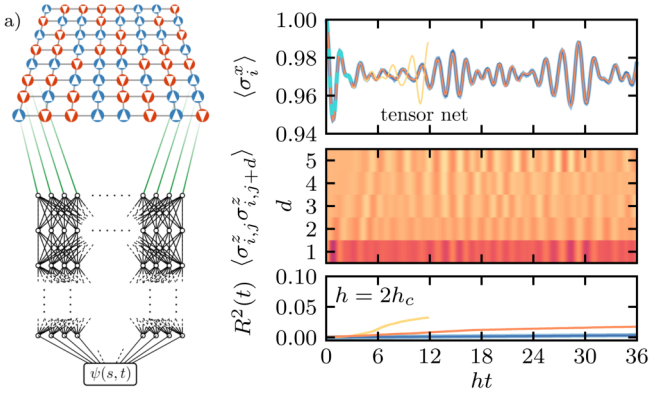

Figure 1: a) Schematic visualization of the neural network wave function. b) Real-time evolution in the two-dimensional quantum Ising model after a quantum quench comparing the neural network solution to state-of-the-art tensor networks. Figures taken from [3].

An essential aspect of the NQS approach is the fact that ANNs are universal function approximators. As a consequence, in principle, any quantum many-body wave function, $\psi_{\vec{\eta}}(s)$, can be represented by ANNs provided the number of parameters, N_p, is sufficiently large. Indeed, ANNs can efficiently encode (i.e., with relatively low N_p) intricately entangled quantum states that other state-of-art variational approaches, such as tensor networks, cannot efficiently describe. The powerful expressivity of ANNs is then expected to provide a way to overcome the inherent complexity growth (associated with the rapid growth of entanglement) during the dynamics of high-dimensional systems.

Recent works, nevertheless, have raised doubts about the applicability of the NQS approach in otherwise inaccessible regimes of quantum dynamics. An important observation is that the issues affecting the NQS approach are not primarily due to the expressivity of ANNs, but, instead, to numerical instabilities inherent to the NQS approach, which, however, in many cases

can be controlled by a series of algorithmic improvements as we aim to demonstrate below.

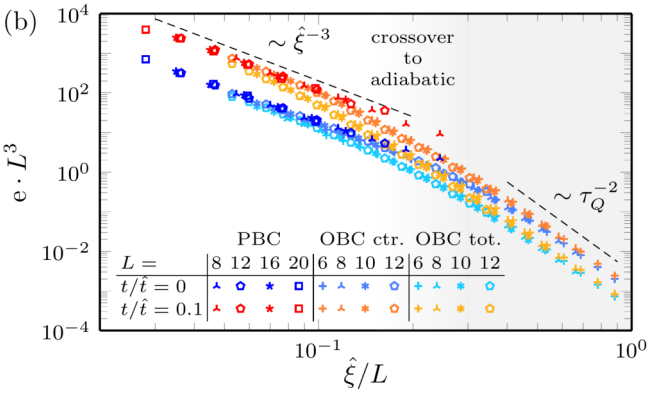

Figure 2: Excitation energy density e for a parameter sweep in the quantum Ising model providing evidence for universal behavior as predicted by the quantum Kibble-Zurek mechanism [4].

Real-time dynamics with neural quantum states Training, i.e., optimizing $\psi_{\vec{\eta}}(s)$ to represent the dynamical quantum many-body wave function, is performed by demanding for each time step τ that the change of parameters $\dot{\vec{\eta}}$ minimizes the distance between the exactly time-evolved state $e^{-i\tau H}|\psi_{\vec{\eta}(t)}\rangle$ and the approximate one $|\psi_{\vec{\eta}(t)+\tau\dot{\vec{\eta}}}\rangle$ in the variational manifold as measured by the Fubini-Study metric $\mathcal{D}$ [2]. Minimization with respect to $\dot{\vec{\eta}}$ yields a first order differential equation $S_{k,k'}\dot{\eta}_{k'} = F_k$ for the variational parameters $\eta_k(t) \in \mathbb{C}$ where $S_{k,k'}$ and F_k with $k, k' = 1, \ldots, N_p$ are some quantities which can be, in principle, straightforwardly computed using some Monte-Carlo sampling procedure. Notice that this differential equation is the well-known time-dependent variational principle (TDVP), which translates the quantum evolution described by the Schrödinger equation to a set of nonlinear differential equations for the variational parameters.

While the TDVP seem to be straightforwardly solvable, it has turned out that the solution faces severe numerical instabilities. Within the recent years we have achieved a set of algorithmic improvements, which finally made the resulting approach competitive and partially superior to state-of-the-art tensor network methods for the simulation of the dynamics of two-dimensional quantum matter. Concretely, we have demonstrated the progress for the paradigmatic quantum Ising model on a square lattice (see also Fig. 1a):

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_j \sigma_j^x \,. \tag{2}$$

Here, the $\sigma_i^{x/z}$ denote the Pauli x and z matrices and $\langle i, j\rangle$ the set of neighboring sites on the square lattice. We have considered two nonequilibrium scenarios: i) a quantum quench [3] and ii) the quantum Kibble-Zurek mechanism [4]. In both cases we chose as the initial condition $|\psi_0\rangle = |\rightarrow\rangle$ the ground state of H for $J = 0$ and $h > 0$. For the quantum quench, the dynamics is performed with a Hamiltonian H constant in time yielding the time-dependent state $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$. Comparing the resulting solution using our NQS approach yields results, which can be competitive or even superior over state-of-the-art tensor network approaches, see Fig. 1b. In the case of the Kibble-Zurek mechanism, the Hamiltonian parameters are tuned in a slow and continuous fashion. Concretely, we have considered $g(t)/g_c = 1 - \epsilon(t), J(t)/J_c = 1 + \epsilon(t)$ with $\epsilon(t) = t/\tau_Q$. Here, g_c and J_c are the parameters where the Ising model undergoes a quantum phase transition. We start the protocol at $t_i = -\tau_Q$ with $J(t_i) = 0$, crossing the critical point at $t = 0$, and ending at $t_f = \tau_Q$. For a sufficiently slow parameter sweep, i.e., large τ_Q, the famous quantum Kibble-Zurek mechanism predicts a universal behavior of the amount of excitations, dictated by the universality class of the underlying quantum phase transition. In Fig. 2 we quantify this amount by plotting the excitation energy density e as a function of an emergent length scale $\hat{\xi}$ in the problem, with L denoting the linear extent of the system so that L^2 is the total number of lattice sites. Notice that the data for PBC has been obtained using the NQS approach whereas for OBC using tensor networks demonstrating again the capabilities of the NQS allowing us to reach significantly larger system sizes. This turns out to be important for identifying sufficient numerical evidence in Fig. 2 for power-law behavior extending over more than one decade.

Outlook The NQS approach described here can also be extended to compute dynamical response functions and excitation spectra of many-body systems. The idea is that NQS can efficiently simulate the real-time dynamics of local excitations related to such dynamical quantities. A direction of interest that we plan to pursue is to characterize the excitation spectra of two-dimensional models relevant to experiments performed with Rydberg atoms in optical arrays [1]. In particular, we plan to analyze the prospect of characterizing interesting quantum many-body phases (e.g., density waves or spin liquid) of Rydberg systems in frustrated lattices using dynamical spectral probes.

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2.4 Disorder-free localization in interacting higher-dimensional lattice gauge theories

PETER KARPOV, NILOTPAL CHAKRABORTY, AND MARKUS HEYL

Introduction Quantum interference can localize the electronic wavefunction of non-interacting quantum matter in the presence of quenched random disorder. Pioneering work in the last two decades has shown that the presence of weak interactions doesn't necessarily destabilize this so-called Anderson localization, which has led to the notion of the many-body localized (MBL) phase. Strongly interacting many-body systems represent a whole new challenge, where it is nowadays understood that MBL can be stable for one-dimensional systems. However, the situation is much less clear for higher dimensions. In the last few years, a new mechanism for localization has been discovered, which doesn't rely on quenched disorder and which can even exist in two-dimensional quantum matter, as we will discuss in more detail below. This phenomenon, dubbed disorder-free localization (DFL) [1], occurs in lattice gauge theories (LGTs), whose so-called gauge superselection sectors can induce an effective internal disorder as a consequence of the local gauge symmetry [2]. Most LGTs hosting localization have been one-dimensional. However, we have recently shown that a large class of strongly interacting LGTs in two dimensions can also localize [3]. Hence, our findings suggest that DFL represents a much more robust localization mechanism as compared to conventional MBL, especially in higher dimensions.

Disorder-free localization The key ingredients of DFL are local conserved quantities enforced by Gauss' law following from local gauge symmetries. These conserved quantities fragment the Hilbert space into so-called superselection sectors, making the Hamiltonian block-diagonal. The existence of these sectors, protected by gauge invariance, can lead to an unconventional scenario for ergodicity breaking. Consider a homogeneous superposition state $|\psi\rangle = \sum_n C_n|\psi_n\rangle$ involving many of such superselection sectors n. As the Hamiltonian and typical observables are block-diagonal, i.e., $H|\psi_n\rangle = H_n|\psi_n\rangle$, the expectation values of an operator O during dynamics also becomes diagonal in the form of $\langle O(t)\rangle = \sum_n |C_n|^2\langle\psi_n|e^{iH_nt}Oe^{-iH_nt}|\psi_n\rangle$ with H_n the corresponding block of the Hamiltonian, which takes the form analogous to an effective disorder average with the disorder strength set by how strongly the amplitudes C_n distribute over different superselection sectors [2]. This can, in principle, lead to nonergodic behavior even though both the initial state and the Hamiltonian are homogeneous. This is the essence of DFL [1].

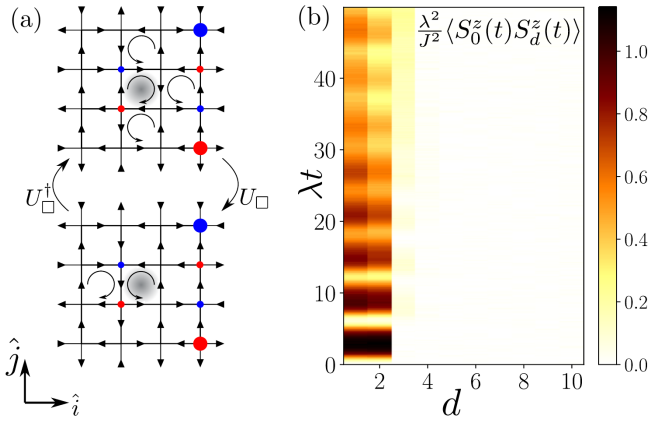

Figure 1: a) Illustration of the $U(1)$ quantum link model (QLM) with spin$-1/2$'s located on the links of the square lattice. Spins pointing $\rightarrow,\uparrow$ correspond to $S^z = +1$ and $\leftarrow,\downarrow$ to $S^z = -1$, respectively. The operators $U_\square$, $U^\dagger_\square$(shown for the darkened central plaquette) flips all spins on a plaquette whenever they are oriented clockwise or counterclockwise. Flippable plaquettes are indicated by circular arrows. Background charges with nonzero in- our out-flow of electric field at a given vertex are indicated by red and blue dots. b) Spatiotemporal buildup of quantum correlations $\langle S^z_{\mathbf{r},y}(t)S^z_{\mathbf{r}+\mathbf{d},y}(t)$ ($\mathbf{d}$ = d $\hat{i}$) starting from $|\psi(\alpha = 0)\rangle = |\rightarrow\rangle$ in the localized phase of the QLM for $J/\lambda = 0.1$ and a system size of 20×20, i.e., 800 spins. The propagation of quantum correlations is clearly limited as a signature of the localized phase of the QLM.

Ergodicity breaking in the two-dimensional quantum link model Here we summarize our results [3, 4] on disorder-free localization for the 2D $U(1)$ quantum link model (QLM). This model can be thought of as a simplification of lattice quantum electrodynamics, where only photonic degrees of freedom are considered (no matter fields such as electrons or positrons) but instead of the local infinite ladder of photon states only the two lowest ones are kept, leading to an effective spin-1/2 description. In the QLM the spins $S_{\mathbf{r},\mu}$ reside on the links of a square lattice connecting vertices $\mathbf{r} = (x, y)$ and $\mathbf{r} + \mu$ (here $\mu = \hat{i}, \hat{j}$ is one of the two unit vectors of the lattice), see Fig. 1 for an illustration, with the Hamiltonian:

$$H = \lambda \sum_{\square} (U_\square + U^\dagger_\square)^2 - J \sum_{\square} (U_\square + U^\dagger_\square). \qquad (1)$$

The sums run over all plaquettes $\square$, $U_\square = S^+_{\mathbf{r},\hat{i}} S^+_{\mathbf{r}+\hat{i},\hat{j}} S^-_{\mathbf{r}+\hat{j},\hat{i}} S^-_{\mathbf{r},\hat{j}}$ induces a collective flip of all spins on plaquette $\square$ as shown in Fig. 1, and $S^\pm_{\mathbf{r},\hat{\mu}}$ denote the usual spin raising and lowering operators. The local gauge symmetry is generated by $G_\mathbf{r} = \sum_\mu (S^z_{\mathbf{r},\mu} - S^z_{\mathbf{r}-\mu,\mu})$ counting the total inflow of the electric field to the vertex $\mathbf{r}$. Since $[G_\mathbf{r}, H] = 0$ for all lattice points and $[G_\mathbf{r}, G_{\mathbf{r}'}] = 0$, eigenstates of H can be classified by the respective eigenvalues $q_\mathbf{r} \in \{-2, -1, 0, 1, 2\}$ of $G_\mathbf{r}$. The set of $\mathbf{q} = \{q_\mathbf{r}\}$ defines the superselection sector of

states $|\psi_{\mathbf{q}}\rangle$ with $G_{\mathbf{r}}|\psi_{\mathbf{q}}\rangle = q_{\mathbf{r}}|\psi_{\mathbf{q}}\rangle$, hence, each of the $q_{\mathbf{r}}$ can be given a physical meaning in terms of static back-

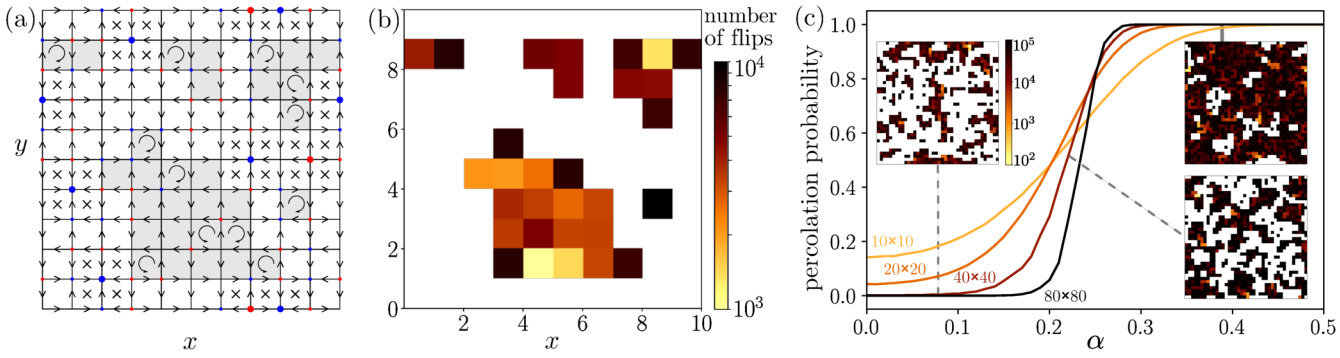

Figure 2: Unconventional classical percolation problem implying a quantum nonergodic phase in the QLM. (a) Typical spin configuration sampled from $|\psi_0(\alpha = 0)\rangle \equiv |\rightarrow\rangle$ with arrows showing the local spin orientation and circular arrows showing flippable plaquettes. Red and blue disks denote positive and negative background charges, respectively. Crosses indicate plaquettes blocked by charges $q = \pm 2$. Grey color indicates plaquettes that can become flippable in the course of the evolution. (b) Result of the Monte Carlo simulation starting from the state (a). The colormap shows the number of times that the individual plaquettes were flipped in the course of the simulation; white color stands only for plaquettes, that have never been flipped. c) Percolation probability vs α. The insets show typical configurations below, at, and above the percolation threshold $\alpha_c \approx 0.25$ for a 40×40 system.

ground charges, whenever the famous "two-in two-out" rule at a vertex $\mathbf{r}$ is violated. For our study we use a one-parametric family of homogeneous initial states $|\psi_0(\alpha)\rangle$ which continuously connects states without background charges at $\alpha = \pi/4$ to states with strongly random background charges at $\alpha = 0$.

As we find, the quantum real-time evolution of the state $|\rightarrow\rangle = |\psi_0(\alpha = 0)\rangle$ is consistent with non-ergodic behavior [3, 4] (see Fig. 1b). We provide further evidence for the existence of an extended non-ergodic phase by employing a classical correlated percolation problem whose percolation threshold provides an upper bound for the quantum ergodicity transition point. For the state $|\rightarrow\rangle$, which is distributed over all superselection sectors, one can for instance choose a typical one (Fig. 2(a)). Such a sector contains many background charges $q_{\mathbf{r}}$ imposing strong kinetic constraints. For instance, one can convince oneself from Fig. 1 that $q_{\mathbf{r}} = \pm 2$ (big red/blue dots) implies that neighboring spins either all point inwards or outwards, hence the adjacent plaquettes remain unflippable forever (denoted by crosses). Are these constraints so strong to fragment the lattice into sets of kinetically disconnected islands or there exists a single extensive connected cluster for state $|\psi_0(\alpha)\rangle$? We answer this question by studying a percolation problem of what one might call active plaquettes. By means of an infinite-temperature classical Monte Carlo simulation we randomly flip flippable plaquettes (which can influence the flippability of nearby plaquettes) and record how often each plaquette is flipped (see Fig. 2(b)). For α close to $\alpha = 0$ we find that small clusters of active plaquettes are surrounded by inactive regions implying a nonpercolating phase. Calculating the percolation probability in the full α range, we obtain a clear non-percolating phase (Fig. 2(c)) and a percolation threshold $\alpha_c \approx 0.25$. For $\alpha < \alpha_c$, the system is localized just because of the small disconnected clusters which don't allow any transport. However, we note that α_c is purely an upper bound for the actual quantum thermalization transition since we have not accounted for quantum interference effects in the considered percolation problem.

Outlook The central result of the presented works is that interacting two-dimensional quantum matter can enter a non-ergodic localized phase as a consequence of local gauge symmetries. In the future it would be important to address the role of quantum interference which is missing in the utilized mapping to a classical percolation problem. A further important aspect would be to study the influence of matter fields. Beyond the question of ergodicity a promising further research direction could be to explore the possibility of localization protected quantum order, which has been very fruitful in the context of conventional disordered systems. Moreover, three-dimensional extensions of this work could also lead to interesting questions about localization of emergent photons in quantum spin ice materials, which have been theorized to host a large fine structure constant realizing an emergent strong coupling version of quantum electrodynamics.

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2.5 Quantum pyrochlore magnet at finite and zero temperature

ROBIN SCHAEFER, IMRE HAGYMÁSI, RODERICH MOESSNER, AND DAVID J. LUITZ

Highly-frustrated spin systems continue to pose challenges for condensed matter physicists, since they are the most likely candidates to realize new exotic phases of matter, inter alia, quantum spin liquids or ice states. While frustrated magnets are a fascinating topic, they are also extremely hard to study since numerical and analytical tools are severely limited. One of the most prominent frustrated material is the antiferromagnetic pyrochlore lattice, composed of corner-sharing tetrahedra. The three-dimensional cousin of the intensively studied kagome lattice is a prime candidate for a quantum spin liquid phase. Even though this model was studied extensively during the last decades only little is known about the spin-$S = \frac{1}{2}$ Heisenberg pyrochlore. We address various properties at zero and finite temperature with and without an external magnet field in a series of papers [1–3].

We focus on the isotropic spin Heisenberg antiferromagnet with nearest neighbor interaction:

$$H = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + h \sum_i S_i^z. \qquad (1)$$

The sum $\langle i, j \rangle$ in Eq. (1) runs over nearest neighbor bonds of the lattice. The underlying Bravais lattice (face centered cubic) is equipped with a tetrahedral unit cell. A characteristic feature of the pyrochlore lattice are two types of tetrahedra resulting from the unit cells and their connecting bonds, see inset in Fig. 3.

Finite temperature properties [1] The three-dimensional and frustrated nature of the system limits the numerical toolbox to study strongly correlated many-body systems. In our first work, we address the finite temperature properties of the model (1) using a combination of cutting-edge numerical techniques suited for this problem. First, we investigate finite sized cluster with two different methods: Canonical typicality yields exact results for a cluster of 2x2x2 unit cells (32 spins) even at very low temperatures. In addition, we demonstrate that tensor-network methods are capable of reaching non-trivial low temperatures in three dimensions (48 sites with periodic boundary conditions) and provide accurate results for thermodynamic quantities. Second, a systematic cluster expansion (NLCE) within the infinite lattice structure opens the possibility to obtain reliable finite temperature results in the thermodynamic limit. Using graph- and group-theoretic approaches, we are able to fully diagonalize the arising configurations of eight tetrahedra (up to 25 spins) in the pyrochlore lattice. By further pushing the linked cluster expansion, we are able to go far beyond the limits of previous works and to obtain converged results for different observables (i.e., specific heat, entropy, and susceptibility) in the thermodynamic limit down the temperatures of 0.2J which already exhibits non-trivial features, see Fig. 1.

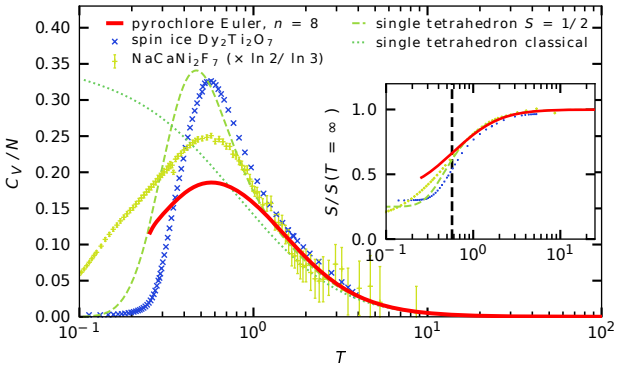

Figure 1: The main plot shows the heat capacity per spin versus temperature for different pyrochlore magnets. The converged part of our NLCE calculation for the $S = 1/2$ Heisenberg model is indicated by the red curve. We compare the data with the behavior of a single tetrahedron for $S = 1/2$ (dashed) and $S = \infty$ (classical case, dots). We scaled T to match with the high-T limit. Furthermore, we compared the theoretical prediction with experimental data of $NaCaNi_2F_7$ [4] (green symbols), a $S = 1$ (approximate) Heisenberg magnet, and the Ising spin ice $Dy_2Ti_2O_7$ [5]. Again, both datasets are scaled in T to coincide with the peak of the $S = 1/2$ model. Additionally, we included a factor $\ln 2/\ln 3$ to account for the larger $S = 1$ entropy. The entropy per spin of the same models are shown in the inset. We use natural units $k_B = 1$, $\hbar = 1$, $J = 1$.

Zero temperature properties [2] The nature of the ground state of the pyrochlore $S = 1/2$ Heisenberg antiferromagnet remains unknown and poses one of most important, unsolved problems of condensed matter theory in spite of several years' active research. Among other frustrated materials, the pyrochlore antiferromagnet is a prominent spin liquid candidate. We provide strong evidence that the lattice inversion symmetry is spontaneously broken in the ground state, which imposes serious constraints on the type of spin liquid state the ground state can assume. Our evidence is based on large-scale SU(2)-symmetric density-matrix renormalization group calculations by pushing this method to three-dimensions including clusters with up to 128 sites. Fig. 2 displays the real space correlations revealing an energy density difference between the two sublattices of tetrahedra coinciding with the starting point of perturbative treatments [5]. Our estimate for the ground state energy, $E_0/N_{\text{sites}} = -0.490(6)J$, is very precise and confirmed by bounds we obtain from high

order series expansion, clarifying contradictory claims in the literature. A finite size scaling for a range of different cluster sizes and the comparison to the literature is shown in Fig. 3. These results where confirmed very recently by independent subsequent work [7].

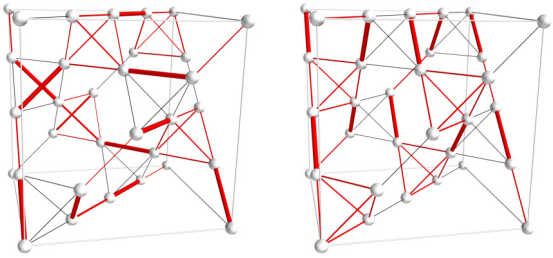

Figure 2: Real space spin-spin correlations for the best variational DMRG wavefunction ($S_z = 0$) for $N = 64$ (left) and $N = 128$ (right) within a cubic cell. The strength of the correlation is encoded via the thickness of the red bonds between neighboring sites. A negligible correlation magnitude is indicated via black lines.

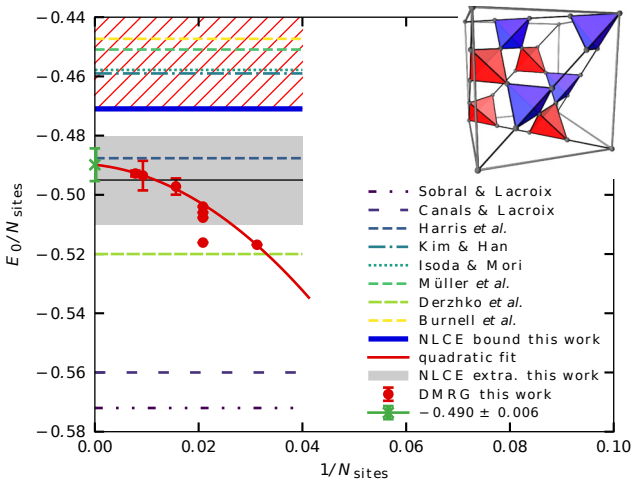

Figure 3: We present a finite-size scaling for ground-state energy and compare it to the various approaches in the literature (horizontal lines) in the thermodynamic limit ($J = 1$). References and values are given in [2]. The DMRG energies are encoded via the red points and extrapolated to infinite bond dimension with a quadratic polynomial. Using the converged NLCE data at finite temperature allows us to assign a robust upper bound and excluding the red hashed area. We further extrapolated the converged NLCE data to zero temperature (solid black line, gray shaded area indicates the confidence interval). The pyrochlore lattice is shown in the inset, highlighting the two tetrahedral sublattices in red and blue.

Magnetization process [3] Frustrated magnets typically display a nontrivial magnetization process with exotic ground states if placed in an external magnetic field. Using our state-of-the-art density-matrix renormalization group method we systematically calculated the ground state in an external magnetic field h for a range of finite clusters with up to 128 sites. Fig. 4 shows the resulting magnetization curve at zero temperature. We find several incompressible magnetic phases visible as pronounced plateaus, the most robust one at $\frac{1}{2}$ magnetization. Our detailed investigation of the nature of the wave function reveals that this state spontaneously breaks (real-space) rotational, but not spin-rotation, symmetry. The symmetry breaking is expressed by *oppositely polarized* spins on alternating kagome and triangular planes. An analogous state, known as kagome ice, is known in spin ice, where however the symmetry-breaking is not spontaneous, raising the question about what range of mechanisms can be responsible for such 'order by disorder'.

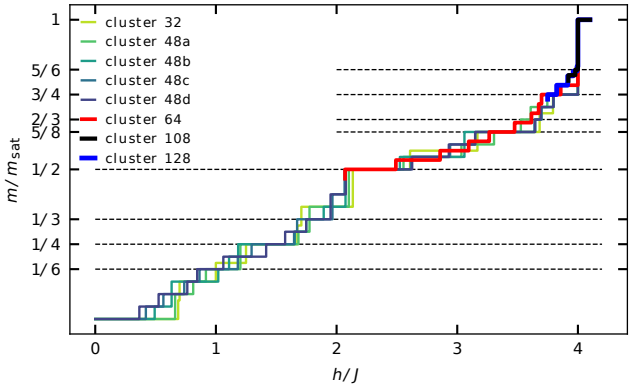

Figure 4: Magnetization curve ($m = \langle\psi_0|S^z_{\text{tot}}|\psi_0\rangle$) of various pyrochlore clusters with different sizes as a function of the external magnetic field h. The saturation magnetization is given by the fully polarized state of N spins: $m_{\text{sat}} = N/2$.

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2.6 Hierarchy of relaxation timescales in local random Liouvillians

KEVIN WANG, OSCAR EMIL SOMMER, FRANCESCO PIAZZA, AND DAVID J. LUITZ

Quantum many-body systems are extremely complex due to the interactions between particles. This has been well understood for unitary quantum systems, for which it was shown that they share many intriguing properties with completely random matrices. This is, for example, the case for the distributions of spectral gaps, or for matrix elements of local operators. The latter observation gave rise to the eigenstate thermalization hypothesis, which provides an excellent description of how and if closed quantum systems can reach thermal equilibrium [1].

Much less was known on such general grounds for open quantum systems until much more recently, when the foundations of a random matrix theory for quantum master equations were set out. Surprisingly, it turned out that a random Liouvillian, which satisfies the crucial properties of positivity and the preservation of the trace of the density matrix, has a peculiar spectral support in the shape of a lemon, located in the complex half plane with nonpositive real parts [2,3]. A very similar behavior was found in the case of classical rate equations, although the specific form of the spectral support differs [4].

Such a random matrix description represents an important first step towards establishing the typical behavior of open quantum many-body systems, but lacks an important physical ingredient: the locality of dissipative interactions.

In our work [5], we generalized models of random and purely dissipative Liouvillians to include only few-body dissipative interactions. This is achieved by limiting the set of allowed Lindblad jump operators L_i in the Lindblad master equation

$$\mathcal{L}_D(\rho) = \sum_{i,j=1}^{N_L} K_{ij}[L_i \rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_i, \rho\}]. \qquad (1)$$

For concreteness, we consider a system of ℓ qubits and write the Lindblad operators L_i as Pauli strings $\sigma_{i_1} \times \sigma_{i_2} \times \cdots \times \sigma_{i_\ell}$, where $i_x \in \{0,1,2,3\}$. A Pauli string is k local if it consists of k nonidentity and $\ell - k$ identity ($i_x = 0$) Pauli matrices. The physically most relevant case is $k = 1$ and $k = 2$, which corresponds to single qubit jump operators as well as two qubit dissipative interactions. Starting from the set $\{L_i\}$ of N_L k-local Lindblad operators, our model (1) is fully parametrized by the Kossakowski matrix K, which we randomly sample by drawing its nonnegative i.i.d. eigenvalues from a box distribution and then rotate to a random basis using a random unitary matrix $U \in \mathrm{CUE}(N_L)$. This procedure guarantees that K is positive semidefinite.

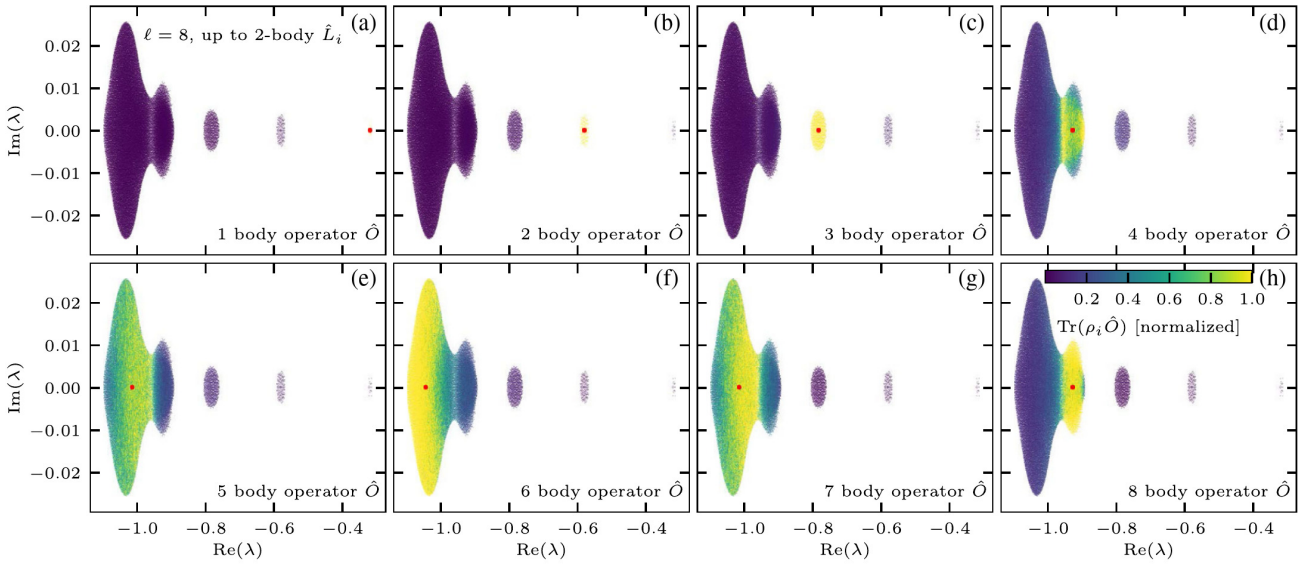

Figure 1: Eigenvalues λ_i of a random 2-local Liouvillian for $\ell = 8$ qubits. The color of each eigenvalue indicates the m-body observable content of each eigenmatrix ρ_i corresponding to the eigenvalue, as quantified by $\mathrm{Tr}(\rho_i O)$, where O is a random superposition of Pauli strings with m nonidentities. Here, $m = 1, 2, 3, 4, 5, 6, 7, 8$ in panels a,b,c,d,e,f,g,h respectively. Figure from Ref. [5].

Based on these simple ingredients, we can build the full matrix representation of the $k = 2$ local Liouvillian $\mathcal{L}_D$ and calculate its eigenvalues and eigenmatrices shown in Fig. 1. The spectrum is composed of several dense eigenvalue clusters unlike in the nonlocal case where only a single cluster exists. The nature of the corresponding eigenvalues can be understood in terms of the locality of observables they correspond to: each panel in Fig. 1 shows the contribution of each eigenpair of the Liouvillian to an m-local observable O (generated from a random superposition of m-local Pauli strings), and the color scale shows the weight of $\mathrm{Tr}(\rho_i O)$ for the eigenmatrix ρ_i corresponding to the eigenvalue λ_i. It is clear that for local observables (low m) the eigenvalue clusters are strictly separated by the locality properties of the corresponding observables. This means that e.g. the relaxation of a two local observable (2-point correlation function) is governed only by eigenpairs from the second eigenvalue cluster from the right and that this relaxation is *faster* than the relaxation of one qubit observables.

In fact it turns out that this emergent hierarchy of relaxation timescales emerges from the positivity of the K matrix, which admits a perturbation theory treatment around the limit of $K \propto 1$. The perturbation theory predicts the precise location of the centers of each eigenvalue cluster, indicated by red dots in Fig. 1, and gives an analytical handle on the predicted timescales of relaxation. The analytical prediction agrees perfectly with larger scale numerical simulations of the dynamical relaxation of m-body observables, confirming the validity of our picture also in the thermodynamic limit.

In order to test our random matrix theory in an experiment, we exploited existing quantum computing platforms which turn out to be ideal for the study of dissipative quantum chaos [6]. While dissipation is the major obstacle for quantum computing, it is omnipresent in all current platforms. Although the dissipation channels can be modeled to some extent, a detailed microscopic knowledge of all dissipation channels is not available. Therefore, it is useful to use random matrix modelling to reflect our absence of precise knowledge, while retaining the physical information on the locality of dissipative interactions.

We designed an experimental protocol to leverage the intrinsic dissipation of the IBM quantum processors generated during the application of two qubit gates. This is achieved by applying a "waiting circuit" W to a set of qubits, where we define units of time by the number of CNOT gates (which inject the largest amount of dissipation). After reaching a target "time" t, we apply the conjugate of the "waiting circuit" $W^\dagger$, such that in a perfect quantum computer the total action of the two circuits $WW^\dagger = 1$ is identity. Due to the presence of dissipation, this is however not true and we expect that the effective action of the waiting circuit is purely dissipative.

Using this protocol, we evolve initial product states, and measure a large set of m local Pauli string observables at time t. From the relaxation of these observables, we can extract various time scales, shown in Fig. 2 for different numbers of qubits ℓ as vertical bars for each operator order m. While the results are subject to noise, due to the large number of different Pauli string observables for each m, we obtain accurate average values (orange), which we can compare to our random matrix theory (blue curve), yielding an excellent match.

From this comparison, we can conclude on very general grounds that the dominant dissipation in CNOT circuits on IBM quantum processors is indeed 2-local.

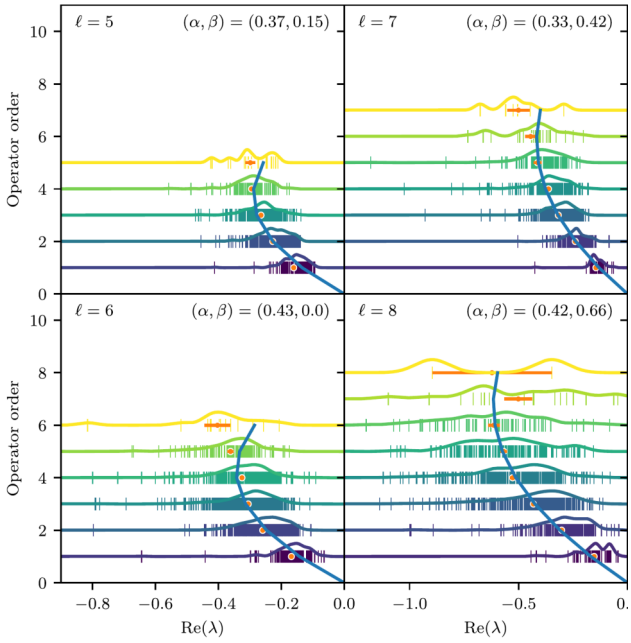

Figure 2: Extracted relaxation rates of m-local (operator order m) Pauli string observables on ℓ qubit subsets of `ibmq_16_melbourne`. The colored curves show distributions of the timescales, orange dots show the average relaxation rate. The theoretical prediction is a quadratic dependence on m, shown by blue curves. Figure from Ref. [6].

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2.7 Photoelectron dynamics from a network of Hamilton matrices

SAJAL GIRI, ULF SAALMANN, AND JAN M. ROST

Machine learning concepts carry the potential for new kinds of spectroscopy, at least in two aspects, since an unprecedented amount of data can be processed routinely with an artificial neural network. Firstly, single (laser shot) spectra can be analyzed in parallel including possible fluctuations from possible noise in the individual spectra without having to recur to averaged spectra. Noise, inherent in the light pulses (as it is the case for SASE FEL light) offers a more detailed photoelectron probe since the light-matter coupling is less restricted by photoionization selection rules. Secondly, one can train the network to recognize a large number of different systems. We will do this in the form of Hamilton matrices. They have random elements representing systems which may but do not necessarily have to exist in nature. Analyzing a photoelectron spectrum with the trained network, will implicitly identify those Hamiltonians whose spectra are closest to the analyzed one [1].
In the SASE FEL context we can purify the spectra from noise by a mapping to corresponding spectra from Fourier-limited Gaussian pulses, and secondly, if the spectra were generated by double pulses of undetermined time-delay varying from shot to shot, we can estimate this time-delay [2].

We will demonstrate this with resonant two-photon ionization, a typical non-linear photon-absorption process. Central to our approach is to cast possible target systems the network will be trained upon in terms of $n_{\rm mat}$ *Synthetic Hamilton Matrices* (SHM). They contain random energies E^k_α and coupling matrix elements $V^k_{\alpha\beta}$ from field-free systems. The field strengths A_k correspond for the present example to intensities in the range of $5\times10^{15}\ldots5\times10^{16}\,\mathrm{W/cm^2}$ (referring to the Fourier-limited pulse). The coupling to the light is augmented by $n_{\rm pul}$ noise realizations $f_l(t)$ to arrive at

$$E_k = E^k_\alpha\delta_{\alpha\beta},\ V_k = V^k_{\alpha\beta},\ H_{kl}(t) = E_k + A_k\, f_l(t) V_k, \quad (1)$$

whereby $k=1\ldots n_{\rm mat}$ and $l=1\ldots n_{\rm pul}$. The paradigmatic field-free Hamilton matrix is obtained by diagonalizing a 1-dimensional example Hamiltonian from the ground state at -24.2 eV up to energies of $\widetilde{E}_\alpha \le E_{\rm max} \approx 48$ eV, resulting in 600 eigenstates mimicking helium with an electron in a softcore potential. We create SHMs by randomly changing energies E_α and matrix elements $V_{\alpha\beta}$ about this matrix through the variation of four parameters [1]. The SHMs can capture dynamics not restricted to 1D, since energies E_k and coupling matrix elements V_k are chosen randomly.

A typical set of learning data is constructed in the following way: For each reference spectrum, we calculate of the order of $n_{\rm pul}=10^2$ fluctuating spectra from noisy pulses f_l obtained with the partial-coherence method [3] using a different noise realization for each SHM. Since solving the TDSE for a single spectrum takes only a few seconds thanks to the highly-optimized propagation scheme [1], this procedure can be executed despite the need to solve about 10^7 TDSEs. For a given SHM, we average over all fluctuating spectra $\overline{P}_k(E) = n_{\rm pul}^{-1}\sum_l P_{kl}(E)$. All averaged fluctuating and reference spectra are normalized, $\int dE\, P(E) = 1$. Finally, the learning data contains of the order of $n_{\rm mat}=10^4$ pairs of spectra. Each pair consists of an averaged noisy spectrum with its respective reference spectrum for the same SHM. A fully connected feed-forward artificial neural network containing 5 layers with 60 neurons establishes the mapping as summarized in Fig. 1.

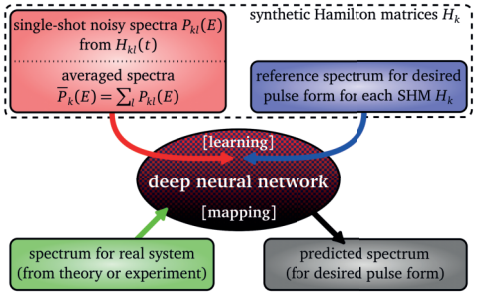

Figure 1: Sketch of deep learning with an artificial neural network using synthetic Hamilton matrices and noisy spectra.

To test the capability of the trained network we feed to it a calculated noisy 3D helium spectrum (completely outside the training space!) and obtain from it the predicted purified spectrum as shown in Fig. 2 in good agreement with the ground truth. Note, that the individual noisy spectra (Fig. 2b) as well as their average (green line in Fig. 2a) look very different.

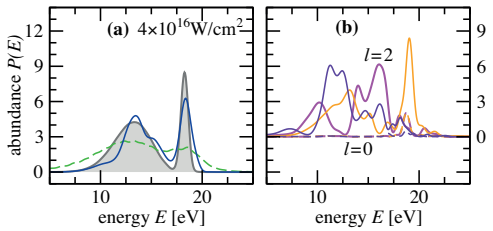

Figure 2: **(a)**Averaged (dashed, green) and predicted (dark blue) photo-electron spectrum for a 3D helium atom compared to the reference spectrum (grey). **(b)** Three single-shot spectra for final angular momentum s (ℓ=0, dashed lines) and d (ℓ=2, solid lines).

Time-delay of noise-free double-pulses We first construct a network-based map to extract the time-delays $T_{\rm d}$ of noise-free double pulses from spectra they generate. The learning data set consists of spectra from 20,000 SHMs, each paired with a single double pulse with delays between 2 and 14 fs. Details of the network can be found in [2].

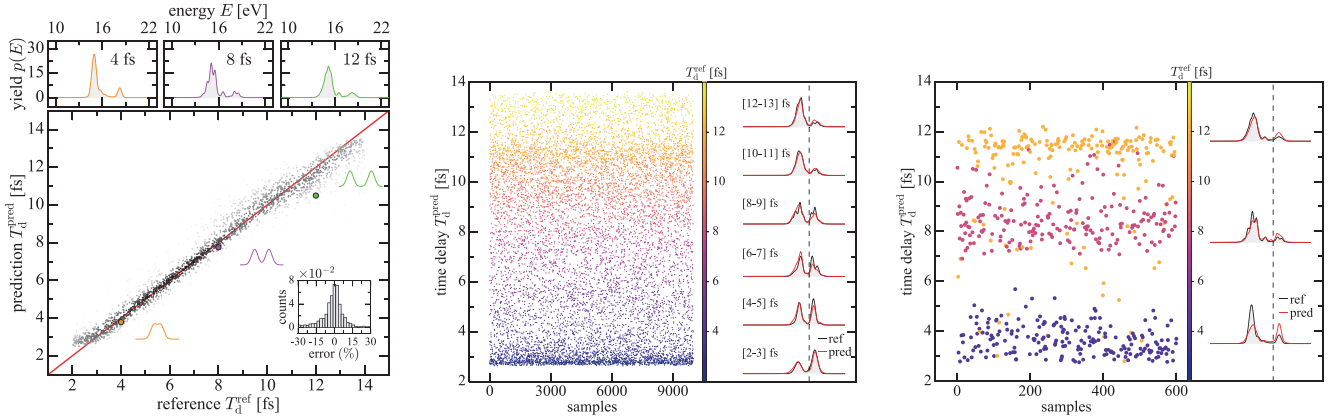

Figure 3: **(left)** Predicted time-delays against reference time-delays for the test data. The pulse energy is $E_p = 1.6\times10^{16}$ W fs/cm^2. The error distribution of the time-delays for the test data is shown in the lower inset. The red line represents error free prediction. The trained network is transferred to the 3D helium spectra for three time delays: 4 fs, 8 fs, and 12 fs with the reconstructed time delays shown as circles and double pulse shapes sketched. The upper inset gives the corresponding photoelectron spectra. **(middle)** Simultaneous reconstruction of time-delay and purification of noisy spectra for a single Hamilton matrix taken from test data. The reconstructed pulse time-delays of single-shot fluctuating spectra are shown as scattered points where the color represents the reference time-delay. We consider 12 intervals of time-delay in the range 2–14 fs with interval length of 1 fs. All single-shot spectra which fall into on interval of time-delay are averaged. The averaged spectra are passed through an another network which maps averaged noisy spectra to purified ones. The predicted purified spectra (red) are compared to reference spectra (black). **(right)** Same as middle panel but for 3D helium for which the network was not trained. The single-shot spectra are averaged over all spectra with time-delays in an interval of 1 fs about the three peaks at 4, 8, 12 fs. The averaged spectra are passed through the trained network to obtain the corresponding purified spectra shown on the right (red). The three averaged reference spectra (black) are obtained in the same way.

Figure 3 (left) shows the training success with the SHMs as well as the transfer of the network to 3D helium spectra, unknown to the network. The trained network reproduces well the delays (results scatter along the ideal red line with an error given in the inset). The deviation for small T_d is expected since the individual pulses in the double pulse have a width of $T = 3$ fs which limits the resolution towards small time-delays. Results for the reconstructed time-delay for full 3D helium spectra are given for T_d of 4, 8, and 12 fs, respectively, and demonstrate the transferability of the network. The upper row shows the corresponding 3D helium spectra. Despite the similarity of these spectra for different time-delays, the trained network can reliably extract the time-delays.

Time-delay in noisy double pulses Finally, we analyze fluctuating single-shot spectra by simultaneously purifying them and extracting the time-delay of the generating noisy double pulse. This scenario is motivated by SASE XFEL pulses, where the pulse is split by a chicane for the relativistic electron bunch which creates the light pulse, or by situations where an XFEL pulse and a time-delayed strong laser pulse are used together, whereby the delay between the two pulses varies from shot to shot due to a jitter. To have reasonable statistics for the map and also reasonably different spectra for different time-delays, we reconstruct from each noisy single-shot spectrum (all for the same SHM) the time-delay but average the spectra afterwards over small intervals (1 fs) of time-delays. Subsequently, the averaged spectra are passed through another trained network to purify them. The result is shown in Fig. 3 (middle). The monotonic change in colors of the reconstructed time-delays demonstrates that the reconstruction for the test data has been successful. The spectra within 1 fs intervals of reconstructed time-delays are averaged and subsequently purified. They are shown on the right of the middle panel in red along with reference spectra (black), averaged over the same interval of time-delays. The generally good agreement demonstrates that reconstruction of time-delays and purification of the single-shot spectra is possible without additional information but the single-shot spectra.

The last step is to proof that the reconstruction and purification can be transferred to spectra unknown to the networks. To this end we take noisy single-shot spectra of 3D helium with three well-defined time-delays and pass them through the trained network for reconstruction of the time-delay shown as scattered points in Fig. 3 (right). We average the corresponding spectra over 1 fs about the three peak time-delays in the scattered points and pass the averaged spectra through the purification network to arrive at the three spectra on the right in red. They agree well with the corresponding reference spectra, averaged over the same intervals of time-delay (black). The successful reconstruction of the time-delay and purification of the corresponding fluctuating spectra renders deep learning as a promising tool for advanced spectroscopy with noisy data.

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2.8 Rydberg composites

MATTHEW T. EILES, ALEXANDER EISFELD, ANDREW HUNTER, AND JAN M. ROST

A ground state atom can bind to a Rydberg atom by strongly polarizing it, resulting in a "trilobite" dimer molecule with a highly localized electronic wave function. Adding more ground state atoms leads to polyatomic molecules [1, 2] and eventually a bound *Rydberg composite* forms with diverse Rydberg electron spectra, depending on the number and geometric arrangement of the atoms. In [3] we propose a systematic description capable of interpolating between molecular and solid state-like features as the number of atoms increases. Reformulating the Hamiltonian of the Rydberg composite, we show its spectrum to be equivalent to that of a tight-binding Hamiltonian, revealing a direct connection between a Rydberg composite and the solid state, detailed below. Moreover, increasing the number of atoms and the Rydberg excitation to infinity realizes a thermodynamic limit for a single Rydberg atom, since the Coulomb potential supplies infinitely many and highly degenerate excited Rydberg states when approaching the ionization threshold. For a ring Rydberg composite with the radius of the Rydberg elecron's outer classical turning point, the interactions reduce to those of next neighbors enabling Anderson localization of a Rydberg electron.

The Rydberg composite's Hamiltonian reads in atomic units $H = H_0 + \hat{h}$ with the hydrogenic Hamiltonian $H_0 = -\frac{1}{2}\nabla^2 - \frac{1}{r}$ and the interaction Hamiltonian

$$\hat{h} = 2\pi \sum_{q=1}^{M} a_s(R_q)\delta^3(\vec{r} - \vec{R}_q) \tag{1}$$

for M ground state atoms at positions $\vec{R}_q$ (relative to the ion) in contact interaction with the electron. They constitute point-like perturbations of the Rydberg wave function with a strength proportional to the S-wave scattering length $a_s(R_q)$, which is dominant due to the low kinetic energy of the electron. For the following derivation we set $2\pi a_s = 1$. H_0 represents the unperturbed hydrogen atom with the Schrödinger equation $H_0|ni\rangle = -\frac{1}{2n^2}|ni\rangle$. Each manifold with principal quantum number n contains $J = n^2$ degenerate eigenstates $|ni\rangle$, $i = 1, \ldots, J$. The degeneracy is lifted to an extent depending on the number M of perturbers and to an excellent approximation each manifold can be considered individually. In the hydrogenic basis and for fixed n, the interaction Hamiltonian reads

$$\hat{h}_{ii'} = W_{iq}W^{\dagger}_{qi'}\,, \quad W_{iq} = \Phi^*_{ni}(\vec{R}_q) \equiv \langle ni|\vec{R}_q\rangle\,, \tag{2}$$

with the convention that the sum is taken over indices appearing twice. $\hat{h}_{ii'}$ is a separable $J \times J$ matrix with rank M. Then $S = (W^{\dagger}W)^{-1/2}W^{\dagger}$ constitutes a semi-unitary transformation which has a right (Moore-Penrose [4]) inverse $S^{\dagger}$ with $SS^{\dagger} = 1_M$ but $S^{\dagger}S \neq 1_J$. The transformation

$$S_{qi}\hat{h}_{ii'}S^{\dagger}_{i'q'} = W^{\dagger}_{qi}W_{iq'} \equiv \hat{h}_{qq'} \tag{3}$$

maps $\hat{h}_{ii'}$ into the interaction Hamiltonian in tight-binding form

$$\hat{h} = \sum_{q,q'=1}^{M} |q\rangle h_{qq'}\langle q'| \equiv \sum_{q=1}^{M} E_q|q\rangle\langle q| + \sum_{q=1}^{M}\sum_{q'\neq q}^{M} V_{qq'}|q\rangle\langle q'| \tag{4}$$

containing only the non-vanishing M eigenvalues in a manifold n. The meaning of the site representation can be illustrated with the so called trilobites [1], $|T_q\rangle = \sum_{i=1}^{J}|ni\rangle\langle ni|\vec{R}_q\rangle = \sum_i |ni\rangle\mathcal{W}_{iq}$. These are eigenstates of a Rydberg dimer, a Rydberg atom and a single perturber at $\vec{R}_q$ and therefore associated with site q. The $|T_q\rangle$ are analogous to the LCAO (linear combination of atomic orbitals) for constructing a molecular electronic orbital centered on several atoms and they are also numerically very convenient, as the trilobite space $|T_q\rangle\langle T_q|$ is for $M < n^2 = J$ smaller than the space spanned by the unperturbed hydrogenic eigenfunctions in a given manifold n.

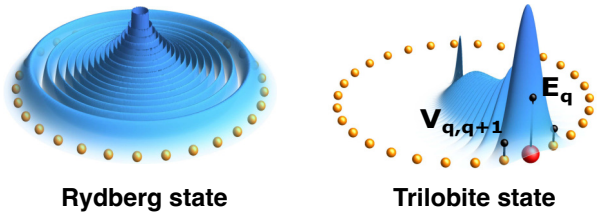

Figure 1: Exemplary states used in the calculation for a Rydberg level $n = 30$. An exemplary trilobite state $|T_q\rangle$ associated with the scatterer $|q\rangle$, marked in red.

Fig. 1 contrasts for scatterers on a ring with radius $R = 2n^2$ a hydrogenic orbital with a trilobite orbital. The "trilobite" representation inspires a pictorial analysis of the composite and its tight-binding Hamiltonian, since the matrix elements $V_{qq'}$ are given by the amplitude of the trilobite state $|T_q\rangle$ evaluated at the perturber q'. For the particular radius $R = 2n^2$ the tight binding is reduced to dominant next neighbour interactions. Thus, the tight-binding Hamiltonian with nearest-neighbor hopping – a paradigmatic model in condensed matter physics – can be directly realized in a ring Rydberg composite [5]. Figure 2 illustrates the resulting level structure in this case. From each Rydberg manifold descends a subspace of dimension M. The

eigenstates of this perturbed spectrum are Bloch waves in the site representation (black spheres) of the Hamiltonian, and show a one-to-one correspondence with the nodal structure of the electronic wave function along the ring. A thermodynamic limit exists when the number of perturbers M and the principal quantum number n are increased to infinity in tandem.

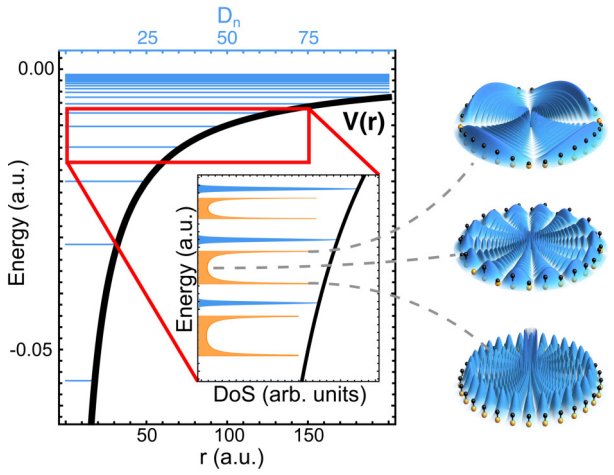

Figure 2: The level structure and exemplary eigenstates of the ring Rydberg composite with radius $2n^2$. The Coulomb potential $V(r)=-1/r$ supports an infinite bound spectrum $E_n=-1/2n^2$ (blue lines). Each line's length represents the level degeneracy $D_n=n^2=J$. The inset highlights the densities of states of three Rydberg levels. A highly structured DoS containing M levels (orange) forms, shifted away from the unaffected $J-M$ states (blue). Both representations of the eigenstate amplitudes located at the marked positions are shown in blue (position representation of the Rydberg electron) and black (site representation).

As demonstrated above, the traditional description of the perturbed Rydberg spectrum from atomic physics (1) is equivalent to the tight-binding Hamiltonian (4) from solid state physics. This equivalence links our studies of Rydberg atoms immersed in an environment (Refs. [3, 5, 6]) conceptually and opens new research perspectives.

Naturally, this equivalence suggests the possibility of Anderson localization of the Rydberg electron in the ring composite, particularly in the case highlighted in Fig. 2 with nearest-neighbor hopping. In [7] we show that Anderson localization of a Rydberg electron can be achieved by adding random disorder to the perturber positions and reaching the thermodynamic limit with $n, M \to \infty$. Moreover, since the hopping amplitudes in Eq. 4 arise from the Rydberg electron's motion in the confluence of infinite-ranged Coulomb and zero-ranged electron-scatterer potentials, a variety of effective interactions are achievable. The trilobite states in Fig. 3 show that ring sizes with $R = 1.5n^2$ and $R = n^2$ give rise to long and even infinite-ranged interactions. Such composites realize localization scenarios in novel regimes of interactions and correlated disorder.

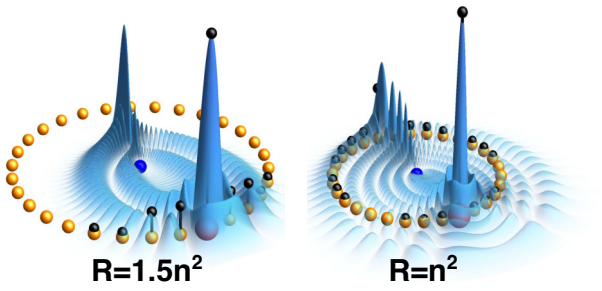

Figure 3: Ring composite trilobite states for different ring sizes.

The generality of Eq. 4 allows us to consider more complicated geometries, for example 2D and 3D lattices as in Ref. [3] or a random gas as in Ref. [6]. These composites are characterized by strong on-site and off-diagonal disorder and a complicated array of hopping amplitudes, and can be analyzed with a similar approach as we have recently developed in the context of interacting Rydberg gases. The dipolar interactions between randomly positioned Rydberg atoms are disordered and long-ranged, creating both localized cluster states and diffuse delocalized states held together by long-range couplings [8]. We find similar behavior here, with cluster states identifiable as the trilobites found to persist in a dense random gas [6] and delocalized states similar to those described in Ref. [3].

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2.9 The stochastic hierarchy of pure states

XING GAO, LIPENG CHEN, AND ALEXANDER EISFELD

The hierarchy of pure states (HOPS) is a stochastic wavefunction based method to solve the dynamics of open quantum systems with coupling to a structured non-Markovian environment [1]. To overcome the rapid growth of the number of coupled differential equations for an increasing number of environmental modes, we reformulate HOPS in the form of stochastic matrix product states and matrix product operators [3]. A localization property of the stochastic processes enables the use of adaptive grids that allow us to handle excitation transport for nearly arbitrary system sizes [2]. Finally, these features of HOPS can be also used in the calculation of correlation functions that are needed, for example, for spectroscopy [4].

The open quantum system: We consider a quantum system coupled linearly to a (infinite) set of harmonic oscillators. The total Hamiltonian is written as $\hat{H}_{\rm tot} = \hat{H}_{\rm S} + \hat{H}_{\rm B} + \hat{H}_{\rm SB}$, with $\hat{H}_{\rm S}$, $\hat{H}_{\rm B}$, and $\hat{H}_{\rm SB}$ describing the system, the bath and the system-bath interaction, respectively. We consider a bath that can consist of several independent parts: $\hat{H}_{\rm B} = \sum_{j=1}^{J} \hat{H}_{{\rm B},j}$ with $\hat{H}_{{\rm B},j} = \sum_\lambda \omega_{\lambda j} \hat{b}^\dagger_{\lambda j} \hat{b}_{\lambda j}$ where $\hat{b}^\dagger_{\lambda j}$ and $\hat{b}_{\lambda j}$ are bosonic creation and annihilation operators. The system-bath coupling Hamiltonian is taken as

$$\hat{H}_{\rm SB} = \sum_j \hat{L}_j \otimes \sum_{\lambda,j} c_{\lambda,j} (\hat{b}_{\lambda,j} + \hat{b}^\dagger_{\lambda,j}), \tag{1}$$

where each system operator $\hat{L}_j$ couples to its own environment. It is convenient to define the spectral densities, $S_j(\omega) = \pi \sum_\lambda c^2_{\lambda,j} \delta(\omega - \omega_{\lambda,j})$, which describe the frequency dependent system-bath coupling strength of the j-th bath. In the time-domain, the bath correlation function,

$$\alpha_j(t) = \frac{1}{\pi} \int_0^\infty {\rm d}\omega S_j(\omega) \big[\coth(\frac{\omega}{2T}) \cos\omega t - i \sin\omega t \big], \tag{2}$$

fully characterizes the influence of the environment at temperature T. We use the units $\hbar = k_B = 1$. We assume a factorized initial state $\rho_{\rm tot}(0) = \rho(0) \otimes \frac{e^{-H_{\rm B}/T}}{Z_{\rm B}}$ with partition function $Z_{\rm B} = {\rm Tr}_{\rm B}\{e^{-H_{\rm B}/T}\}$.

HOPS: To improve readability, we use in the following only a single coupling operator $\hat{L}$ with $\hat{L} = \hat{L}^\dagger$. The general case is discussed in Ref. 3. Within the HOPS method the reduced density operator $\rho(t)$ is obtained from

$$\rho(t) = \mathbb{E}\big\{ |\psi_t(Z_t^*)\rangle\langle\psi_t(Z_t^*)| \big\}, \tag{3}$$

where the $|\psi_t(Z_t^*)\rangle$ are vectors in the system Hilbert space that depend on stochastic processes Z_t, and $\mathbb{E}[\cdots]$ denotes the average over trajectories. The Z_t are complex valued and fulfill $\mathbb{E}[Z_t] = 0$ and $\mathbb{E}[Z_t Z_s] = 0$ and $\mathbb{E}[Z_t Z_s^*] = \alpha(t-s)$. To obtain the HOPS, the bath-correlation function (2) is approximated by a sum of exponentials (which we denote as modes),

$$\alpha(t) \approx \sum_{k=1}^{K} d_k e^{-\nu_k t} \;\; (t \geq 0), \tag{4}$$

with complex numbers ν_k. Then HOPS reads [1],

$$\begin{aligned} \partial_t \psi_t^{\mathbf{n}} = & \big[-i\hat{H}_{\rm S} + \hat{L} Z_t^* - \sum_{k=1}^{K} n_k \nu_k \big] \psi_t^{\mathbf{n}} \\ & + \hat{L} \sum_{k=1}^{K} \Big[\frac{d_k}{\sqrt{|d_k|}} \sqrt{n_k}\, \psi_t^{\mathbf{n}-\mathbf{e}_k} - \sqrt{|d_k|} \sqrt{n_k+1}\, \psi_t^{\mathbf{n}+\mathbf{e}_k} \Big]. \end{aligned} \tag{5}$$

The superscript $\mathbf{n} = \{n_1, \cdots, n_k, \cdots, n_K\}$ consists of a set of non-negative integer indices, and $\mathbf{e}_k = \{0, \cdots, 1_k, \cdots, 0\}$. The initial conditions are $\psi^{\mathbf{0}}_{t=0} = \psi_{\rm ini}$ and $\psi^{\mathbf{n}}_{t=0} = 0$ for $\mathbf{n} \neq \mathbf{0}$. The trajectories entering Eq. (3) are $\psi_t(Z_t^*) = \psi_t^{\mathbf{0}}(Z_t^*)$. In practice the hierarchy has to be truncated by approximating the last term on the right hand side based on a condition on $\mathbf{n}$. For example one can set this term equal to zero, for $\sum_k n_k < n_{\rm max}$. Unfortunately, the size of the HOPS grows rapidly with an increasing number of modes K or more independent environments. To overcome this problem, we show that HOPS can be rewritten in terms of matrix product states (MPS) and matrix product operators (MPO) [3].

Formulation of HOPS using Matrix Poduct states: First, we formally define states $|\mathbf{n}\rangle = |n_1, \cdots, n_K\rangle$ and introduce $|\Psi(Z^*)\rangle_t = \sum_{\mathbf{n}} \psi_t^{\mathbf{n}}(Z^*) |\mathbf{n}\rangle$ with the auxiliary vectors $\psi_t^{\mathbf{n}}$ of HOPS as expansion coefficients. With $\langle \mathbf{n}|\mathbf{n}'\rangle = \delta_{\mathbf{n}\mathbf{n}'}$, these coefficient can be obtained from $\psi_t^{\mathbf{n}} = \langle \mathbf{n}|\Psi\rangle_t$. The HOPS, Eq. (5), is then expressed as $\partial_t |\Psi(Z^*)\rangle_t = -i\hat{H}_{\rm eff}(Z^*) |\Psi(Z^*)\rangle_t$, with the effective stochastic Hamiltonian

$$\begin{aligned} \hat{H}_{\rm eff}(Z^*) = & \hat{H}_{\rm S} + i\hat{L} Z_t^* - i \sum_{k=1}^{K} \nu_k\, \hat{b}_k^\dagger \hat{b}_k \\ & - i\hat{L}^\dagger \sum_{k=1}^{K} \sqrt{|d_k|}\, \hat{b}_k + i\hat{L} \sum_{k=1}^{K} \frac{d_k}{\sqrt{|d_k|}}\, \hat{b}_k^\dagger, \end{aligned} \tag{6}$$

where creation ($\hat{b}_k^\dagger$) and annihilation ($\hat{b}_k$) have been defined by $\hat{b}_k^\dagger |\mathbf{n}\rangle = \sqrt{n_k+1} |\mathbf{n} + \mathbf{e}_k\rangle$ and $\hat{b}_k |\mathbf{n}\rangle = \sqrt{n_k} |\mathbf{n} - \mathbf{e}_k\rangle$. Now the labels $\{n_k\}$ of the hierarchy play the role of occupation numbers. It is worth mentioning that the third term in the right hand side looks like a collection of harmonic oscillators, however with complex frequencies $\{\nu_k\}$.

This reformulation of HOPS has not only an esthetic appeal, but the form of Eq. (6) is also

convenient for an implementation in terms of MPSs and matrix product operators (MPOs). We represent the wavefunction MPS: $|\Psi\rangle_t = \sum_{\ell,\mathbf{n},\mathbf{a}} A^{\ell}_{1,a_0} A^{n_1}_{a_0 a_1} \cdots A^{n_K}_{a_{K-1},1} |\ell, n_1, \cdots, n_K\rangle$. Each $A^{n_i}_{a_{i-1}a_i}$ is a rank-3 tensor with 'physical index' n_i and 'virtual indices' a_{i-1} and a_i. The ranges of the virtual indices are denoted as bond dimensions M_i. Increasing the bond dimensions can systematically improve the accuracy of an MPS. The bond dimensions can also be optimized adaptively in each time-step during propagation. In conjunction with the MPS, Eq. (6) is written as a MPO. Introducing MPOs allows one to calculate $\hat{H}_{\text{eff}}|\Psi\rangle_t$ using contractions of local matrices. The computational cost is then only polynomial in the number of effective modes K. We stress that all tensors of the MPS and the MPO depend on the stochastic processes.

Typically a non-linear, normalizable version of Eqs. (5) and (6) is required to achieve convergence with respect to the number of trajectories [1]. It is obtained through the following replacements: $\hat{L}^\dagger \to \hat{L}^\dagger - \langle \hat{L}^\dagger \rangle_t$ and $Z_t^* \to Z_t^* + \int_0^t \mathrm{d}s\, \alpha^*(t-s)\langle \hat{L}^\dagger \rangle_s$. Expectation values $\langle \cdot \rangle_t$ are calculated using the normalized state.

Example: As an example, we consider the motion of (electronic) excitations under the influence of damped vibrational modes, along a long linear chain, as shown in Fig. 1(a). This model describes e.g. molecular aggregates or biological light harvesting systems with coupling to vibrations of the molecules. Treating each molecule as an electronic two-level system, the system Hamiltonian can be written as $\hat{H} = \sum_{j=1} \hat{H}_j + \sum_{jj'} \hat{V}_{jj'}$, where the Hamiltonian $\hat{H}_j$ of the jth site is characterized by a system part $\hat{H}_{\mathrm{S},j} = \epsilon_j \hat{a}_j^\dagger \hat{a}_j$, system-bath coupling operators $\hat{L}_j = \hat{a}_j^\dagger \hat{a}_j$ and a corresponding spectral density $S_j(\omega)$, which contains molecular vibrations and the coupling to the local surroundings. The coupling between sites is typically the long-range dipole-dipole interaction and assumed not to couple directly to the environment. For this problem we use a MPO/MPS as shown in Fig. 1b, where each local system Hamiltonian $\hat{H}_{\mathrm{S},j}$ is followed by its modes from the decomposition of the respective bath-correlation function. This allows us to also conveniently treat the case of several electronic excitations, needed for example to describe exciton-exciton annihilation experiments or multidimensional femtosecond experiments. In Fig. 1(c) and (d) we show examples for two different bath-correlation functions. In (c) it comes from a Debye spectral density at high temperature and in (d) it represents damped intramolecular vibrations at low temperature. In both cases around 500-1000 trajectories are sufficient to achieve converged results. The efficiency of the approach can be seen by looking at the bond dimensions, which remain small for all times. Note that with 100 sites we are dealing with system sizes that are not treatable using the standard HOPS.

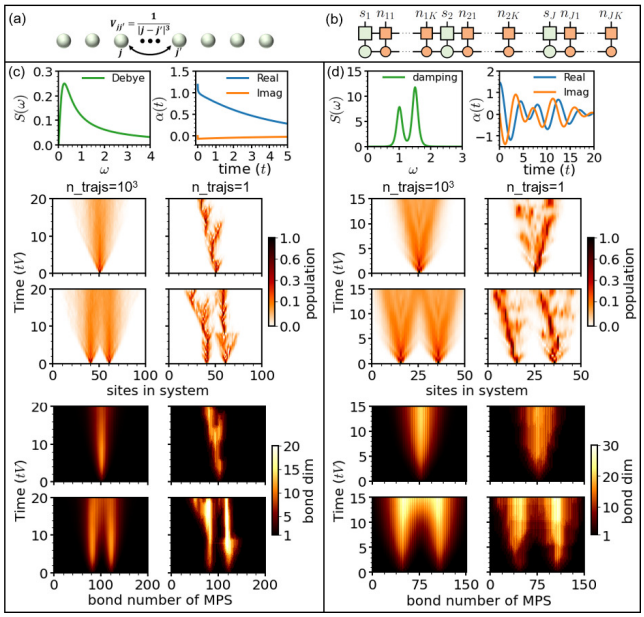

Figure 1: Application of HOMPS to a linear chain. (a) one dimensional chain with intermolecular coupling strength $V_{jj'} = \frac{1}{|j-j'|^3}$. (b) The used MPS/MPO structure. (c), (d): Evolution of population and bond dimension for both average (with $n_{\text{traj}} = 1000$ trajectories) and single trajectories. The corresponding spectral densities and bath-correlation functions are shown in the upper row of each panel. Parameters of HOMPS are (c) $K = 1$ and $n_{\max} = 40$. (d) $K = 2$, $n_{\max} = 20$.

Conclusions: The combination of the stochastic hierarchy of pure states with matrix product states opens the door to treat large molecular aggregates with realistic coupling to internal vibrations and the environment. To go to even larger sizes it is straightforward to use the adaptive algorithm that we developed previously for stochastic trajectories [2],since both the site populations and also the bond dimensions remain well localized (see the examples in Fig. 1). This allows in principle to handle arbitrarily large systems as long as the interaction to the environment is not too weak.

Typically experiments probe the aggregates by linear and non-linear spectroscopy. We developed a framework to apply the stochastic HOPS directly to the calculation of the corresponding dipole-dipole time-correlation functions [4]. We want to stress that our formalism is not restricted to aggregates but can be applied to general open quantum systems.

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2.10 Eigenstate reconstruction from spatially resolved near-field spectra

FULU ZHENG, XING GAO, AND ALEXANDER EISFELD

A general problem in quantum mechanics is the reconstruction of eigenstates from measured data. In the case of molecular aggregates, information about excitonic eigenstates is vitally important to understand their optical and transport properties. Here we show that from spatially resolved near field spectra it is possible to reconstruct the underlying delocalized aggregate eigenfunctions. Although this high-dimensional non-linear problem defies standard numerical or analytical approaches we have found that it can be solved using a convolutional neural network. For both one-dimensional and two-dimensional aggregates we find that the reconstruction is robust to various types of disorder and noise.

States where electronic excitation is coherently shared by several particles appear in many areas of physics. Examples that we investigate are biological and artificial light harvesting systems [1], assemblies of Rydberg atoms [5] or molecules deposited on surfaces [2]. For the latter case, near-field spectroscopy allows one to obtain spatially resolved spectra [3]. On dielectric surfaces at low temperatures, one has very sharp absorption lines, that allow one to distinguish the eigenstates energetically [2]. In the following we show that from the position dependence of such spectra one can reconstruct the underlying eigenstates. Our procedure is sketched in Fig. 1.

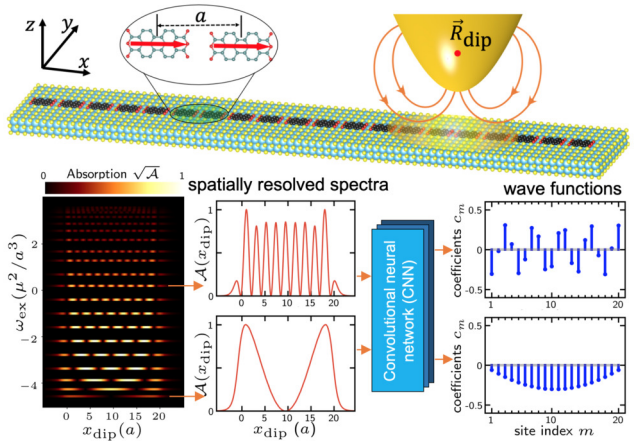

Figure 1: Top: Sketch of the setup. Molecules form an aggregate on the surface (here a one-dimensional linear chain). The red arrows represent the transition dipole moments $\vec{\mu}$ of the molecules. We use distance a as our unit of length. The aggregate is located in the x-y-plane. Bottom: Left: spatially and frequency resolved near-field spectrum stemming from a Hertzian dipole located $2a$ above the aggregate and with dipole pointing along the z axis. Middle: spatially resolved spectra for fixed frequency are fed into a convolutional neural network (CNN). Right: extracted wave functions corresponding to the respective spectra.

Theoretical description: For each of the N individual molecules comprising the aggregate, we consider two electronic states: 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 is in the global ground state $|g_{\rm agg}\rangle = |g\rangle_1 \cdots |g\rangle_N$. For linear absorption we are interested in states with one excitation. Using basis states $|m\rangle = |e\rangle_m \prod_{n\neq m}^{N} |g\rangle_n$ the excited state Hamiltonian for the system is written as

$$H_{\rm ex} = \sum_{m=1}^{N} \varepsilon_m |m\rangle\langle m| + \sum_{m} \sum_{n\neq m} V_{mn} |m\rangle\langle n|. \qquad (1)$$

Here, ε_m is the transition energy of molecule m and V_{mn} is the transition dipole-dipole interaction, which we take as $V_{mn} = \frac{1}{R_{mn}^3}\left(\vec{\mu}_m \cdot \vec{\mu}_n - 3(\vec{\mu}_m \cdot \frac{\vec{R}_{mn}}{R_{mn}})(\vec{\mu}_n \cdot \frac{\vec{R}_{mn}}{R_{mn}})\right)$ with $\vec{R}_{mn}$ the distance vector from molecule m to n and $R_{mn} = |\vec{R}_{mn}|$. From the Schrödinger equation $H_{\rm ex}|\phi\rangle = E|\phi\rangle$, one obtains the N eigenenergies E_ℓ with corresponding eigenstates,

$$|\phi^{(\ell)}\rangle = \sum_{m=1}^{N} c_m^{(\ell)} |m\rangle. \qquad (2)$$

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

We model the electromagnetic field stemming from the tip as a Hertzian dipole $\vec{d}$, located at position $\vec{R}_{\rm dip}$ a few nanometers (tip distance + radius of the tip) above the aggregate. The resulting field has a strong spatial variation on the scale of a few nanometers in the plane of the aggregate. With $\vec{E}(\vec{R}_m; \vec{R}_{\rm dip})$ we denote the electric field component at the position of monomer m. The absorption strength from the ground state to the eigenstate $|\phi^{(\ell)}\rangle$ can be written as [3]

$$\mathcal{A}^{(\ell)}(\vec{R}_{\rm dip}) = |\sum_{m=1}^{N} c_m^{(\ell)}\, \vec{\mu}_m \cdot \vec{E}(\vec{R}_m; \vec{R}_{\rm dip})|^2. \qquad (3)$$

Eq. (3) is valid for fields which vary strongly over the extent of the aggregate but only very weakly over the extent of a single molecule. For brevity we often drop the eigenstate-index ℓ and write c_m for the wavefunction coefficients and $\mathcal{A}(\vec{R}_{\rm dip})$ for the corresponding absorption strength. In the following we choose $\vec{d}$ to be perpendicular to the surface. In Ref. 6 we discuss the case of arbitrary orientation of the dipole direction $\vec{d}$ and relate it to the incoming far-field of a scanning optical near-field microscope setup. We also validated the model presented above by modeling the tip within the discrete dipole approximation, calculating the response of both aggregate and tip self consistently.

Reconstruction of the wave function coefficients using a convolutional neural network: To reconstruct the eigenstate wave functions Eq. (2) from the near-field absorption spectra we use CNNs with several convolutional layers (for details see Ref. 4). The inputs are spatially discretized near-field spectra $\mathcal{A}(\vec{R}_{\rm dip})$ evaluated at a finite number $N_{\rm tip}$ of positions $\vec{R}_{\rm dip}$ at fixed distance from the aggregate. The input for the CNN is therefore a real-valued array with $N_{\rm tip}$ elements. The outputs are the corresponding predicted coefficients $c_m^{\rm pre}$ of the wave function, which we have normalized to fulfill $\sum_m |c_m^{\rm pre}|^2 = 1$. The dimension of the output is equal to the number of molecules N. To evaluate the quality of the prediction of the CNN we use the "loss function" $L = \frac{1}{4}\sum_{m=1}^{N} |c_m - c_m^{\rm pre}|^2$, where $c_m - c_m^{\rm pre}$ is the difference between true and predicted coefficients. This loss function, which takes values between 0 and 0.5, is minimized to optimize the parameters inside the CNN during the training. Adequate network training requires a sufficient amount of appropriate training data which in our case is pairs of wavefunctions and corresponding spatial spectra. We use a physically motivated procedure to construct a viable data set for training. We calculate the wavefunctions by diagonalizing Hamiltonian (1) for random values of the parameters ϵ_n and V_{nm}, physically corresponding to static disorder typically caused by 'defects' of the surface. Finally, we augment the date by random noise. This augmentation on the one hand makes the network more robust, on the other hand it allows us also to extract the eigenstate coefficients from non-ideal spectra, as it would be the case in an experiment.

Results: In Fig. 2 examples of reconstructed wavefunction amplitudes for a one dimensional linear chain are shown. In Ref. [4] also the cases of disordered chains and two-dimensional arrays is discussed. We find that for all cases considered we can very accurately predict the eigenstate coefficients $c_m^{(\ell)}$ of Eq. (2). Even when the spectra become very noisy, this reconstruction is still possible; examples can be seen in the right column of Fig. 2. We also investigated the situation homogeneously broadened lines of the spectra, such that the peaks corresponding to eigenstates start to partially overlap. Even in this situation, a reasonable reconstruction was possible.

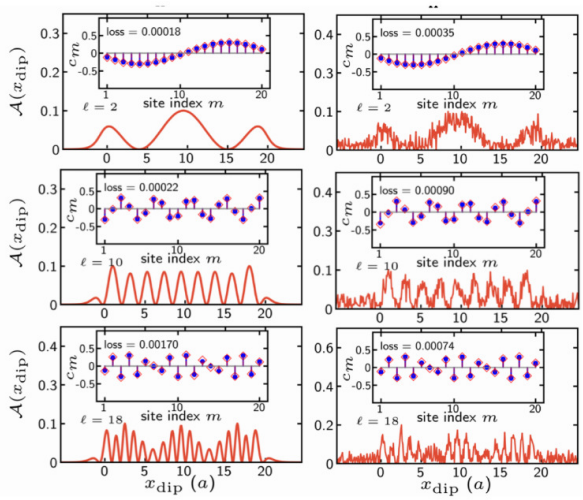

Figure 2: Examples of reconstructed wavefunction amplitudes for a one dimensional chain. The main panels show the spatially resolved spectra at fixed frequency and the insets show the reconstructed wavefunction coefficients (magenta diamonds) together with the exact ones (blue dots). The spectra on the right are the same as on the left, but with added random noise. Examples of two-dimensional arrangements can be found in Ref. 4

Conclusions: To conclude, we have shown that properly trained CNNs can obtain wave functions from their spectra to a very high accuracy even in the presence of significant experimental noise and imperfect conditions, thus confirming that that the inversion of Eq. (3) is possible and providing a method for doing so. We have tried to obtain the wave-function coefficients by using various optimizers, including Gaussian process regression. We only obtained reasonable results for quite small aggregates ($N \lesssim 10$) and wave functions with a small number of nodes, cementing the need for sophisticated machine learning techniques.

In addition to the application to near-field spectra of molecular aggregates, the methodology adopted in present work can be applied to spectra of other systems, such as those of electron energy-loss spectroscopy of silver nanowires where a similar inversion as Eq. (3) is required. Hence the implementation of CNNs, as shown here, opens new possibilities to extract key insight from experimental spectra.

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2.11 Ultracold collisions between Rydberg atoms and ground state atoms

PANAGIOTIS GIANNAKEAS AND MATTHEW T. EILES

When a ground state "perturber" atom encounters a highly excited Rydberg atom, the two particles can either bind together into a long-range Rydberg molecule or react, changing the state of the Rydberg atom. We have developed a semi-analytical theoretical method based on the generalized local frame transformation (GLFT) to calculate the Rydberg atom-perturber potential energy curves (PECs). This powerful method is more accurate than conventional approaches and provides a more general framework. By using the GLFT method in conjunction with physically-motivated analytic models we have uncovered two novel effects in interacting Rydberg-ground state atom systems.

Background: A Rydberg atom is characterized by a high principal quantum number n and, in the perturber's absence, angular momentum l. The partial wave expansion allows the Rydberg-perturber interaction to be parametrized by the electron-atom scattering phase shifts $\delta_L(k)$, where L and $k^2/2$ are respectively the electron's angular momentum and energy relative to the perturber. Previous studies included only $L = 0$ and $L = 1$ terms and have almost universally relied on diagonalization in a large basis of Rydberg states [1, 2]. The failure of this basis expansion to rigorously converge has impeded efforts to obtain spectroscopic accuracy [2]. The GLFT method, which we extended to long-range Rydberg molecules in Ref. [3], capitalizes on the presence of local symmetries in this system. These lead to the near-separability of the Hamiltonian in different regions of space. Far from the perturber, l and n form a set of good quantum numbers for the electronic wave function, while close to it, the Coulomb potential is nearly constant and L and k characterize the approximate eigenstate. The GLFT describes how to project these incompatible sets of quantum numbers onto each other and allows us to match the solutions from different regions of space together on a surface centered around the perturber. This determines the reaction matrix and, subsequently, the molecular PECs.

Dressed ion-pair states: With these converged PECs we examined the vibrational spectra of Sr_2 Rydberg molecules and extracted improved estimates of the $e-$Sr scattering phase shifts from a comparison with experimental measurements [3]. Encouraged by this evidence of the improved accuracy of the GLFT framework, we then took advantage of its additional generality to calculate, for the first time, the effect of higher ($L \geq 2$) scattering partial waves [4]. We calculated the D- and F-wave scattering phase shifts for rubidium using a two-electron R-matrix code [2]. Fig. 1 shows the resulting Rb(n)+Rb($5s$) PECs (blue), labeled by the approximate L value of their respective electronic states. We have set M, the projection of L onto $\vec{R}$, to zero. Not only does $L \geq 2$ scattering produce PECs capable of supporting vibrational states, but these PECs are, to leading order in the internuclear distance R, Coloumbic, i.e. $U_{L\geq 2}(R) \propto R^{-1}$.

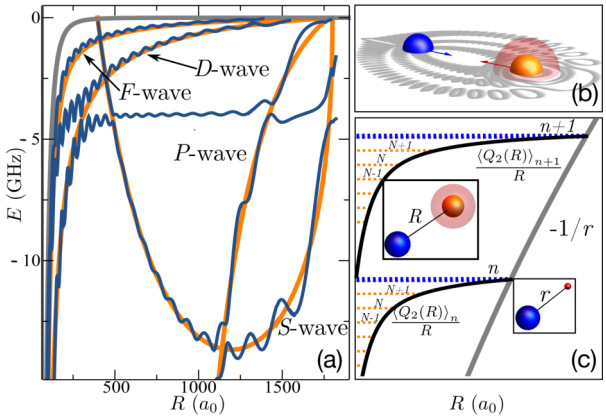

Figure 1: (a) $M = 0$ PECs of the Rb(30)+Rb($5s$) molecule, calculated using the GLFT method (blue) and Eq. 2 (orange). (b) An illustration of the dressed ion-pair state, composed of the Rydberg core (blue) and perturber (orange) dressed with excess charge (red). (c) A schematic (not to scale) of the nested D-wave electronic and vibrational energy levels, both obeying the Rydberg formula.

A re-interpretation of the binding mechanism of these molecules provides clarity to this unexpected Coulomb attraction emerging between the Rydberg atom and the perturber. The S-wave "trilobite" wave function depicted with a gray contour in Fig. 1(b) shows that the perturber breaks the spherical symmetry with respect to the core and mixes many high$-l$ Rydberg components. Close to the perturber this wave function amplitude peaks prominently. This represents an accumulation of excess electronic charge, depicted by the red sphere, which is spherically symmetric with angular momentum L. Intuitively, this excess charge is related to the Wigner-Smith time delay, which controls how the perturber speeds or slows the electron as it scatters. We derived an expression for the excess charge,

$$\langle Q_L(R)\rangle_n = -\frac{1}{2n^3}\left(\frac{2}{\pi k}\frac{d\delta_L(k)}{dk}\right), \qquad (1)$$

which reveals this connection explicitly through the appearance of the time delay in brackets. Eq. 1 implies that the molecule behaves as *a dressed ion-pair*, with the positive Rydberg core interacting with the perturber, dressed by the excess charge. This leads to a semiclassical formula for the PECs,

$$U_L(R) = -\int_\infty^R \mathrm{d}R' \frac{Q_L(R')}{R'^2} = -\frac{1}{2(n-\delta_L(k)/\pi)^2}. \qquad (2)$$

The excellent agreement between Eq. 2 and the exact results shown in Fig. 1 supports the dressed ion-pair interpretation, which in turn explains the Coulombic $L \geq 2$ PECs. Unlike S- and P-wave scattering, where the charge fluctuates as a function of R, the $L \geq 2$ PECs demand that the effective charge is constant. The Born approximation, in excellent agreement with our numerical phase shifts, gives $\delta_{L\geq 2} \propto k^2$. Eq. 1 then predicts an R-independent charge. The vibrational spectra supported by these Coulomb PECs must conform to a Rydberg formula, confirmed numerically with the GLFT and analytically using the effective charge. As illustrated in Fig. 1(c), this results in a nested Rydberg *vibrational* spectrum inside of the Rydberg *electronic* spectrum [4]. The oscillations in these potentials can be suppressed by setting $M = 2$.

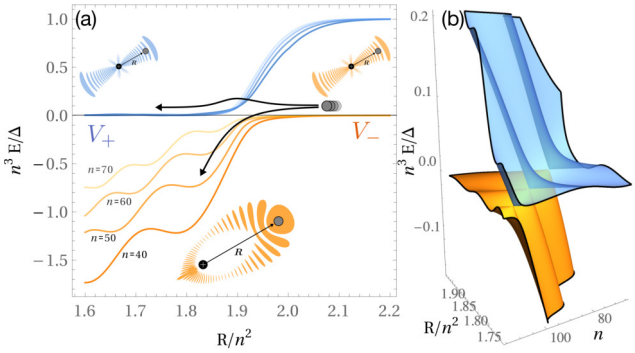

Figure 2: (a) Adiabatic potential curves governing the collision Rb(nf)+Rb($5s$). An incoming particle can either adiabatically follow V_- or non-adiabatically hop onto V_+. By scaling the energies and distances as a function of n, similarities between n levels become clear. (b) The full potential energy surfaces treating n as a synthetic dimension. Conical intersections appear at certain (n, R) tuples.

Conical intersections and l-changing collisions: The PECs govern not only the formation of molecules, but also the outcomes of ultracold collisions. Recently measured lifetimes of Rb(nf) states were incongruously short [5], and we surmised that the reaction Rb(nf) + Rb($5s$) $\rightarrow$ Rb(nl) + Rb($5s$) was the mechanism for their fast decay. Based on GLFT calculations of the PECs, we developed a two-level model (Fig. 2a) including only the coupled diabatic trilobite and nf PECs. The nf level's energetic proximity to the trilobite PEC results in a strong coupling near the classical turning point of the Rydberg atom. Adiabatically proceeding along the V_- PEC from large R, an incoming atom induces a change from the electron's initial nf state to the trilobite state (see orange insets). Such a collision changes the l quantum number rapidly and limits the lifetime of Rydberg nf states. However, if the non-adiabatic coupling is sufficiently strong, the perturber can "hop" over the avoided crossing and continue along the V_+ potential, preserving the diabatic state's character (blue inset). We account for this in the l-changing collision rate by including the Landau-Zener curve-hopping probability, giving a total rate

$$\gamma = \sigma \rho v \left[1 - \exp\left(\frac{-\pi d(n, R_0)}{4v|\mathcal{P}(n, R_0)}\right)\right], \qquad (3)$$

where $\sigma = \pi R_0^2$ is the geometric cross section associated with the l-changing collision radius R_0, v is the collision velocity, ρ is the gas density, $d(n, R_0)$ is the separation between adiabatic potential curves, and $\mathcal{P}(n, R_0)$ is the off-diagonal P-matrix element giving the strength of the non-adiabatic coupling. The non-adiabatic transition probability is negligible for most n, resulting in l-changing rates proportional to n^4 at typical ultracold temperatures, consistent with available experimental data [5]. However, certain Rydberg states – e.g. $n = 79, 99, 111$ in Rb – have anomously small l-changing collision rates, nearly independent of v. This suggests very strong non-adiabatic effects. By promoting n to a continuous variable, we computed potential energy surfaces as a function of the real parameter R and the *synthetic parameter* n. This reveals that the strong non-adiabatic physics is inherited from conical intersections embedded in the higher-dimensional surfaces. Two conditions must be met at a conical intersection: the perturber lies in a radial node of the nf wave function, and the diabatic trilobite PEC intersects the diabatic nf PEC. The dressed-ion PEC (Eq. 2) reveals that this latter condition is satisfied when $\delta_{L=0} = \delta_{l=3}$, i.e. when the scattering phases of both the perturber and the short-range core potentials of the Rydberg atom are identical. At integer n values in the vicinity of these conical intersections, the Rydberg nf states will have demonstrably longer lifetimes in spite of collisions with ground state atoms [5].

Outlook: The generality of the GLFT method allows us to readily employ it elsewhere. We have recently studied photoionization in an ultracold gas using the GLFT, finding that the interference between photoelectron pathways – one directly from the ion and one backscattered from a perturber – imprints an oscillatory fine structure onto the photoionization cross sections, akin to a low energy variant of the extended X-ray absorption fine structure [6]. The GLFT can also be used to study polyatomic molecules with a molecule replacing the atomic perturber, and we expect that pairing it with simpler analytic models will continue to be fruitful in studying non-adiabatic physics in Rydberg systems.

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2.12 Electrohydraulic Activity of Tissues

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Active matter approach to tissue dynamics. Tissues are assemblies of large numbers of cells, which form an active soft material. These materials are governed by chemical signals between cells which coordinate active mechanical processes but which can also give rise to fluid flows and to electric fields and currents. Tissues are therefore not only chemical and mechanical devices but also electrohydraulic systems. Indeed, cell fluid pumping is mediated by ion pumps which create differences in osmotic pressures, thus generating fluid flows that can lead to the formation of fluid-filled lumens inside tissues. Ion transport also generates electric fields, which, in turn, can influence cell proliferation and differentiation, adding an additional layer of complexity to tissue dynamics. Here we develop a coarse grained active matter approach to tissue electrohydraulics based on hydrodynamic concepts.

Hydrodynamic theory of tissue electrohydraulics. To capture the hydraulic properties of tissues, we also adopt a two-fluid description, where the cells, which form the first fluid, are permeated by the interstitial fluid. In the long-time limit (several days or weeks) that we consider, cells are able to reorganize such that an effective description of the tissue as a viscous active fluid can be used.

The stress tensor of the system is decomposed into $\boldsymbol{\sigma}^{\rm c} + \boldsymbol{\sigma}^{\rm f}$ with $\boldsymbol{\sigma}^{\rm c}$ the cell stress and $\boldsymbol{\sigma}^{\rm f}$ the interstitial fluid stress, and the force balance reads (inertia is negligible):

$$\mathrm{div}\boldsymbol{\sigma}^{\rm c} + \boldsymbol{f}^{\rm int} = 0\,, \quad \mathrm{div}\boldsymbol{\sigma}^{\rm f} - \boldsymbol{f}^{\rm int} = 0\,, \tag{1}$$

where $\boldsymbol{f}^{\rm int}$ represents the internal force densities that are exerted between cells and interstitial fluid. To a first approximation, the interstitial fluid stress is simply defined by pressure $\boldsymbol{\sigma}^{\rm f} = -P^{\rm f}\mathbf{1}$ with $P^{\rm f}$ the fluid pressure. To capture the directional ion transport performed by cells, we define a cell polarity field $\boldsymbol{p}$ with unit norm. We also consider the electric field $\boldsymbol{E}$ and the electric current density $\boldsymbol{j}$ within the tissue. The constitutive equations for the internal force density and electric current read [1]:

$$\boldsymbol{f}^{\rm int} = -\kappa(\boldsymbol{v}^{\rm c} - \boldsymbol{v}^{\rm f}) + \lambda_1\boldsymbol{p} + \lambda_2\boldsymbol{E}\,, \tag{2}$$

$$\boldsymbol{j} = -\bar{\kappa}(\boldsymbol{v}^{\rm c} - \boldsymbol{v}^{\rm f}) + \Lambda_1\boldsymbol{p} + \Lambda_2\boldsymbol{E}\,. \tag{3}$$

Eq. (2) provides a generalization of Darcy's description of porous media to the case of active material with electric properties. In this description, κ is a friction coefficient, $\lambda_1\boldsymbol{p}$ accounts for active fluid pumping by the cells, while the term proportional to λ_2 corresponds to an electroosmotic transport. Similarly, Eq. (3) is a generalized Ohm law where Λ_2 is the electric conductivity of the tissue, $\bar{\kappa}$ is a reverse electroosmotic coefficient and Λ_1 characterizes the contribution of ion pumping to the electric current. Finally, the constitutive equation for the cell stress tensor $\boldsymbol{\sigma}^{\rm c}$ is also obtained by symmetry arguments. Its isotropic part is given by:

$$\sigma^{\rm c} + P^{\rm c}_{\rm h} = \bar{\eta}\nabla\cdot\boldsymbol{v}^{\rm c} - \nu_1\boldsymbol{p}\cdot\boldsymbol{E} - \nu_2\boldsymbol{p}\cdot(\boldsymbol{v}^{\rm c} - \boldsymbol{v}^{\rm f})\,, \tag{4}$$

where $-\sigma^{\rm c}$ is the local cell pressure. We have introduced the tissue bulk viscosity $\bar{\eta}$ and the homeostatic pressure $P^{\rm c}_{\rm h}$, a property specific for tissues that results from a balance of cell growth and cell death. The terms proportional to ν_1 and ν_2 represent bioelectric and biohydraulic stresses induced by a coupling to the electric field or by a (relative) fluid flow, respectively. The anisotropic part of the stress is obtained in a similar way, thus introducing the tissue shear viscosity η and two anisotropic bioelectrohydraulic coefficients ν_3 and ν_4 [1,2].

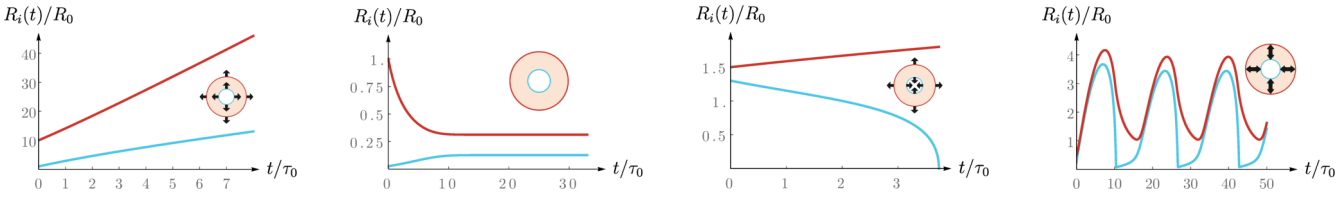

Figure 1: Interplay of lumen and spheroid growth. Lumen (blue) and spheroid (red) radius as a function of time for different choices of parameters. From left to right: spheroid and lumen growth; relaxation to a stable steady-state; lumen closure and spheroid growth; lumen and spheroid oscillations.

Dynamics of lumen formation. Lumen formation is driven by the interplay of tissue electrohydraulics and mechanics that can be described in the framework introduced above. Considering a tissue with a spherical symmetry, the quasistatic dynamics of the cell spheroid, i.e. of the lumen radius $R_1(t)$ and of the outer radius $R_2(t)$, is obtained by solving Eq. (1) using the appropriate boundary conditions [2], see Fig. 1.

Considering lumen nucleation ($R_1 \ll R_2$), the dynamics of R_1 takes a simple form and reads:

$$\frac{\mathrm{d}R_1}{\mathrm{d}t} \simeq P^{\mathrm{eff}} + \lambda^{\mathrm{eff}} R_2 - \frac{2\gamma^{\mathrm{app}}}{R_1}\,. \tag{5}$$

Eq. (5) has a form analogous to a nucleation equation of a droplet in a fluid, where three crucial parameters can be identified. The first one is the effective pressure difference P^{eff} supplemented with the tissue homeostatic pressure and active stress terms. The second parameter is the coefficient λ^{eff},which combines active pumping and electroosmosis. When $\lambda^{\mathrm{eff}} > 0$, fluid pumping is directed inwards and promotes lumen formation, and a sufficiently large spheroid (R_2 large) necessarily develops a lumen. The third key parameter is the surface tension γ^{app}, which resembles a Laplace pressure term and which we discuss below.

Active flexoelectricity of tissues. In a spherical geometry, cell shape anisotropy permits an active flexoelectric term $\Lambda_3 \boldsymbol{p}(\nabla \cdot \boldsymbol{p})$ in Eq. (3), which characterizes the generation of an electric field due to the splayed geometry of the cells. As a consequence, the bare tissue surface tension at the lumen/tissue interface is modified by a flexoelectric contribution, defining the apparent surface tension γ^{app} introduced above. If the flexoelectricity contribution dominates, γ^{app} can even become negative, giving rise to the spontaneous formation of a lumen or allowing tissue thickness oscillations in time (see Fig. 1).

Controlling tissue dynamics with external hydraulic and electric perturbations. An overwhelming majority of experiments in developmental biology use genetic, chemical and mechanical perturbations to test hypotheses and the robustness of biological mechanisms, while perturbations of hydraulic or electrical properties of tissues are rarely used. Using the formalism discussed above, we have explored how tissue dynamics can be manipulated by hydraulic or electric perturbations.

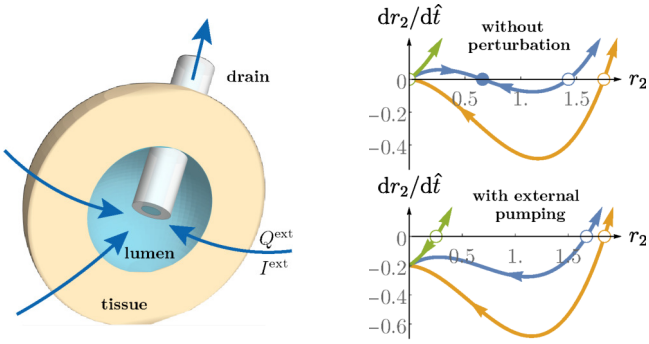

Figure 2: Left. Schematic representation of a cell spheroid with a drain. Right. Phase portraits of the spheroid radius r_2 for spheroids with different proliferating behaviours (different colors). Their proliferation is decreased by the imposition of an external pumping (bottom).

In the case of a cell spheroid, such perturbations could be imposed by inserting a drainage tube or a micrometer-sized electrode to its center [3], see Fig. 2. An order-of-magnitude analysis reveals that imposing an external electric current of the order of $1 - 100$ nA or a volume flow rate of the order of $10^3 - 10^5$ $\mu\mathrm{m}^3/\mathrm{s}$ results in the suppression of a millimeter-sized spheroid. Such values are close to those measured in tissues, for example during the formation of cysts, and therefore seem realistic for practical applications. We find that such perturbations would have to be imposed over sufficiently long time (several days or weeks) to achieve complete suppression of a spheroid [3]. Our work suggests that such electric or hydraulic perturbations could be used to suppress cancerous tumors in a medical context, without the use of chemicals or radiations.

Our work reveals that tissues are not only chemical and mechanical devices but also employ electricity and hydraulics to perform various biological functions. Other examples where tissue hydraulics play a central role is for instance the liver bile fluid network [4]. Fluid flows have also been shown to govern the sequential formation of *C. Elegans* oocytes [5]. Electrohydraulics also opens novel methods for perturbing tissues, with application both in experimental biology and medicine. Whether electrohydraulics could also play a role during morphogenesis and for growth control is an open question that we will address in the future.

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2.13 Self-Organization of Active Surfaces

ALEXANDER MIETKE, IVO SBALZARINI, AND FRANK JÜLICHER

Mechano-chemical self-organization of shape. Morphogenesis is the process of generation of shape or form, for example when the morphology of an organism emerges from active pattern forming processes in an embryonic tissue. Shape is also generated when single cells form protrusions or when cells form a constriction during division. Such morphogenetic processes are in general active, i.e. they require the supply of energy which is transduced to mechanical work by force generating processes at molecular scales.

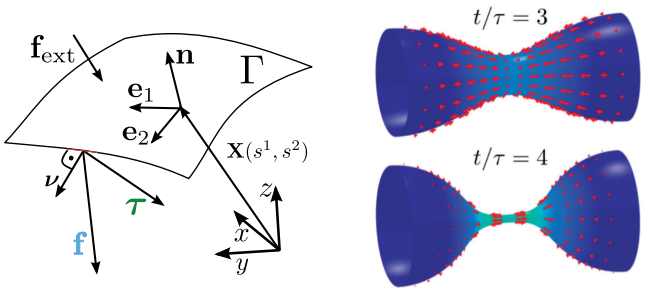

Figure 1: (a) Parametrization of a curved surface. The surface $\mathbf{X}(s^1, s^2)$ is parametrized by the parameters s^1 and s^2. The normal vector is denoted $\mathbf{n}$. External forces act on the surface and the in plane tension implies tangential forces at the surface boundaries. (b) Instability of a cylinder by mechano-chemical self-organization. The cylindrical shape constricts as contractile tension builds up and flows toward the constriction emerge (red arrows).

Active soft matter can exhibit a rich variety of dynamic states and spatiotemporal patterns which are often studied in the bulk [1]. In order to generate shapes, surfaces play an important role. Active processes on surfaces can induce shape changes [2]. Chemical patterns on a surface can coordinate the generation of patterns of active stresses which induce surface flows and via force and torque balances enable surface deformations. Such systems represent a deep integration of mechanical and chemical processes and via mechano-chemical feedback represent systems that can generate shapes of deforming surfaces by the self-organized interplay of active mechanical and chemical processes.

The dynamics of self-organized active surfaces embedded in three dimensional space can be studied using numerical and analytical techniques [3, 4]. We represent the geometry of a smooth surface by a parameterization $\mathbf{X}(s^1, s^2, t)$ and define tangent vectors $\mathbf{e}_i = \partial_i \mathbf{X}$ and the metric tensor $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$, see Fig. 1 (a). The constitutive equation for the stress tensor in the tangent plane reads

$$T_{ij} = T^{\rm eq}_{ij} + 2\eta(v_{ij} - \frac{1}{2} v^k_k g_{ij}) + \bar\eta v^k_k g_{ij} + T^{\rm act} g_{ij} \quad (1)$$

where η and $\bar\eta$ are shear and bulk viscosity, $T^{\rm eq}_{ij}$ is the passive or equilibrium stress, $T^{\rm act}$ is an active stress, and $v_{ij} = (\nabla_i v_j + \nabla_j v_i)/2 + v_n C_{ij}$ is the symmetric velocity gradient tensor, where C_{ij} is the curvature tensor. For simplicity, we use $T^i_n = \kappa \nabla^i C^k_k$, which is the equilibrium stress and κ a bending rigidity of the surface. The force balance then reads

$$\begin{aligned} \nabla_i T^{ij} + C^j_i T^i_n &= -f^j_{\rm ext}, \\ \nabla_i T^i_n - C_{ij} T^{ij} &= -f_{{\rm ext},n}. \end{aligned} \quad (2)$$

where $\mathbf{f}_{\rm ext}$ is the force that acts on the surface by the bulk. The active stress $T_{\rm act} = T_0 f(c)$ is regulated by the concentration c of a diffusing and advected molecular species, which obeys

$$\partial_t c = D \nabla_k \nabla^k c - \nabla_k (c v^k) - C^k_k v_n + j_n \quad . \quad (3)$$

The stress activation function $f(c)$ is nonlinear and saturates for large c.

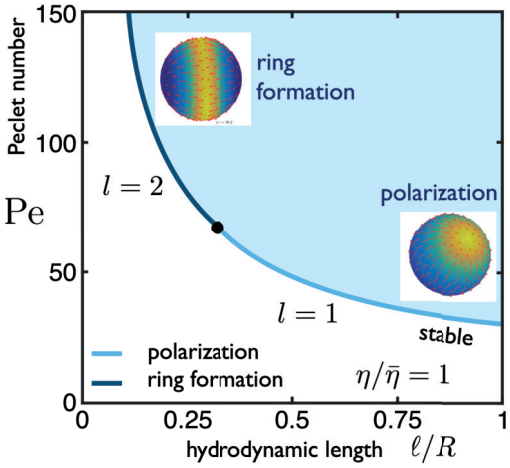

Figure 2: Stability diagram of a sphere as a function of Peclet number and of the hydrodynamic length ℓ. For increasing Peclet number, an isotropic sphere becomes unstable with respect to symmetry breaking modes. For small hydrodynamic length the instability is nematic, leading to a contractile ring. For larger hydrodynamic length the instability generates a polar asymmetry of the sphere.

Here D is a diffusion coefficient and j_n a normal flux describing exchange with the bulk. For given shape and concentration field, the velocity $\mathbf{v} = v^i \mathbf{e}_i + v_n \mathbf{n}$ can be determined form the instantaneous force balance, where $\mathbf{n}$ is the normal vector. This then allows to evolve the shape and the concentration in time by integration of Eq. (3) and by using the normal velocity v_n on the surface to evolve the shape as $\partial_t \mathbf{X} = v_n \mathbf{n}$.

We have investigated the stability diagram for spherical and for cylindrical shapes. In the case of cylinders,

the stability depends on the cylinder length. As the magnitude T_0 of the active stress is increased, the initially stable cylindrical shape becomes unstable. This instability can lead to a stationary constriction or to an oscillatory dynamics. Fig. 1 (b) shows an example of the full nonlinear dynamics of a self-organized active surface starting from a cylinder. As T_0 is increased above the shape instability threshold, a constriction emerges which is driven by a ring-like accumulation of stress activator and active stress. This constriction and the corresponding concentration profiles and velocity profiles are shown for two time points. The radius of the cylinder at the constriction shrinks and can eventually reach at a finite time a singularity where the radius shrinks to zero.

Minimal model of cell symmetry breaking. This system of active surfaces can be used to build minimal models of cell like systems by considering an active surface of spherical shape enclosing a simply Newtonian fluid. We therefore combine the active surface with Stokes equation for an incompressible bulk fluid with viscosity η_f

$$\eta_f \nabla^2 \mathbf{u} = \nabla p \quad , \tag{4}$$

where $\mathbf{u}$ is the flow field and p denotes hydrostatic pressure to satisfy the incompressibility constraint $\nabla \cdot \mathbf{u} = 0$. We impose no slip boundary conditions at the surface Γ as $\mathbf{e} \cdot \mathbf{u}|_\Gamma = v_i$ and $\mathbf{n} \cdot \mathbf{u}|_\Gamma = v_n$. The force boundary conditions read $\mathbf{f}_{\rm ext} = -\mathbf{n} \cdot \sigma$, where

$$\sigma = \eta_f(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - p\mathbf{1} \tag{5}$$

is the stress tensor in the fluid. For the exchange flux we write $j_n = k_{\rm on}\bar{c}|_\Gamma - k_{\rm off}c$, where $k_{\rm on}$ and $k_{\rm off}$ are on and off rates of molecules that exchange between surface and bulk and $\bar{c}$ is the bulk concentration.

Fig. 2 shows the stability diagram of an active spherical surface enclosing a viscous fluid. Stability depends on the Peclet number ${\rm Pe} = T_0 R^2/(D\eta)$ and the hydrodynamic length $\ell = \eta/\eta_f$, scaled by the sphere radius R. For large hydrodynamic length, a homogeneous state on the sphere becomes unstable with respect to a polar mode as the Peclet number is increased. The resulting state exhibits a concentration maximum of the stress regulator at one pole on the sphere and a flow pattern towards this high concentration region. The shape of the sphere deforms and takes an asymmetric shape that is flattest in the high stress region. Such a polar symmetry breaking of the sphere provides a minimal model for the establishment of cell polarity which is characterized by asymmetric concentration profiles defining a cellular axis and poles. Note that if immersed in a fluid, the polarized sphere becomes a swimmer. The polar surface flow field imply a slip velocity that propels the swimmer in the external fluid.

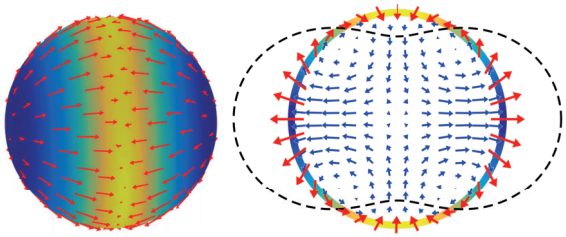

Figure 3: Nematic instability on a sphere generates a contractile ring and a nematic flow pattern. The resulting deformation (dashed line) corresponds to a constriction of the contractile ring.

For small hydrodynamic length, the instability has nematic symmetry, see Fig. 3. As a result, a ring shaped pattern of high concentration of stress activator emerges at the equator of the sphere. The flow field points toward this ring from opposite sides. The self-organized ring that forms via the mechano-chemical feedback corresponds to a region of high contractile stress. Therefore it acts as a contractile ring that induces a constriction of the spherical shape. Indeed in the linearly unstable mode that combines the concentration field, the flow field and the shape deformation reveals the constriction by the ring, see Fig. 3. This suggests that the mechano-chemical self-organization of an active surface can provide key features and shape changes required for division.

The self-organization of an active spherical surface in a passive fluid background can therefore serve as a simple physical model that can generate key processes that are characteristic of living cells. Within a single minimal model of mechano-chemical self-organization based on a diffusible regulator of active stress we obtain phenomena such as polarity establishment, swimming locomotion, contractile ring formation and constriction. This minimal model can serve as a framework to introduce increasing levels of complexity, such as nematic and polar order, chiral asymmetries, viscoelasticity and chemical complexity. It will be interesting to see in the future if these systems can be realized experimentally in reconstituted systems.

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2.14 Understanding collective processes underlying cell fate decisions using single-cell genomics

FABRIZIO OLMEDA AND STEFFEN RULANDS

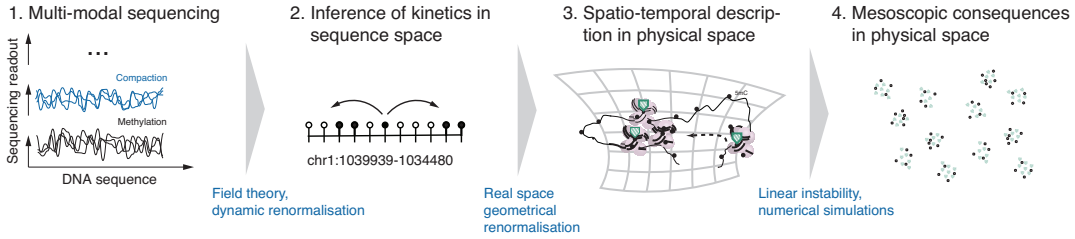

Figure 1: Overview over the theoretical steps used to infer emergent processes in space and time from sequencing measurements along the linear sequence of the DNA.

On the molecular level, different kinds of processes are involved in regulating cellular fate: besides the expression of genes it has, in recent years, 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.

Recent technological breakthroughs in single-cell biology now allow probing all of these processes with unprecedented microscopic detail in living organisms (*in vivo*) [3]. For the first time, it is now possible to obtain information on the expression of thousands of genes, on epigenetic modifications of the DNA or on which positions of the DNA are in contact for thousands of single cells from living organisms. These technological developments have led to detailed descriptions of the molecular processes underlying cellular behaviour along the linear DNA sequence. Biological function, such as cell differentiation, proliferation or death, however, crucially relies on the spatial arrangement of molecular states in the three-dimensional space of the cell. Further, it is determined by emergent (collective) states on the cellular and tissue scale which arise from interactions between processes occurring at many different loci on the molecular scale. But how can detailed quantitative information on the microscopic scale inform on emergent processes that determine biological function at the cellular and tissue scale?

In 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 rules that govern on the microscopic scale (emergence). Therefore, the collective dynamics underlying biological function cannot be straightforwardly inferred from detailed molecular measurements. Hence, despite the excitement that novel developments in single-cell genomics are causing, insights from these technologies remain descriptive until matched with methods to identify collective degrees of freedom. Concepts from non-equilibrium statistical physics such as field theory and renormalisation provide a powerful framework to begin to understand the collective processes underlying cellular behaviour.

By combining for the first time the possibilities of single-cell technologies and tools from nonequilbrium statistical physics, we developed theoretical frameworks that overcome these conceptual limitations of an emerging technology in biology.

From sequence to space and time in single-cell genomics In one project, we used field theory, renormalisation group theory and differential geometry methods to show that emergent phenomena in physical space, such as phase separation, can be unveiled from single-cell sequencing along the one-dimensional DNA sequence. We demonstrated this approach by revealing the interplay between the establishment of epigenetic marks during early mouse development and nanoscale topological changes in the way the DNA is folded spatially.

DNA methylation is a primary layer of epigenetic regulation where a methyl group is deposited on a cytosine [2]. It plays key regulatory roles during development, ageing, regeneration and the emergence of cancer. In this project, using a novel theoretical framework combining field theory, renormalisation group theory and differential geometry method, we first inferred the stochastic kinetics of epigenetic processes in sequence space and then employed a dynamic geometric mapping between distances in sequence space

and distances in physical space to derive the kinetics in physical space. This then allowed us to infer collective mesoscopic epigenetic phenomena in the physical space of the cell (Fig. 1) [1].

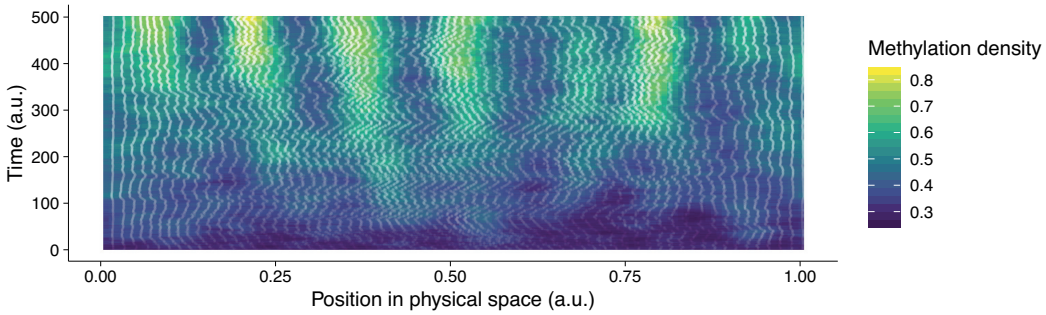

Figure 2: Stochastic simulation of the time evolution of the concentration of DNA methylation marks in space and time. White lines denote the position of fixed positions on the DNA over time.

Specifically, applied to the establishment of DNA methylation marks in the embryo, we used this theory to unveil the dynamical and spatial processes that govern this key process in development. We predicted that this process relies on a positive feedback between the deposition of methyl groups and the DNA and local changes in DNA topology. In physical space and dimensionless units, the concentration of methylation marks is then governed by a partial differential equation of the form

$$\partial_t \phi = \phi^\lambda + \phi^{\lambda-3}\partial_{xx}\phi - \phi^\lambda \partial_{xx}\phi + \dots , \qquad (1)$$

with and exponent $\lambda = 1/3$. If the local concentration of DNA methylation marks exceeds a threshold value we predict the emergence of condensates of methylated DNA of a size of 30-40nm, which is also confirmed by numerical simulations of the stochastic spatio-temporal dynamics (Fig. 2). With this parameter-free theory, using renormalisation group methods, we were able to predict the time evolution of the empirical spatial distribution of DNA methylation patterns (correlation functions) in the embryo. Further, renormalisation showed that these nanoscale processes dominate the time evolution of global DNA methylation levels, giving rise to stereotypic scaling behaviour and self-similarity of the form $t^{5/2}$.

This work showed that methods from non-equilibrium statistical physics are able to overcome conceptual limitations of an emerging technology in biology.

Glassy fluctuations in gene regulatory networks The expression of genes and their interaction in large gene regulatory networks is typically considered to be the primary layer of the regulation of cell identity. The abundances of immediate gene products, mRNA molecules, can be quantified using sequencing technologies and methods that allow profiling the expression of thousands of genes in single-cells (single-cell RNA sequencing) have become the workhorse in single-cell genomics. However, due to a large number of technical and statistical steps involved in the quantification of these experiments their read-outs are usually non-stoicheiometric quantities and do not allow experimental data to be predicted by theories.

In this project, we showed that the macroscopic propagation of fluctuations in gene regulatory networks gives direct information on the physical mechanisms governing cell state transitions, independent of technical noise. Specifically, we started with a full Master equation description of the stochastic dynamics of gene expression and showed that steady-state fluctuations in such systems are effectively described by bipartite spin glasses of Sherrington-Kirkpatrick type. We showed that such spin glasses exhibit a phase transition between a paramagnetic phase, where fluctuations between genes are uncorrelated, and a glassy phase, where fluctuations show strong correlations both across genes and in time. We found biologically plausible parameter pose cells in the vicinity of the phase transition point.

By analysing a range of single-cell RNA sequencing experiments we validated that cells indeed exhibit hallmark signatures of glassy fluctuations in mRNA levels. These findings highlight the possibility that glassy gene expression noise can be a carrier of biological information. Our work also shows how understanding collective properties of fluctuations in gene regulatory networks can reveal physical mechanisms of how cells select and maintain their identity.

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2.15 Multiscale propagation of fluctuations in active biosystems

ADOLFO ALSINA, FELIX J. MEIGEL, AND STEFFEN RULANDS

In statistical and condensed matter physics, we are usually interested in systems that are defined by microscopic symmetries. We then ask how these symmetries are broken on the macroscopic scale. Biological systems, by contrast, are organised in a hierarchy of spatial scales: on the smallest scale, molecules interact with each other and with the DNA, giving rise to emergent states at the level of protein concentration, DNA configuration or gene expression. These processes are often embedded in subcellular structures, called organelles. On the cellular scale, the interaction of many cells leads to the formation of complex organs and organisms which are sometimes organised in societies with a varying degree of complexity.

In a further contrast to condensed matter systems, biological systems usually perform specific functions. Striking examples of such functions are the capacity of cells to sense fluctuating signals from their environment, to interpret these signals, and finally to trigger the correct molecular programs in response to these signals. In several projects, we investigated how active biosystems make use of this peculiar spatial architecture in order to perform biological functions. Specifically, we asked how fluctuations propagate through a hierarchy of spatial scales, and how biological systems can manipulate the propagation of fluctuations to sense and respond to fluctuating extrinsic signals.

Specialisation and plasticity in a primitively social insect Biological systems have the remarkable capacity to build and maintain complex spatio-temporal structures. Such structures are often surprisingly robust in noisy environments and their formation relies on the integration of regulatory processes on vastly different spatial scales of organisation, from the molecular level to tissue or population-level feedback.

While historically theoretical and experimental research has focused on the processes underlying the formation of complex structures, such as the self-organisation of cells into tissues, in recent years it has become clear that biological systems also have the remarkable capacity to break up and rebuild these structures. As an example, colonies of social insects rely on the long-term specialisation of individuals into distinct castes, such as queen and workers. Although such phenotypes can be stable over years in the presence of environmental noise, individuals are nevertheless capable of being rapidly reprogrammed [2]: upon receipt of specific cues they undergo a transient phase in which an individual's behaviour normally associated with a specific caste is rapidly altered in order to perform a different task from the one it performed initially (plasticity).

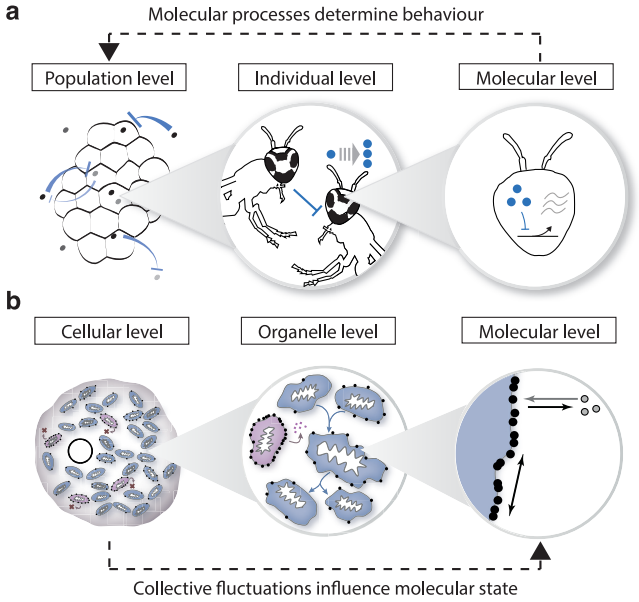

Figure 1: Schematic illustrating the interplay between fluctuations on different levels of biological organisation in **(a)** primitively social insects and **(b)** the regulation of cell death.

In this project, we asked how biological systems can achieve rapid plasticity under specific environmental changes and simultaneously retain stable specialisation over time [3]. We used a unique model system of phenotypic plasticity, colonies of primitively social paper wasps (Fig. 1(a)). Such colonies consist of a single reproductive queen and 8-30 non-reproductive workers (specialisation). After queen removal, the remaining workers can rapidly reprogram to generate a single new queen (plasticity). In order to understand how the paper wasp society simultaneously achieves robust specialisation and rapid plasticity we developed a unique experimental approach that allowed us to track the relaxation process of the nest into the social steady state simultaneously across vastly different spatial scales: from detailed molecular profiling of wasps' brains and anatomical measurements of reproductive organs, to characterising individual behaviours and nest dynamics.

Based on these experiments we derived a theory that allows us to understand specialisation and plasticity as an emergent property of the interplay between molecular and colony-level processes. Specifically, we showed that the interplay between antagonistic processes on the molecular and colony scale allows paper wasps to distinguish between intrinsic perturbations of molecular states while reacting plastically to extrinsic cues

affecting the society as a whole, and thereby to simultaneously achieve rapid plasticity and robust specialisation. Specifically, the society undergoes a saddle-node bifurcation governed by the population structure as a bifurcation parameter, therefore simultaneously achieving bistability in the steady state and transient, rapid convergence to the queen phenotype after colony-level perturbations (Fig. 2(a)).

Our study provides a general principle of how both specialization and plasticity can be achieved in biological systems.

Multiscale fluctuations in the regulation of cell death
The establishment and maintenance of complex tissues relies on a precise regulation of the behaviour of cells, which continuously sense and respond to environmental signals. Understanding the processes underlying such cell fate decisions is one of the central topics in biology. Historically, research on cell fate decisions has focused on the molecular processes underlying the behaviour of cells, such as biochemical signalling cascades.

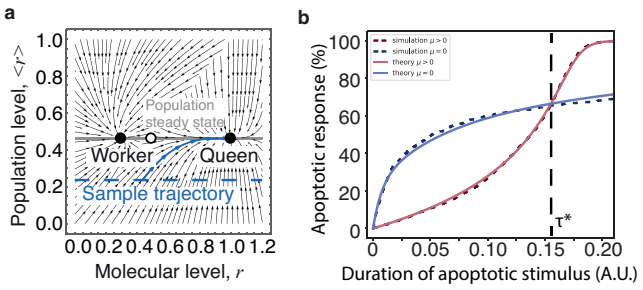

Figure 2: **a)** Phase portrait depicting the co-evolution of the population composition, represented by the average molecular state in the population, $\langle r \rangle$, and the molecular degree of freedom, r. **b)** Contrasting the response of cells to stress signals for interacting ($\mu > 0$) and non-interacting ($\mu = 0$) mitochondria. Interacting mitochondria suppress the response on short time scales and strengthen the response on long time scales.

In this project, we found an entirely different way of how cells decide their fate. We showed that important cell fate decisions rely on cells manipulating how fluctuations propagate across a hierarchy of spatial scales. Together with experimental collaborators, we demonstrated this paradigm in the context of the paradigmatic decision of cells to commit suicide (apoptosis) and their decision to trigger an immune response to viral threats. Specifically, both decision-making dynamics are regulated by protein complexes that localise on the membranes of cellular organelles called mitochondria. Protein complexes, that are dynamically formed in response to varying stress levels of cells, act here as central regulators that trigger a cascade of events ultimately leading to cellular inflammation responses or the death of a cell [4]. Interestingly, not only the formation of protein complexes is highly dynamic, but also mitochondria themselves undergo rapid fusion and fission on a time scale of minutes which leads to a stochastic redistribution of protein complexes on mitochondrial membranes. By this, mitochondrial dynamics feedback to the protein complex formation dynamics (Fig. 1(b)).

By a combination of analytical and numerical calculations, we showed that the interplay between molecular and organelle dynamics leads to quasi-particle solutions of the multi-scale dynamics. The kinetics of these quasi-particles reflect those of non-Newtonian fluids, exhibiting a weak response on small time scales and a strong response on long time scales (Fig. 2(b)). This intriguing response behaviour allows cells to distinguish between fast noise and slow, biologically relevant trends, thereby constituting a kinetic low-pass filter of fluctuating cellular stress levels [5]. We showed that this effects dominates the cell death decision by orders of magnitude and validated our predictions with experiments, where cells were subjected to temporally modulated stress levels.

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2.16 Phase transitions at surfaces controlled by molecular binding processes

XUEPING ZHAO, SUSANNE LIESE, FRANK JÜLICHER, AND CHRISTOPH A. WEBER

Liquid droplets at intra-cellular surfaces. Biological function inside cells is realized 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, such as mitochondria, have a membrane, others are not enclosed by a membrane [1]. Many membrane-less compartments have been found to exhibit properties reminiscent of liquid droplets [2]. Strikingly, such intra-cellular condensates form via liquid-liquid phase separation and their formation and dissolution is governed by local thermodynamics. It has been suggested that such condensates can dampen concentration fluctuations in cells [4]. A further striking property of such intra-cellular droplets is that they can wet membrane surfaces and that the main droplet constituents can also bind to such surfaces [1]. However, a theory that captures the interplay between molecular binding and phase transitions at the surface such as wetting and prewetting transitions was lacking.

We studied how membrane binding of molecules affects wetting, prewetting and surface phase transitions, see Fig. 1(a-c). We have developed a thermodynamic theory taking into account for molecular binding processes between bulk and membrane surface [5]. Our theory goes beyond the classical thermodynamics of wetting transitions by introducing additional surface states. Recently, we also extended our theory to non-equilibrium conditions. We studied the relaxation of condensates toward equilibrium but also cases where binding is maintained away from equilibrium [2].

Theory for phase transitions at surfaces driven by molecular binding reactions. We focus on a binary mixture that interacts with a surface layer of molecules that are bound to a flat and rigid membrane. In addition, molecules can bind and unbind according to (top left in Fig. 1)

$$\phi \rightleftharpoons \phi_m \,, \tag{1}$$

where ϕ and ϕ_m are the volume fractions of the solute and of the surface bound state, respectively. We consider a bulk binary mixture of volume V which is composed of solute molecules and solvent. The free energy contains contributions from the bulk $f_b(\phi)$, the membrane $f_m(\phi_m)$ and coupling free energy between them, $J(\phi|_0, \phi_m)$:

$$F[\phi,\phi_m] = \int_V d^3x \Big[f_b(\phi) + \frac{1}{2}\kappa |\nabla\phi|^2 \Big] \tag{2}$$
$$+ \int_m d^2x \Big[f_m(\phi_m) + \frac{1}{2}\kappa_m |\nabla_{||}\phi_m|^2 + J(\phi|_0,\phi_m) \Big] \,,$$

where $\phi|_0$ is the bulk volume fraction at the membrane surface. Moreover, κ and κ_m characterize the corresponding free energy contribution for gradients in bulk and membrane, respectively, and $\nabla_{||} = (\partial_x, \partial_y)$ denotes the gradient vector in the membrane plane. Using this theory, we determined the phase transition lines for wetting, prewetting and bulk phase separation.

Using our theory, we show that membrane binding can lead to a variety of thermodynamic surface states at undersaturated conditions with rich surface phase diagrams (see Fig. 2). Such states are described by a pair of order parameters, i.e., the fraction of bound molecules in a single surface layer and the excess surface concentration of the condensates adjacent to the surface. Interestingly, we find cases where phase transitions at and adjacent to surfaces occur under conditions where the bulk cannot phase-separate at any concentration. More generally, a layer of bound molecules on the membrane effectively modifies the properties of the surface which can for example lead to a shift of the prewetting line to low concentrations. Finally, surface binding affects the wetting transition and the contact angle of bulk droplets that wet the surface.

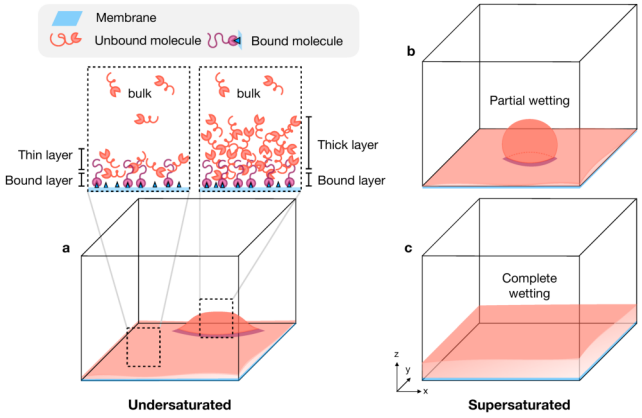

Figure 1: **Schematics of phase separations at surfaces in the presence of membrane binding**. Molecules from the bulk can bind to specific sites (blue triangles) on the membrane (blue surface). Unbound bulk molecules can also accumulate adjacent to the membrane surface, leading to the formation of three dimensional layers on the membrane surface (red surfaces). **(a)** If the system is undersaturated, prewetted thin and thick layers can transiently form. At thermodynamic equilibrium, either thin or thick layers are stable except at the prewetting transition where both states coexist. At phase coexistence, condensates either partially wet **(b)** or completely wet the membrane surface **(c)**, depending on the interactions.

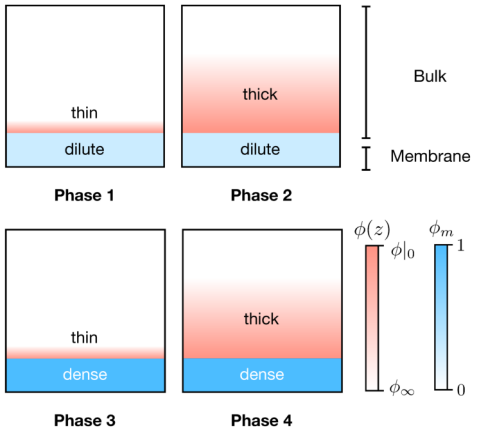

Figure 2: **Overview of surface states for systems where molecules can bind to a membrane surface.** We find four surface states which are each characterized by a pair of order parameters, i.e., the volume fraction of molecules bound to the surface, ϕ_m, and the excess surface concentration, c_s. Depending on the interactions between bulk and surface, the membrane can be either dilute (light blue, low ϕ_m) or dense (dark blue, high ϕ_m), and the bulk layer can be either thin (low c_s) or thick (high c_s). The shades of red show the bulk profile $\phi(z)$ which ranges between the bulk volume fraction ϕ_∞ and the volume fraction at the membrane surface $\phi|_0$ (see colorbar).

In our work, we also find that surface binding alters the prewetting behavior and the occurrence of surface phase transitions. When molecules bind to the membrane surfaces, phase-separation can occur in the membrane (surface phase transition). This alters the prewetting behavior by effectively modifying the properties of the surface. Moreover, while the classical prewetting transition line is very close to the saturation concentration without binding processes, the transition lines of prewetting and surface phase transitions can shift to lower values when molecules can bind to membrane surfaces. Interestingly, the actual physiological concentrations of many membrane-binding proteins in living cells (typically $(10-100)nM$) are far below their saturation concentrations (typically $(1-10)\mu M$). Further research is required to scrutinize whether the low physiological concentrations of membrane-binding proteins serve the purpose to form condensates on intracellular surfaces rather than droplets in the bulk.

Our findings show that the binding of molecules provides a versatile mechanism to control the position and size of condensed states at surfaces. In recent years, a growing number of intra-cellular condensates were shown to adhere to membrane-bound organelles or the intra-cellular surfaces. Many of such surface-bound droplets were suggested to act as scaffolds for biochemical processes [4]. A striking example are supramolecular assemblies such as the tight junction, where protein droplets at the cell membranes were suggested to provide an assembly hierarchy by successively recruiting specific tight junctional building blocks. In collaboration with Alf Honigmann at MPICBG, we aim to understand the governing principles of tight junction formation. Our joint project is also supported via the DFG SPP Program entitled, "Molecular Mechanisms of Functional Phase Separation". We together consider genetically modified cells in combination with in-vitro assays including reconstituted tight junction proteins at supported lipid bilayers. A key finding of these joint studies are condensed patches that form on the membrane far below the saturation concentration of phase separation in the bulk. These patches are of fixed size in the bilayer plane and have a height of a few molecular layers. Currently, our theory suggests that such patches correspond to prewetted condensates which are controlled by molecular binding processes to a receptor that is confined to the bilayer.

Conclusion. Membranes surfaces have an essential role in living cells. This role is reflected in a plethora of biological processes ranging from cell division to intra- and extra-cellular transport. Binding to such surfaces together with surface phase transitions gives rise to a new level of complexity with a rich variety of phases and variability of phase diagrams that cells can make use of to realize cell biological processes. Complex patterns at surface are expected when binding processes are maintained away from thermodynamic equilibrium [2, 7], which is the case in living cells. In biological systems, ATP-driven cycles of kinase and phosphatase can alter binding equilibria. Future research will clarify how such active binding processes modify the properties of wetted and prewetted states out of equilibrium.

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2.17 Quantitative models for phase-separated systems

LARS HUBATSCH AND CHRISTOPH A. WEBER

Relevance of quantifying droplet dynamics. Liquid-liquid phase separation is an important organizing principle in biology and is thought to be involved in the formation of various membrane-less cellular organelles. Hallmark properties of such organelles are their rapid formation and dissolution, their fusion, and their wetting to membranes [1]. Another key property is that phase-separated organelles exchange material with their environment leading to dynamic sequestration of molecules. This sequestration can affect biochemical processes by spatially redistributing reacting components. Probing the dynamics of condensate components is thus crucial for a quantitative understanding of how condensates affect the cellular biochemistry.

To probe the dynamics of condensates, biomolecules are typically labelled with fluorescent tags. In general, in systems with tagged molecules, various methods exist to characterize molecular properties such as binding rates and diffusion coefficients, including fluorescence correlation spectroscopy (FCS), single-particle tracking (SPT), and fluorescence recovery after photobleaching (FRAP). However, interpretation of the experimental data acquired from such methods requires a rigorous derivation of a theory accounting for the underlying physicochemical processes. This derivation has been achieved for some biological systems and processes, but is lacking for condensates formed by liquid-liquid phase separation. To fill this gap, we have derived the quantitative theory for FRAP [2] and SPT [3]. Both theories can be used to quantify the kinetic parameters such as diffusivities inside liquid droplets but also thermodynamic properties such as partition coefficients. We have already applied our theory for FRAP to experimental measurements. Below we discuss the theory for FRAP and its application to experiments; see Fig. 1 for an illustration.

Theory for FRAP of liquid droplets. Here, we first introduce a quantitative FRAP method to extract the diffusion coefficient inside, D_{in}, purely based on fluorescence measurements inside droplets. Strikingly, this method works without requiring knowledge about the partition coefficient P or the diffusion coefficient outside, D_{out}. Using irreversible thermodynamics, we have derived the theory that connects dynamics inside and outside of the droplet via transport across a finite interface. We find that the concentration of unbleached components c_u follows

$$\partial_t c_u = \nabla \cdot \left[D(\phi_{\mathrm{tot}}) \left(\nabla c_u - c_u \frac{\nabla \phi_{\mathrm{tot}}}{\phi_{\mathrm{tot}}} \right) \right] , \qquad (1)$$

where $\phi_{\mathrm{tot}}(\vec{x},t) = \phi_u(\vec{x},t) + \phi_b(\vec{x},t)$ is the total volume fraction of unbleached and bleached components. Moreover, the diffusivity $D(\phi_{\mathrm{tot}}) = k_{\mathrm{B}}T\Gamma_0(\phi_{\mathrm{tot}})$ depends on $\phi_{\mathrm{tot}}(\vec{x})$ via the mobility Γ_0. As we have shown in Ref. [3], a similar approach can be used to investigate single-molecule dynamics across phase boundaries.

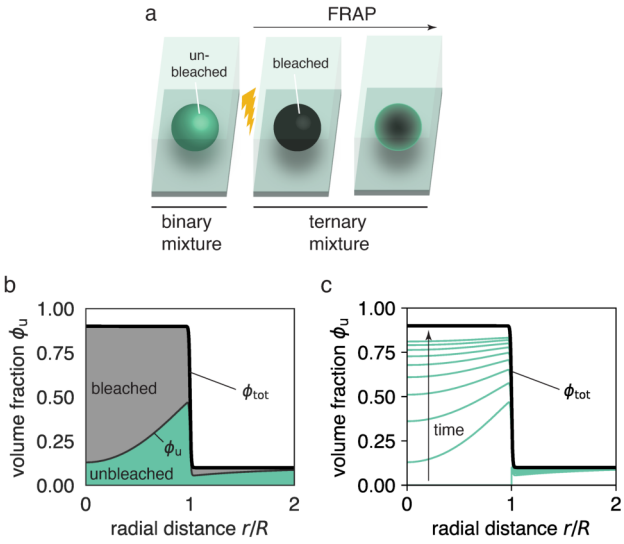

Figure 1: **Ternary mixture accounts for the dynamics of bleached and unbleached molecules.** (**a**) Before bleaching, a droplet that is composed of fluorescently labelled molecules can be described by a binary mixture, namely unbleached molecules and solvent. After bleaching, the system is composed of three components, bleached molecules, unbleached molecules and solvent. If the system was at equilibrium prior to bleaching, the sum of bleached and unbleached molecules forms a stationary, non-uniform profile $\phi_{\mathrm{tot}}(r)$ (see panel b). (**b**) Snapshot of model dynamics at $t = 0.22R^2/D_{\mathrm{in}}$. Initial conditions are $\phi_{\mathrm{u}}(r, t = 0) = \phi_{\mathrm{out}} \cdot \Theta(r - R)$, corresponding to a fully bleached droplet. Note that at any time we have $\phi_{\mathrm{tot}} = \phi_{\mathrm{u}} + \phi_{\mathrm{b}}$. (**c**) Time course of spatial recovery. For long times, when nearly all bleached material has been exchanged, ϕ_{u} approaches ϕ_{tot}. Panels (c,d) use radial symmetry with r denoting the radial position.

Quantifying liquid droplet dynamics. Our theory, essentially represented by Eq. (1), governs the dynamics of labeled molecules through interfaces of condensates. This equation can be applied to spherical condensates, as well as to non-spherical condensates and arbitrary bleach geometries. By means of our theory, we were also able to quantify the impact of neighbouring droplets and the coverslip on the recovery dynamics. In these studies, we found that neighbouring droplets caused an appreciable speed-up in overall recovery, while emulating a coverslip caused a weak slow-down. In order to experimentally verify our theory, we have used different *in vitro* droplet systems.

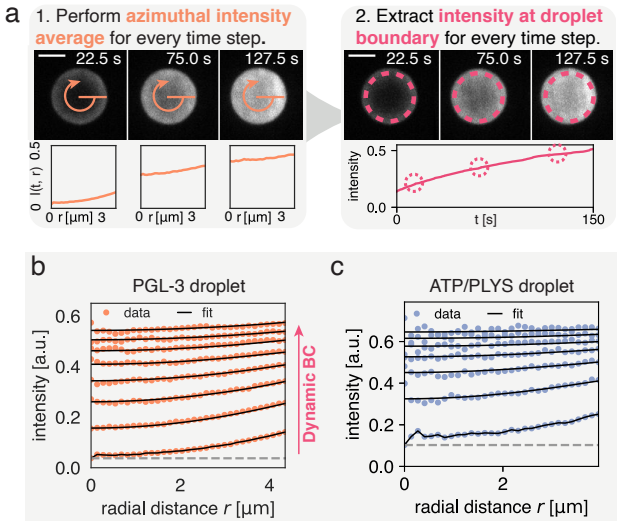

Figure 2: **Quantitatively measuring D_{in} by extracting intensity at condensate interface.** (**a**) *(1)* Spatial time course of FRAP recovery after full bleach for PLYS/ATP coacervate droplet. Azimuthal average (orange) is highlighted. *(2)* To obtain the boundary condition $c(r = R_-, t)$, fluorescence intensity is extracted approximately $1.4\mu m$ away from the interface (see methods). Data closer to the droplet boundary can be subject to optical artefacts giving rise to an artificially broad interface. Lower panel shows azimuthal averages at different time points.For each fitting step, a numerical solution to Eq. (1) is calculated with a trial D_{in} and the experimentally measured boundary condition from step (2). Subsequently simulation and experiment are compared according to the cost function, before choosing the next trial D_{in}. Scale bar, $5\mu m$. (**b**) Fluorescence recovery inside a PGL-3 condensate, along the radial direction (azimuthal averages, see (a)). D_{in} is extracted by global fitting of Eq. 1b to the experimental profiles, using the experimentally extracted initial and boundary conditions (see panel (a) (1) and (2)). The grey line indicates an offset that comes about due to incomplete bleaching, and a small but visible, fast and uniform recovery with unknown cause (see Methods). (**c**) Same as (b) but for ATP/PLYS coacervates.

There is remarkable quantitative agreement between our theory and the diffusion dynamics observed inside such droplets. This agreement shows that proteins and charged, synthetic polymers can form droplets that follow simple diffusive dynamics. Crucially, we have used the full spatio-temporal data for fitting and can thus distinguish the timescale set by intra-droplet diffusion from the timescales at play in the dilute phase. We extracted the intensity directly at the inside of the droplet interface and fit a spatially resolved diffusion equation to the ensuing recovery. We use the boundary intensity as a dynamic boundary condition and the experimentally measured profile as initial condition. Within the statistical fluctuations the numerical solutions and the experimental data are not distinguishable (see Fig. 2b,c). Throughout the time course, we find excellent agreement with the data and have thus found a method with minimal approximations that can precisely measure the inside diffusion coefficient D_{in}.

Building on the analysis inside the droplet, we also showed that there is a relationship between partition coefficient P and the diffusion coefficient in the dilute phase, D_{out}. Data obtained from FRAP experiments define a line in (D_{out}, P) space, along which a range of parameter sets can reliably account for the boundary dynamics. This relationship allowed us to characterize changes in P upon salt addition, opening an alternative avenue for characterizing P without relying on fluorescence intensities. This approach is particularly important in light of recent results obtained by quantitative phase microscopy which show that measuring partition coefficients based on fluorescence intensity can lead to strong underestimation of P (McCall et al. (2020)).

Conclusion. Our approach of quantifying liquid droplets can be readily extended to multi-component systems with an arbitrary number of components, which is particularly useful *in vivo*. This would be hardly possible for techniques that do not use labeled components, such as quantitative phase microscopy or other scattering methods. Of particular interest are multi-component systems with chemical reactions away from equilibrium [4]. Our approach is currently extended with the goal to determine the diffusion coefficients and concentration levels of reactants, and thereby provide insights into reaction kinetics. Interestingly, introducing the bleached molecules via a ternary mixture also enabled us to derive the Langevin equation governing single-molecule motion in phase-separated media, thus providing a link to SPT. In Ref. [3], we use this approach to theoretically derive the theory for the stochastic dynamics of single molecules across phase boundaries. The resulting stochastic equations provide insights into how single labeled molecules experience a phase boundary and how phase separation properties can be extracted from single molecule trajectories. Approaches for single labelled molecules are relevant since high labelling fractions can alter the kinetics in dense protein phases.

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2.18 Yield stress phenomenology in cellular systems

MARKO POPOVIĆ

Introduction Developing tissues grow into functional shapes, which requires them increase in size and change their shape in a controled way. They are often described as viscoelastic fluids, motivated by the fact that over long developmental times active cellular processes lead to fluidisation. However, on shorter time scales tissues should behave as yield stress materials, such as clay, changing their shape only when under a sufficiently high mechanical stress Σ_c. For stresses close to Σ_c yield stress materials flow through collective rearrangements of large parts of the material, which suggests that this regime might be identified in developing tissues by imaging their geometry. Here, we make first steps towards understanding yield stress properties of developing tissues using the vertex model of epithelial tissues.

Vertex model The vertex model describes a confluent epithelial tissue as a network of polygons that represent individual cells. The mechanics of the vertex model is specified by the energy function

$$E = \sum_{c\in\text{cells}} \frac{1}{2}\left[K_c\left(A_c - A_{0,c}\right)^2 + \Gamma_c P_c^2\right] + \sum_{b\in\text{bonds}} \Lambda_b L_b \tag{1}$$

where A_c is cell area, K_c is cell area elastic constant, $A_{0,c}$ is the cell preferred area, L_b is bond length, Λ_b is bond tension, P_c is cell perimeter and Γ_c is perimeter elastic constant. The dynamics of a cellular network is then described by the overdamped dynamics of the cell vertex positions $d\vec{r}_\alpha/dt = -\nu\vec{\nabla}_\alpha E$, where ν is a mobility that we set to 1. In numerical simulations we use an ensemble of disordered networks with $N = 400$ and $N = 2500$ cells, as shown in Fig. 1 a) *left*. To prevent crystallisation we introduce polydispersity of preferred area $A_{0,c}$. Technical details are described in [1]. We perform simulations of simple shear at strain rate $\dot{\gamma}$, as illustrated in Fig. 1 a). Initially, the shear stress component Σ grows almost linearly, see Fig. 1 b), but as the strain γ increases cells rearrange and the stress relaxes, visible as sudden drops in the stress-strain curve. We visualise cell rearrangements in Fig. 1 a) *right* by coloring cells that have rearranged during a strain increment $\Delta\gamma = 0.15$. As the steady state is reached the imposed simple shear is balanced by stress relaxation due to cell rearrangements. We find that the steady state flow is well described by the classical Herschel-Bulkley law $\dot{\gamma} \sim (\Sigma - \Sigma_c)^\beta$ [2] with the flow exponent estimate $\beta \simeq 1.3$, as shown in Fig. 1 c).

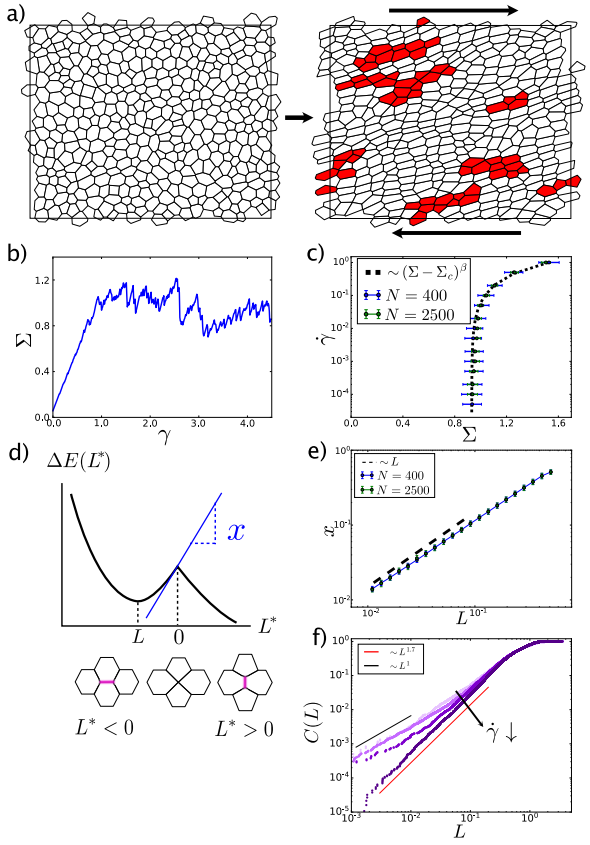

Figure 1: a) A polydisperse disordered network of $N = 400$ cells undergoes a simple shear deformation. Cells that have undergone a recent rearrangement are shown in red. b) Stress-strain curve shows the initial elastic regime, followed by steady state plastic flow. c) Strain rate *vs* stress measured in steady state with the fit of the Herschel-Bulkley law shown by the dotted black line. d) Schematic of the vertex model energy landscape in the vicinity of a T1 transition. e) Numerical measurement of the force x required to shrink a bond as a function of the bond length L. f) The cumulative bond length distribution converges to a power law $C(L) \sim L^{1+\theta}$. Strain rate values (top to bottom) $\dot{\gamma} = 10^{-1}, 10^{-2}, 10^{-3}$, the bottom curve is obtained using a quasistatic protocol.

Cusp in the energy landscape The elementary cell rearrangement in epithelial tissues, called a T1 transition, consists of two cells losing a shared bond and creation of a new bond between the previously unconnected cells. To characterise the energy landscape in the vicinity of a T1 transition, we define $E(L^*)$ to be the energy of the cellular network with an imposed length L^* of the bond rewired in the T1 transition. Values $L^* < 0$ and $L^* > 0$ represent the lengths of disappearing and created bonds, respectively, see Fig. 1 d) *bottom*. The energy difference $\Delta E(L^*) \equiv E(L^*) - E(L)$, where L is the unconstrained equilibrium value of the bond length, exhibits a cusp at the onset of the T1 transition where

$L^* = 0$, a well known feature of the vertex model energy landscape. The presence of the cusp allows us to relate the length of a short bond to the additional force x required to shrink its length to 0. As illustrated in Fig. 1 d) we find $x \simeq \Delta E''(L)L$. Since the stiffness $\Delta E''(L)$ is expected to remain finite at $L^* = 0$ we propose that $x \sim L$. This property generically follows from existence of cusps in the energy landscape and we expect to find it in 2d cellular systems in general. In the vertex model we test this relationship directly by measuring the force required to shrink a bond of length L and we show the results in Fig. 1 e).

Network stability Each T1 transition induces a stress change in the cellular network that can trigger a new T1 transition if there are bonds with small x in the network. Stability of the cellular network at the yield stress, with respect to avalanches of T1 transitions, imposes a constraint that $P(x)$ scales as $P(x) \sim x^\theta$, with $\theta > 0$ [3]. The importance of the linear relation between x and L is now clear, as a measurement of the bond length distribution $P(L)$ allows us to characterise the stability of the cellular network. In particular, we measure the cumulative bond length distribution $C(L) = \int_0^L P(L')dL'$ at different strain rates $\dot{\gamma}$, with a small numerical cutoff required by the implementation of T1 transitions subtracted from the actual bond lengths. As shown in Fig. 1 f), at finite strain rates the cumulative distribution $C(L)$ vanishes linearly, revealing a constant $P(0)$, which is expected in a flowing network. However, as $\dot{\gamma}$ is reduced and the system is driven closer to the yield stress, the number of short bonds is depleted and $P(L)$ approaches the power law behavior required for the stability at the yield stress. Finally, we measure $C(L)$ in the yield stress regime obtained using a quasistatic simple shear driving protocol, shown as the lowest curve in Fig. 1 f). We find power-law behavior with exponent $\theta \simeq 1.7$, consistent with values reported in the literature for models of 2d amorphous solids [4].

Experimental data To test the relevance of these results in biological tissues we use experimental data obtained in the group of Suzanne Eaton and Natalie Dye at MPI-CBG. In particular, we analyse the bond length distribution in the wing epithelium of the fruit fly at two stages of development: i) during pupal morphogenesis [5] and ii) in third instar larval wing disc [6], see Fig. 2. We find that in both tissues the bond length of short bonds follows the power-law distribution with effective exponent $\theta \simeq 0.7 - 0.9$, similar to the one measured in the slowly flowing vertex model. This suggests that the relation $x \sim L$ might hold in real tissues and in future it will be interesting to perform more direct tests of this hypothesis.

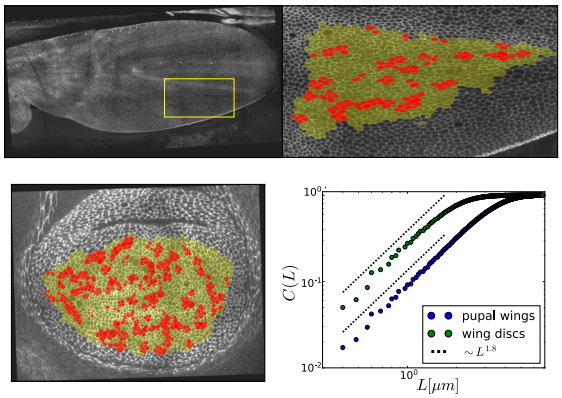

Figure 2: Pupal wing (*top*) and wing disc (*bottom left*) of a developing fruit fly. Regions used for analysis are shown in yellow. Red colored cells have participated in a T1 transition during the last 5 min. The cumulative bond length distribution (*bottom right*) in both tissues shows a power-law scaling with exponent $\theta \simeq 0.7 - 0.9$.

Conclusion We have shown that, as a consequence of cusps in the energy landscape, the distribution of cell bond lengths reflects the stability of the cellular network. Furthermore, the distribution of bond lengths follows a power law at the yield stress, consistent with the requirement of stability with respect to avalanches of T1 transitions, suggesting that the flow regime of a yield stress tissue can be inferred from the statistics of bond lengths. Finally, we find power law distributions of short cell bonds lengths in biological tissues, consistent with the vertex model results in the yield stress regime. Although the comparison is not yet conclusive, as the model did not include active cellular processes such as cell divisions, our results raise the possibility that biological tissues might operate in the yield stress regime.

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2.19 A gelation transition enables the self-organization of bipolar metaphase spindles

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The mitotic spindle is a dynamic structure that emerges from the self-organization of microtubules, molecular motors, and other proteins. Motor-driven poleward flows of microtubules play a key role in the bipolar organization of spindles. However, it is not understood how the local activity of motor proteins generates these large-scale coherent poleward flows. Here, we show that a gelation transition enables long-range microtubule transport causing spindles to self-organize into two oppositely polarized microtubule gels. Laser ablation experiments reveal that local active stresses generated at the spindle midplane propagate through the structure thereby driving global coherent microtubule flows. Simulations show that, in the presence of branching microtubule nucleation, either disrupting such flows or decreasing the network connectivity can lead to a microtubule polarity reversal in spindles. We experimentally confirm this inversion of polarity by abolishing microtubule transport in spindles. Overall, we uncover a connection between spindle rheology and architecture in spindle self-organization.

Active flows in the spindle are polarity-independent. In *Xenopus laevis* egg extract spindles, microtubule flux depends on the activity of Eg5, a kinesin motor that can slide antiparallel microtubules [1]. Microtubule sorting by Eg5 implies that forces between microtubule pairs should depend strongly on their relative orientation [3]. To test this mechanism in *Xenopus* spindles, we quantified microtubule transport and the density of antiparallel overlaps throughout the spindle structure. To visualize the motion of individual microtubules in spindles, we used single-molecule speckle microscopy [2] (Fig. 1A). We compared the microtubule velocity profiles to the antiparallel microtubule overlaps and found that the number density of antiparallel overlaps was maximal at the spindle center and decreased by $\sim$ 90 % at the poles (Fig. 1B). In contrast, microtubule transport was found to be constant throughout the spindle, Fig. 1B).

Active flows are a consequence of long-range stress propagation. Our speckle analysis suggests that local sorting is not sufficient to explain microtubule transport in spindles. One possible explanation for the polarity-independent flows observed throughout the spindle is that the local stresses generated by Eg5 in the region of antiparallel overlaps are propagated over long distances. To test this hypothesis, we designed an assay combining fluorescent speckle microscopy and laser ablation (Fig. 1C). If Eg5 activity is mainly restricted to the spindle midplane and propagates throughout the structure, disconnecting a region of the spindle that is far from the midplane using laser ablation should reduce microtubule transport within that disconnected region. Alternatively, if Eg5 is acting homogeneously in the structure via local sorting, microtubule motion should remain mainly unaffected. We achieved complete disconnection of a spindle pole by a series of three consecutive laser cuts across the spindle (Fig. 1D).The microtubule velocity was significantly reduced after ablation in the disconnected region (DR) from 1.8 $\pm$ 0.1 μm/min before the cut to 0.8 $\pm$ 0.1 μm/min after the cuts. In contrast, microtubule velocity remained unaffected in the connected region (CR) (Fig. 1D). The instantaneous slow down of speckles after the cuts indicates that connectivity is essential to sustain poleward flux at the poles and suggests that microtubule flux in that region is not a consequence of local microtubule sorting. Instead, local stresses generated by Eg5 propagate throughout the structure from the spindle midplane region to the poles, driving microtubules poleward.

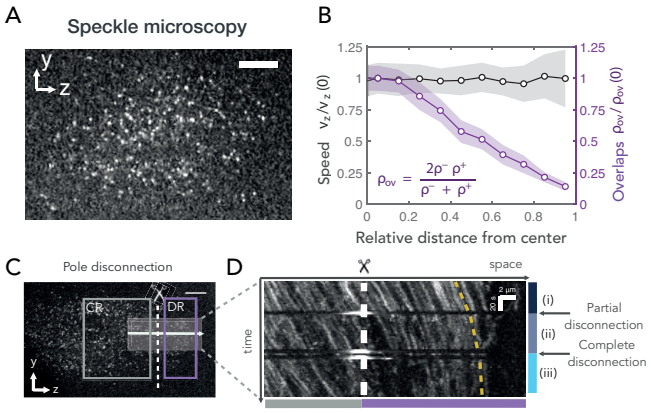

Figure 1: **Local sorting of antiparallel microtubule overlaps is not sufficient to explain poleward microtubule transport**. (A) Speckle microscopy ($\sim$ 1 nM Atto565 frog tubulin) is used to measure microtubule transport. Scale bar: 10 μm. (B) Normalized value of the averaged velocity profiles of the plus and minus networks $v_z/v_z(0)$ compared to the normalized number density of antiparallel overlaps $\rho_{ov}/\rho_{ov}(0)$ (mean $\pm$ SD, $n = 10$ spindles). (C) Fluorescent speckle image before laser ablation. Scale bar: 10 μm. CR: connected region, DR: disconnected region. The arrow denotes the direction along which the kymograph in (D) is studied and the width of the gray region denotes the averaged region. (D) Kymograph from (C) showing how speckle trajectories stop in the disconnected region after consecutive laser ablation events.

A gelation transition enables long-range stress propagation. Mixtures of filaments and motors can behave

as fluids or gels depending on the filament connectivity [4]. To test whether a gelation transition underlies the long-range propagation of stresses in the spindle we turned to large-scale simulations. For simplicity, we simulated the dynamics of one filament network and substituted the second network for a pinning field structure of fixed, polar aligned filaments. To study the effect of connectivity on transport, we systematically varied the number of motors in the system (Fig. 2A). We found that for motor concentrations below 0.5 motors/filament, flows decayed abruptly beyond the overlap region with a length-scale close to the mean filament length. Above this concentration, we observed the emergence of coherent flows that spanned the entire channel (up to a range $\sim$ 10 times larger than the mean filament length, Fig. 2A). We confirmed that the emergence of these long-range flows corresponds to the onset of a gelation transition by measuring the connectivity within the cross-linked filament networks and calculated the distribution of cluster sizes as a function of motor concentration (Fig. 2B).

Microtubule gelation controls a polarity-reversal transition. We reasoned that long-range and polarity independent flows may be required to maintain the proper spindle polarity. Indeed, microtubule transport is necessary to counteract branching microtubule nucleation in spindles, which is known to occur in the form of autocatalytic waves that propagate away from mother microtubules [5, 6]. To test this, we simulated spindles by considering two interacting networks of opposed polarity. Above the gelation point, we observed the emergence of a gradient of polarity at steady-state similar to those observed in experiments (Fig. 2C). Strikingly, when we reduced the connectivity below the gelation point while keeping motor activity constant, filaments self-organized with a reversed polarity profile, with autocatalytic waves of filaments growing towards the poles (Fig. 2C) and polarity-dependent velocity profiles. Similarly, when we reduced the motor activity in a gelated system, we observed the same polarity reversal. We tested this prediction by perturbing spindles with the Eg5 inhibitor FCPT, a drug that suppresses Eg5 ATP hydrolysis while keeping motors bound to microtubules and thought to maintain spindle bipolarity. In spindles, this drug abolished microtubule flows while maintaining a spindle-like structure. When measuring microtubule polarity in these structures using laser ablation, we found a reversed microtubule polarity profile (Fig. 2D). Altogether, these findings support that a gelation transition, together with molecular motor activity, is necessary for correct spindle self-organization. Our study shows the key role of gelation in spindle assembly and highlights the important balance between autocatalytic microtubule nucleation, microtubule transport, and crosslinking, in organizing and maintaining the proper spindle architecture.

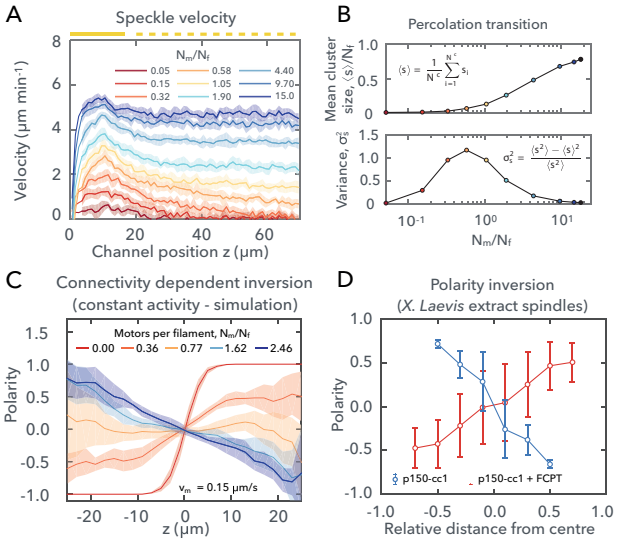

Figure 2: **A gelation transition enables long-range flows in filament networks**. (A) Computer simulations of filament networks show that the length-scale of the filament velocity profiles increases with increasing Eg5 concentration (mean $\pm$ SD, $n = 10$ simulations). (B) Mean and the normalized variance for the cluster size distributions from (A). s_i is the size of the i^{th} cluster, N^{c} is the total number of clusters, and n is the upper cluster size. (C) Polarity reversal enabled by gelation in active systems (steady-state at $t = 12$ min and constant $v_0^k = 0.15\ \mu\text{m s}^{-1}$). Varying connectivity by Eg5 population size ($N_{\text{CL}}/N_{\text{MT}} = 0.0, 0.36, 0.77, 1.6, 2.5$ from red to blue), N_{m} - number of motors, N_{f} - number of filaments, v_{m} - motor speed. (D) Polarity reversal in *Xenopus* extract spindles measured using laser ablation (mean $\pm$ SD, $n = 39$ cuts; red circles).

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2.20 Force generation by protein-DNA co-condensation

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Interactions between liquids and surfaces generate forces that are crucial for many processes in biology, physics, and engineering [1]. In the nucleus, biomolecular condensates are thought to drive transcription [2], heterochromatin formation [3], and DNA repair [4]. Here, we show that the interaction between liquid-like condensates and DNA generates forces that might play a role in bringing distant regulatory elements of DNA together, a key step in transcriptional regulation. We combine quantitative microscopy, in vitro reconstitution, optical tweezers, and theory to show that the transcription factor FoxA1 mediates the condensation of a DNA-protein phase via a mesoscopic first-order phase transition. After nucleation, co-condensation forces drive growth of this phase by pulling non-condensed DNA. Altering the tension on the DNA strand enlarges or dissolves the condensates, revealing their mechanosensitive nature [5].

FoxA1 co-condenses DNA in a tension-dependent manner. To investigate how transcription factors physically organize DNA, we attached linearized λ-phage DNA to a coverslip via biotin-streptavidin linkers and used TIRF microscopy to image the interactions between single molecules of DNA and Forkhead Box Protein A1 (FoxA1), Fig. 1A. In our assay, DNA molecules displayed a broad distribution of end-to-end distances (L), which tunes the DNA's tension. For end-to-end distances greater than approximately 10 μm, FoxA1 generated protein condensates on DNA (Fig. 1A) without influencing DNA. Strikingly, for end-to-end distances below 10 μm, FoxA1 pulled DNA into highly enriched condensates of FoxA1 and DNA, Fig. 1A. Consistent with the ability of FoxA1 to form FoxA1-DNA condensates at low tensions, the cross-correlation of the FoxA1 and DNA signals decayed from one to zero with increasing end-to-end distance, Fig. 1B,C. The observation that FoxA1 drives DNA condensation suggests that it can overcome the DNA molecule's entropic tension set by the end-to-end distance. Incorporating DNA into the condensates increases the tension on the strand, thereby reducing the transverse DNA fluctuations of the non-condensed DNA. To quantify this, we measured the DNA envelope width of the non-condensed DNA fluctuations, Fig. 1B. In buffer, the DNA envelope width decreased as a function of end-to-end distance, consistent with the corresponding increase of DNA strand tension for increasing end-to-end distances, Fig. 1D. However, in the presence of FoxA1, the DNA envelope width remained constant for all end-to-end distances as FoxA1 pulled DNA into one or more condensates, Fig. 1D. The magnitude of the DNA envelope width was lower in the presence of FoxA1 than in buffer conditions for all end-to-end distances. Taken together, this suggests that FoxA1-DNA condensates generate forces that can overcome the entropic tension of the non-condensed DNA and buffer its tension.

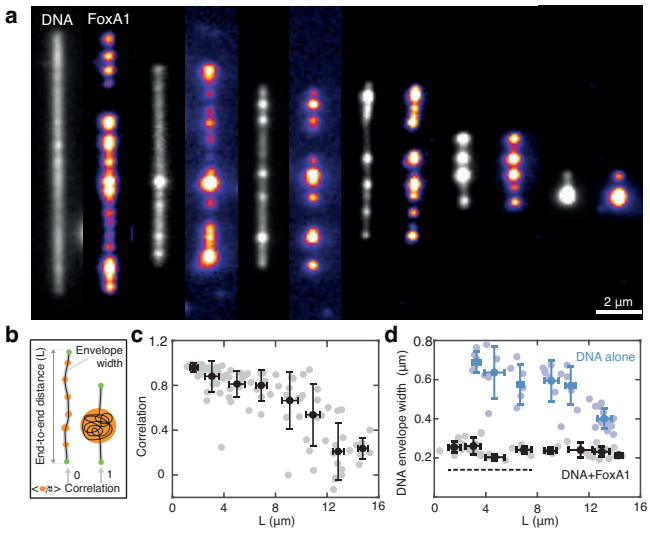

Figure 1: **FoxA1 forms protein-DNA condensates in a tension-dependent manner**. (A) Representative time-averaged projections of FoxA1 and DNA. (B) Schematic displaying three main quantities used to characterize DNA-FoxA1 condensation: the end-to-end distance L; Cross-correlation of DNA and FoxA1 intensities; and DNA envelope width, a measure of transverse DNA fluctuations. (C) Cross-correlation of FoxA1 and DNA signals shows that FoxA1 condenses DNA below a critical end-to-end distance. (D) DNA envelope width measurements reveal that FoxA1-DNA condensation buffers DNA tension. The dashed black line represents the theoretical diffraction limit.

Thermodynamics of protein-DNA co-condensation. To explore the thermodynamics of condensation, we developed a theoretical description based on a semi-flexible polymer partially condensing into a liquid-like condensate. Here, the semi-flexible polymer is DNA and the condensation is mediated by the transcription factor. The free energy of this process contains volume, ($\nu\frac{4}{3}\pi R^3$), and surface contributions, ($\gamma 4\pi R^2$), as well as a term representing the free energy of the non-condensed DNA, where ν is the condensation free energy per volume, R is the condensate radius, and γ is the surface tension of the condensate. We assume that DNA is fully collapsed inside the condensate and thus its volume is proportional to the condensed DNA contour length, $V = \alpha L_d$, where $1/\alpha$ describes the packing density given as DNA length per

condensate volume. The free energy of the polymer, $F_p(L, L_d) = \int_0^L f(L, L_p)dl$, can be obtained from the force-extension curve of the polymer $f(L, L_p)$, where L_p is the contour length of the non-condensed polymer. Using $L_p = L_c - L_d$ where L_c is the contour length of λ-phage DNA (16.5 μm), the free energy is as follows,

$$F(L, L_d) = -\nu\alpha L_d + \gamma 4\pi \left(\frac{3\alpha}{4\pi}\right)^{2/3} L_d^{2/3} + \kappa\left(\frac{(L_c-L_d)^2}{4(L_c-L_d-L)} - \frac{L}{4} + \frac{L^2}{2(L_c-L_d)} - \frac{(L_c-L_d)}{4}\right) \quad (1)$$

where $\kappa = \frac{k_B T}{P}$, k_B is the Boltzmann constant, T is the temperature, and P is the persistence length of DNA. For fixed L, the minimum of $F(L, L_d)$ determines the preferred size of the condensate, Fig. 2A. This free energy predicts upon variation of L a stochastic first-order phase transition for the formation of DNA–protein condensates. The distribution of condensate sizes is then given by $P(L_d)\, e^{-\beta F(L,L_d)}$ for fixed L, Fig. 2B. This accounts for a sharp transition of DNA condensation controlled by the end-to-end distance and thus the tension of the DNA molecule. Our theory also predicts that the condensation forces exerted on the non-condensed DNA are kept roughly constant.

To test this theory, we first measured DNA condensate volumes and found that they increase linearly with the length of condensed DNA (L_d), with $\alpha = 0.04 \pm 0.01 \mu m^2$, Fig 2C. This confirms that DNA is in a collapsed conformation inside the condensates. We simultaneously fit the average amount of DNA contained in the condensates (L_d), Fig. 2D, and the probability of nucleating a DNA condensate (P_{cond}) as a function of end-to-end distance$L$, Fig. 2F. Our fits agree quantitatively with the data and show that L_d decreases with L until a critical end-to-end distance beyond which DNA condensates do not form, Fig. 2D. Below this critical length, the force exerted by the condensate is buffered at 0.21 pN (0.18 $\pm$ 0.30 pN CI), consistent with theory, Fig. 2E. Finally, P_{cond} exhibits a sharp transition at L=10.5 μm (9.4 $\pm$ 10.9 μm CI), in agreement with a stochastic first-order phase transition, Fig. 2F. Our fits allowed us to extract the condensation free energy per volume ν = 2.6 pN/μm2 (2.3 $\pm$ 5.2 pN/μm^2 CI) and the surface tension γ=0.04 pN/μm (0.04 $\pm$ 0.28 pN/μm CI). The forces we measure are similar to those recently measured for DNA loop extrusion [6], and those estimated in intact nuclei from nuclear condensate fusion.

We speculate that these weak forces we find in vitro may be of relevance to the mechanics of chromatin organization. Owing to the tension-dependent nature of DNA–protein co-condensation, our work also suggests that these forces could play a key and, as yet, underappreciated role in genome organization and transcriptional initiation. It is appealing to imagine that transcriptional outputs not only respond to concentrations of transcription factors in the nucleus, but also to mechanical cues from chromatin.

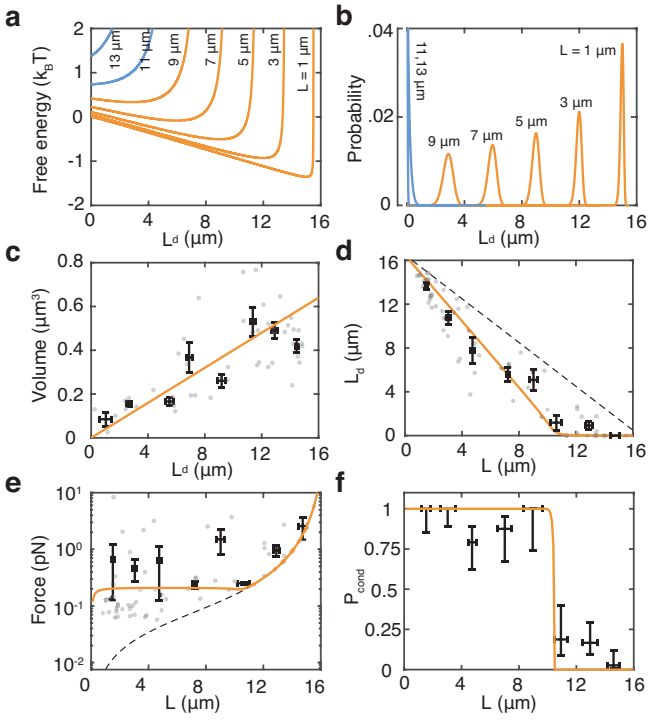

Figure 2: **Thermodynamic description of FoxA1-mediated DNA condensation**. (A) Free energy profiles as a function of condensed DNA (Ld) for different L (orange and blue correspond to favorable and unfavorable condensation, respectively). (B) Boltzmann distributions corresponding to the free energy profiles in (A). (C) Condensate volume linearly increases with L_d. The orange curve represents a linear fit to individual strands (n=47). (D) Amount of condensed DNA as a function of L (n=63). Orange curve represents theoretical fit. The gray dashed-line corresponds to the limit of maximum condensation where L_d is equal to the contour length of DNA minus L. (E) Condensation forces that DNA-protein condensates exert on non-condensed DNA are buffered (n=62). Orange curve is the theoretical prediction. The gray dashed line represents the force when L_d=0. (F) Probability to nucleate a DNA-FoxA1 condensate (P_{cond}) reveals a sharp transition at a critical end-to-end distance.

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2.21 Multiplicative topological phases

ASHLEY M. COOK

Symmetry-protected topological phases of matter have challenged our understanding of condensed matter systems and harbour exotic phenomena promising to address major technological challenges. Considerable understanding of these phases of matter has been gained recently by considering additional protecting symmetries, different types of quasiparticles, and systems out of equilibrium. In this work, we return to the roots of efforts to understand these phases by showing that symmetries may be enforced not just on full Hamiltonians, but also on their components, to construct a large class of previously unidentified *multiplicative* topological phases of matter characterized by tensor product Hilbert spaces similar to the Fock space of multiple particles. To demonstrate our methods, we introduce multiplicative topological phases of matter based on the foundational Hopf and Chern insulator phases, the multiplicative Hopf and Chern insulators, or MHI and MCI, respectively. The MHI shows distinctive phenomena of the parent phases may be combined to create a child phase with exotic non-trivial topology, and we comment on a similar structure in some topological superconductors. We then introduce the MCI phase of matter and show it can realize topologically-protected gapless states that do not extend from the valence bands to the conduction bands for open boundary conditions that respect the symmetries protecting the topological phase. The MCI therefore serves as a blueprint for novel band connectivity in gapped, non-interacting topological phases of matter that illustrates the potential of multiplicative topology to realize exotic phenomena.

The search for novel phases of matter – and particularly phases of matter beyond the Ginzburg-Landau paradigm, known as topological phases of matter – is now a vast and influential topic in condensed matter physics [1–5]. The search has more recently focused primarily on considering an extended set of protecting symmetries [6,7], and on realizing topology in systems that are non-electronic, driven, or coupled to an environment [8–14], as our understanding of electronic topology in equilibrium and in isolation was thought to be complete for effectively non-interacting systems.

However, rather than realizing non-trivial topology by imposing symmetries only on the entire Hamiltonian for a system as has been done in the past, here we generalize by imposing symmetries on components of the Hamiltonian as well, introducing methods for construction of a large class of previously unidentified topological phases, including two examples of new phases as proof of concept of these methods along with an example of how a known phase can be viewed in this framework. This approach considerably expands the possible set of symmetry-protected topological phases of matter, as the large set of symmetries already considered in studying topology may be combined, allowing a set of parent phases of matter to be combined into a single child phase of matter synthesizing the properties of the parents, as illustrated in Fig. 1. Many of these symmetries are commonplace, indicating multiplicative topology is likely widespread.

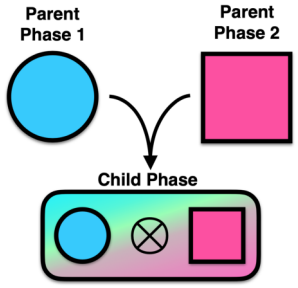

Figure 1: **Realization of multiplicative topology** Parent Hamiltonians 1 and 2, each possessing some symmetries and corresponding to a topological phase of matter, may be combined in a multiplicative manner to construct a single child Hamiltonian. This child Hamiltonian can possess an additional set of symmetries and inherit non-trivial topology from the parents in novel combinations.

We demonstrate this method explicitly by constructing two novel symmetry-protected topological phases of matter, the multiplicative Hopf insulator and the multiplicative Chern insulator, although the concept is broader; indeed we show that a product structure is naturally also present in one kind of topological superconductor. We begin by constructing an example of a multiplicative Hamiltonian that is the child of two non-degenerate parent Hamiltonians, $\mathcal{H}_1(\boldsymbol{k})$ and $\mathcal{H}_2(\boldsymbol{k})$. We then show that this form may be symmetry-protected such that it describes phases of matter, before introducing foundational examples of multiplicative phases of matter, the multiplicative Hopf and Chern insulators (MHI and MCI). To construct the multiplicative Hamiltonian, we first determine the expressions for the matrix elements of the multiplicative Hamiltonian in terms of the matrix elements of the parent Hamiltonians. To do this, we consider parent Hamiltonians which are each acted upon by elements of the special unitary group, $\mathrm{SU}(2)$. Such Hamiltonians have two bands and may describe both the Chern insulator and the Hopf insulator topological phases of matter. A child Hamiltonian constructed from such parents would then be acted upon by the semisimple Lie group $\mathrm{SU}(2)\times\mathrm{SU}(2)$. As this Lie group is isomorphic to

the double cover of $\mathrm{SO}(4)$, this direct product indicates there is a mapping from a pair of parent Hamiltonians, each with 2×2 matrix representation, to a child Hamiltonian with 4×4 matrix representation.

The explicit construction of the isomorphism is given in the methods, and here we state the resulting expression for the child Hamiltonian. We take $\mathcal{H}_1(\boldsymbol{k}) = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ and $\mathcal{H}_2(\boldsymbol{k}) = \begin{pmatrix} \alpha & \beta \\ \kappa & \delta \end{pmatrix}$ to be the two parent Hamiltonians in the construction, with momentum dependence suppressed. The expressions can of course be simplified further given hermiticity of $\mathcal{H}_1(\boldsymbol{k})$ and $\mathcal{H}_2(\boldsymbol{k})$, which gives $c = b^*$ and $\kappa = \beta^*$, ensuring hermiticity of the child Hamiltonian, but we leave the expressions more general to more clearly show the underlying dependence of the child Hamiltonian on the parent Hamiltonians. We may then write the child Hamiltonian $\mathcal{H}_c(\boldsymbol{k})$ in terms of $\mathcal{H}_1(\boldsymbol{k})$ and $\mathcal{H}_2(\boldsymbol{k})$ as

$$\mathcal{H}_c(\boldsymbol{k}) = \begin{pmatrix} a\delta & -a\kappa & b\delta & -b\kappa \\ -a\beta & a\alpha & -b\beta & b\alpha \\ c\delta & -c\kappa & d\delta & -d\kappa \\ -c\beta & c\alpha & -d\beta & d\alpha \end{pmatrix}, \qquad (1)$$

Some physical examples of Hamiltonians of this product form, derived from underlying two-by-two Hamiltonians that can be expanded over Pauli matrices, appear in the theory of 2D Dirac materials, where the two-by-two components can represent spin, valley, or layer degrees of freedom.

To realize Hamiltonians with observables acted on by $\mathrm{SO}(2N)/\mathrm{SO}(N)$, we require that $\mathcal{H}_1(\boldsymbol{k})$ and $\mathcal{H}_2(\boldsymbol{k})$ each lie in class D. This restricts U_1 and U_2 to $\mathrm{SO}(N)$ rather than $\mathrm{U}(N)$. Thus, the desired multiplicative form is realized for Hamiltonians in class DIII with an additional particle-hole symmetry corresponding to class D.

In conclusion, Hamiltonians describing symmetry-protected topological phases of matter may be combined to construct multiplicative topological phases of matter that exhibit properties of their parent phases as well as phenomena beyond our current understanding of non-trivial topology in materials. As any symmetries may be used, in principle, to protect multiplicative topological phases, they should be broadly realizable in materials and cold atom systems [15]. Counterparts of these topological phases are also expected in systems that are not purely electronic and/or not in equilibrium. Given the exception to band connectivity discovered here in the case of the multiplicative Chern insulator, a foundational diagnostic of non-trivial topology in condensed matter systems, it is especially important to fully understand the phenomena that may result from this multiplicative topology.

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2.22 Large Bending Deformations of Cell Sheets During Development

PIERRE A. HAAS

Introduction. Deformations of cell sheets during development are driven by an intricate interplay of cell division, cell shape changes, and related processes, which, in elastic continuum models, appear as changes of the intrinsic geometry of thin elastic shells. A common cell shape change is apical constriction, causing one side of the cell sheet to constrict and hence the cell sheet to bend. This involves "large bending deformations" (Fig. 1), in which a radius of curvature κ^{-1} of the cell sheet becomes comparable to its thickness h. Classical shell theories assume $\kappa^{-1} \gg h$, so $\kappa^{-1} \sim h$ is a new biological scaling limit of elasticity, requiring a shell theory to be derived from first principles, i.e. by asymptotic expansion of three-dimensional elasticity.

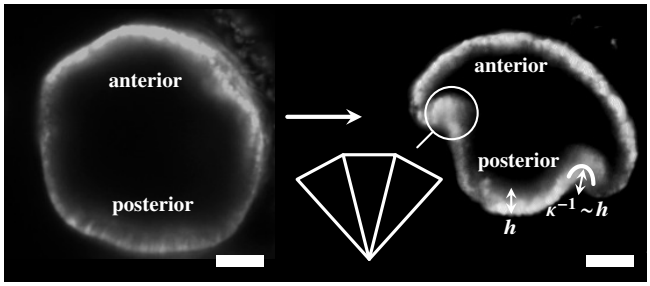

Figure 1: Large bending deformations during invagination in the spherical alga *Volvox globator*: in the midsagittal cross sections, the radius of curvature κ^{-1} of the cell sheet becomes comparable locally to its thickness h. Inset: cartoon of constricted triangular cells in the bend region separating the anterior and posterior hemispheres (labelled in the cross sections). Scale bars: 20 μm. All figures in this report are redrawn from Ref. [1].

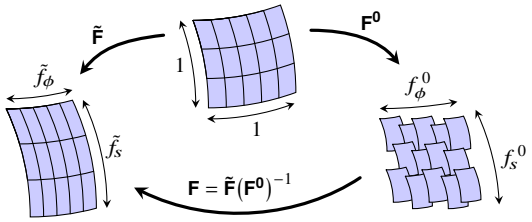

Figure 2: Undeformed (top), deformed (bottom left), and intrinsic (bottom right) configurations of the shell; definition of the deformation gradient tensors $\tilde{\mathbf{F}}$, $\mathbf{F^0}$, $\mathbf{F} = \tilde{\mathbf{F}}(\mathbf{F^0})^{-1}$ and of the meridional (s) and circumferential (ϕ) stretches $\tilde{f}_s, \tilde{f}_\phi$ and f_s^0, f_ϕ^0 of the deformed and intrinsic midsurfaces.

Elastic model. We describe the axisymmetric large bending deformations of an elastic shell of thickness εh, where $\varepsilon \ll 1$ is an asymptotic parameter. We need to distinguish between the undeformed, deformed, and intrinsic configurations of the shell (Fig. 2); the latter differs from the undeformed configuration because of the biological processes, such as cell shape changes, driving the deformations. The relations between these configurations (Fig. 2) are expressed by the tensors $\tilde{\mathbf{F}}$, $\mathbf{F^0}$, $\mathbf{F} = \tilde{\mathbf{F}}(\mathbf{F^0})^{-1}$. The relative meridional and circumferential stretches $\tilde{f}_s, \tilde{f}_\phi$ and f_s^0, f_ϕ^0 of the midsurfaces are defined in Fig. 2. We denote by $\tilde{\kappa}_s, \tilde{\kappa}_\phi$ the curvatures of the deformed midsurface, and correspondingly introduce the intrinsic curvatures $\kappa_s^0, \kappa_\phi^0$. The latter need not equal the curvatures of the intrinsic midsurface, and it is this geometric incompatibility that elastic deformations resolve by "gluing" intrinsically deformed patches of cell sheet back together (Fig. 2). This incompatibility is limited by the "small-strain" assumptions

$$\tilde{f}_s - f_s^0, \tilde{f}_\phi - f_\phi^0 = O(\varepsilon), \quad \tilde{\kappa}_s - \kappa_s^0, \tilde{\kappa}_\phi - \kappa_\phi^0 = O(1). \quad (1)$$

Large bending deformations are introduced by the scaling $\kappa_s^0 = O(\varepsilon^{-1})$, replacing the classical $\kappa_s^0 = O(1)$.

Deriving the shell theory entails reducing the three-dimensional elastic energy of the shell to a two-dimensional, effective energy of its midsurface. The energy of the shell is

$$\mathcal{E} = \iiint_{\mathcal{V}^0} e \, \mathrm{d}V^0, \quad \text{with } e = \frac{C}{2}(\mathcal{I}_1 - 3), \quad (2)$$

where the integration is over the intrinsic configuration $\mathcal{V}^0$ of the shell. In the expression of the incompressible neo-Hookean energy density e, $C > 0$ is a material parameter, and $\mathcal{I}_1 = \operatorname{tr} \mathbf{F}^\top \mathbf{F}$. The effective two-dimensional energy is

$$\mathcal{E} = \iint_{\mathcal{S}} \hat{e} \, \mathrm{d}S, \quad (3)$$

where the integration is over the undeformed midsurface $\mathcal{S}$ of the shell, and the effective energy density $\hat{e}$ is obtained by asymptotic expansion of the energy (2) in the limit $\varepsilon \ll 1$. A long calculation [1] yields

$$\hat{e} = \hat{e}_{\text{stretch}} + \hat{e}_{\text{couple}} + \hat{e}_{\text{bend}} + O(\varepsilon^4), \quad (4)$$

with

$$\hat{e}_{\text{stretch}} = \frac{Ch}{2}\varepsilon^3(\alpha_{ss}E_s^2 + 2\alpha_{s,\phi}E_sE_\phi + \alpha_{\phi\phi}E_\phi^2), \quad (5a)$$

$$\hat{e}_{\text{couple}} = Ch^2\varepsilon^3(\beta_{ss}E_sK_s + \beta_{s\phi}E_sK_\phi + \beta_{\phi s}E_\phi K_s + \beta_{\phi\phi}E_\phi K_\phi), \quad (5b)$$

$$\hat{e}_{\text{bend}} = \frac{Ch^3}{2}\varepsilon^3(\gamma_{ss}K_s^2 + 2\gamma_{s,\phi}K_sK_\phi + \gamma_{\phi\phi}K_\phi^2). \quad (5c)$$

The strain coefficients $\alpha_{ss}, \alpha_{s,\phi}, \alpha_{\phi\phi}, \beta_{ss}, \beta_{s\phi}, \beta_{\phi s}, \beta_{s\phi}, \beta_{\phi\phi}, \gamma_{ss}, \gamma_{s,\phi}, \gamma_{\phi\phi}$ in these definitions are functions, computable in closed form [1], of the large bending parameter $\eta = \varepsilon\kappa_s^0 h/2f_s^0 f_\phi^0$. The shell strains E_s, E_ϕ and curvature strains K_s, K_ϕ are, consistently with Eqs. (1),

$$E_s = \frac{\tilde{f}_s - f_s^0}{\varepsilon f_s^0}, \qquad K_s = \frac{\tilde{f}_s\tilde{\kappa}_s - f_s^0\kappa_s^0}{(f_s^0)^2 f_\phi^0}, \quad (6a)$$

$$E_\phi = \frac{\tilde{f}_\phi - f_\phi^0}{\varepsilon f_\phi^0}, \qquad K_\phi = \frac{\tilde{f}_\phi \tilde{\kappa}_\phi - f_\phi^0 \kappa_\phi^0}{f_s^0 \left(f_\phi^0\right)^2}. \tag{6b}$$

The limit $|\eta| \to 1$, in which all strain coefficients diverge, corresponds to the geometric singularity of apical constriction (Fig. 1, inset). The detailed calculation [1] shows that expansion (4) is valid only if $1 - |\eta| \gg \sqrt{\varepsilon}$. The limit $\eta \to 0$ recovers the classical theory for "small" bending deformations, which replaces Eq. (4) with

$$\hat{e}_0 = \hat{e}_{0,\text{stretch}} + \hat{e}_{0,\text{bend}} + O\left(\varepsilon^4\right), \tag{7}$$

where, on setting $\alpha = 4$, $\gamma = 1/3$,

$$\hat{e}_{0,\text{stretch}} = \frac{Ch}{2}\varepsilon^3 \left(\alpha E_s^2 + \alpha E_s E_\phi + \alpha E_\phi^2\right), \tag{8a}$$

$$\hat{e}_{0,\text{bend}} = \frac{Ch^3}{2}\varepsilon^3 \left(\gamma K_s^2 + \gamma K_s K_\phi + \gamma K_\phi^2\right). \tag{8b}$$

As $\alpha_{\phi\phi} \neq \alpha_{ss}$, $\gamma_{ss} \neq \gamma_{\phi\phi}$ [1], there is thus, in the large bending theory, a new effective, geometric anisotropy, even for a constitutively isotropic shell.

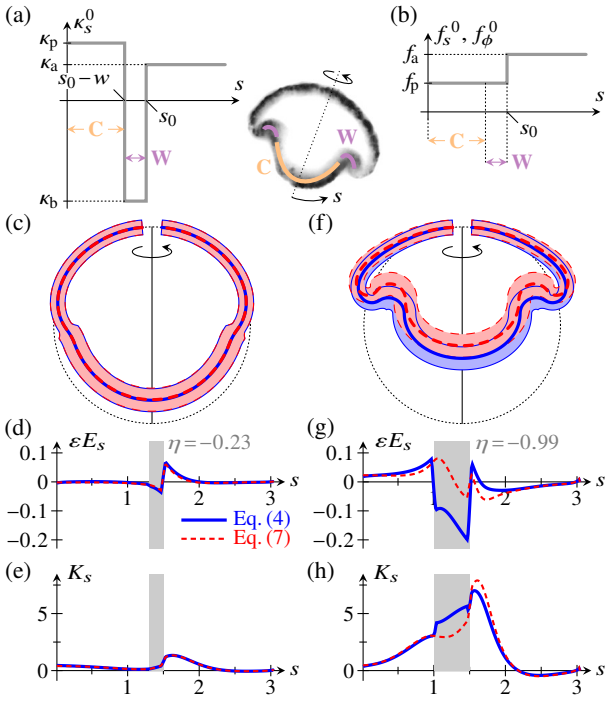

Figure 3: Invagination in *Volvox*: comparison of the elastic model for large bending deformations and the classical model. (a) Plot of the intrinsic curvature κ_s^0 against arclength s. The inset defines s and the regions of wedge-shaped cells [W] and contracted cells [C]. (b) Plot of the intrinsic stretches f_s^0, f_ϕ^0. (c) Early invagination stage: the two models yield very similar shapes. Solid lines: large bending model with energy density (4); dashed lines: classical model with energy density (7). (d) Corresponding plot of E_s. The shaded area is the bend region $s_0 - w < s < s_0$. (e) Corresponding plot of K_s. (f) Late invagination stage: as the constriction limit is approached, the shapes from the two models start to differ. (g) Plot of E_s. (h) Plot of K_s.

Application: Invagination in *Volvox*. The embryos of the alga *Volvox* are spherical sheets of thousands of cells that turn themselves inside out at the close of their development. The first part of this inversion involves a circular invagination (Fig. 1), resulting from two types of cell shape changes bending and contracting the cell sheet [2]: (i) cells in the "bend region" near the equator constrict to become wedge-shaped, and (ii) cells in the posterior contract in the meridional direction.

We model this invagination by the large bending deformations of an incompressible elastic shell; these cell shape changes driving invagination are represented, because of their slow speed [2], by quasi-static changes of the intrinsic stretches and curvatures of the shell. Functional forms for these that encode these cell shape changes are in Figs. 3(a),(b). We solve the boundary value problems associated with the Euler–Lagrange equations of the large bending theory (4) and the classical shell theory (7) numerically.

For early stages of invagination, the two models yield very similar shapes [Fig. 3(c)], mirrored by very similar profiles of shell [Fig. 3(d)] and curvature [Fig. 3(e)] strains. The contraction of the posterior hemisphere leads to thickening of the cell sheet there [Fig. 3(c)]. However, for later stages of invagination, as the intrinsic configuration of the shell approaches the constriction singularity, the shapes resulting from the two models start to differ [Fig. 3(f)]. Correspondingly, the shell [Fig. 3(g)] and curvature [Fig. 3(h)] strains show quantitative and even qualitative differences. There are thus true mechanical differences between the two models.

Discussion. The mechanical differences between the large bending theory and the classical theory revealed by the example of *Volvox* invagination emphasise the importance of this geometric effect for quantitative understanding of the mechanics of morphogenesis. Does the theory presented here then give a complete mechanical description of processes of invagination? For the late invagination stage in Fig. 3, the condition $1 - |\eta| \gg \sqrt{\varepsilon}$, which is particularly restrictive for biological tissues as they are often not "that thin", breaks down. Extending the theory to the limit $|\eta| \to 1$ to regularise the constriction singularity fully thus remains an important challenge. The same large-bending theory applies to other elastic constitutive laws [1], but the continuum mechanics of biological tissues are described, even at equilibrium, by more general, nonelastic constitutive relations: indeed, the continuum limit of a simple discrete model involves nonlocal, nonelastic terms [3]. Hence understanding the interplay of nonelastic constitutive nonlinearities and these large geometric deformations is also a key open problem.

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2.23 Reference quality bat genomes illuminate the molecular basis and evolution of bat adaptations

MICHAEL HILLER

Introduction With more than 1400 species identified to date, bats account for 20% of all mammal species and successfully occupy diverse ecological niches. Their global success is attributed to an extraordinary suite of adaptations including powered flight, laryngeal echolocation, exceptional longevity, and a unique immune system that enables bats to tolerate viruses that are typically lethal in other mammals (e.g., rabies, SARS, MERS) [1]. Therefore, bats represent important model systems to uncover the molecular basis and evolution of extended healthspan and enhanced disease tolerance. To understand the evolution of such traits, we generated the first reference-quality genomes of six bats and performed a comprehensive comparative genomic analysis. This project was a collaboration with the CSDB in Dresden and the Bat1K global genome consortium [2] (http://bat1k.com).

Genome Assembly To assemble high-quality genomes, we generated for each of the six bats long read (PacBio), short read (10X Genomics Illumina) and scaffolding (Bionano optical maps, Hi-C read pairs) data. This sequencing strategy produced assemblies with contig N50 values ranging from 10.6 to 22.2 Mb, which is orders of magnitude more contiguous than previous assemblies generated from short read data. Scaffold N50 values ranged from 80.2 to 171.1 Mb and were often limited by the size of chromosomes. We estimated that 87 to 99% of each assembly is in chromosome-level scaffolds.

Genome Annotation To comprehensively annotate protein-coding genes, we integrated different types of gene evidence, including short read (RNA-seq) and long read (Iso-seq) transcriptomic data from our bats, gene projections by our TOGA (Tool to infer Orthologs from Genome Alignments) method, aligned protein and cDNA sequences of related mammals, and de novo gene predictions. For the six bats, we annotated between 19,122 and 21,303 protein-coding genes. Using the 4,104 mammalian BUSCO (Benchmarking Universal Single-Copy Orthologs) genes, we achieved 99.3-99.7% completeness, showing that our assemblies and annotations are highly complete in protein-coding sequences. Importantly, the completeness of our gene annotations is higher than available annotations of dog, cat, horse, cow and pig, and is only surpassed by those of human and mouse, which have received extensive manual curation of gene models.

Genome-wide screens for gene selection, losses and gains To study the genomic basis of exceptional traits shared by bats, my group performed three unbiased genome-wide screens for gene changes that occurred in the six bats. First, we screened 12,931 genes classified as 1:1 orthologs for signatures of positive selection on the ancestral bat (stem Chiroptera) branch. This revealed 9 genes with a robust signal of positive selection at the bat ancestor. While these 9 genes have diverse functions, they included two genes with hearing-related functions, which may relate to the evolution of echolocation. These genes, LRP2 (low-density lipoprotein receptor-related protein 2, also called megalin) and SERPINB6 (serpin family B member 6) are expressed in the cochlea and associated with human disorders involving deafness. In general, experimental studies are required to test whether the pattern of positive selection on the stem Chiroptera branch affect hearing-related functions of these three genes. If so, this would provide molecular support for laryngeal echolocation as a shared ancestral trait of bats and subsequent loss in pteropodids, informing a long-standing debate in bat biology of whether ancestral bats had the ability to echolocate.

In addition to hearing-related genes, our genome-wide screen also revealed bat-specific selection on several immunity-related genes; the B-cell specific chemokine CXCL13 (C-X-C motif chemokine ligand 13), the asthma-associated NPSR1 (neuropeptide S receptor 1), and INAVA (innate immunity activator), a gene involved in intestinal barrier integrity and enhancing NF-kB signalling in macrophages. Changes in these genes may have contributed to the unique pathogen tolerance of bats.

Second, we used our previously developed approach to systematically screen for gene loss. This revealed 10 genes that are inactivated in our six bats but present in the majority of related non-bat species. Two of these genes again point to changes in immune function in bats, having immune-stimulating and pro-inflammatory functions; LRRC70 (leucine rich repeat containing 70, also called synleurin) and IL36G (interleukin 36 gamma) (Fig. 1a). LRRC70 is expressed in a broad range of tissues and potentiates cellular responses to multiple cytokines and is well conserved among Laurasiatheria. Importantly, LRRC70 strongly amplifies bacterial lipopolysaccharide-mediated NF-kB activation. Our finding of LRRC70 loss in bats makes this poorly characterized gene an interesting target for future mechanistic studies. IL36G, encodes a pro-inflammatory interleukin belonging to the interleukin-1 family. Increased expression of IL36G

was detected in psoriasis and inflammatory bowel disease patients, and IL36G is likely involved in the pathophysiology of these diseases by inducing the canonical NF-kB pathway and other proinflammatory cytokines. Together, genome-wide screens for gene loss and positive selection revealed several genes involved in NF kB signalling (Fig. 1b), suggesting that altered NF kB signalling may contribute to immune related adaptations in bats.

Third, we investigated changes in gene family size, which revealed 35 cases of significant gene family expansions and contractions at the bat ancestor. Among these, we inferred an expansion of the APOBEC gene family, which is known to exhibit a complex duplication/loss history in flying foxes (genus Pteropus) and other mammals. Our detailed analysis indicates a small APOBEC3 expansion in the ancestral bat lineage (Fig. 1c), followed by multiple lineage-specific expansions involving up to 14 duplication events. APOBEC genes are DNA and RNA editing enzymes that have been previously associated with restricting viral infections and transposon activity. Expansion of APOBEC3 genes in multiple bat lineages suggests these duplications may contribute to viral tolerance in these lineages.

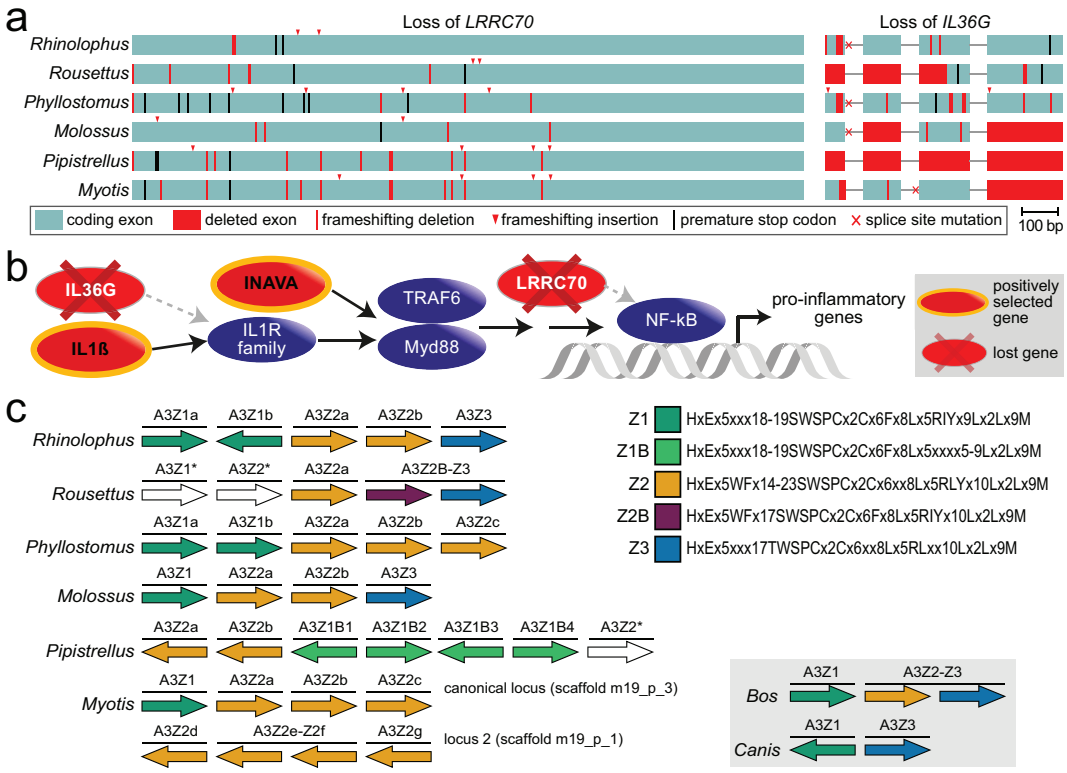

Figure 1: Genome-wide screens highlight changes in genes potentially involved in the unique immunity of bats. (a) Inactivation of the immune-stimulating genes LRRC70 and IL36G. Boxes represent coding exons proportional to their size, overlaid with gene-inactivating mutations present in the six bats. (b) Diagram showing the canonical NF-kB signalling pathway (purple) and interacting proteins which have experienced positive selection (red background) or have been lost in bats (crossed out). (c) Expansion of the APOBEC3 gene locus in bats. Each arrow represents a cytidine deaminase domain, coloured by domain subtypes as defined by given motifs, with likely pseudogenes are in white. Genes containing multiple deaminase domains are indicated with a single bar over more than one domain. A transposition event in Myotis has created two APOBEC3 loci on different chromosomes. Cow and dog are shown as two Laurasiatheria outgroups, where cow also represents the likely, mammalian ancestral state.

Discussion Using a combination of state-of-the-art methods including long-read, short-read, and scaffolding technologies, we generated the first chromosome level, near-complete assemblies of six bats that represent diversity within Chiroptera. These reference-quality genomes improve on all published bat genomes. Our comprehensive and conservative genome-wide screens investigating gene gain, loss and selection provide candidates that are likely related to the unique immunity of bats. Furthermore, our screens reveal selection in hearing genes in stem Chiroptera, which is consistent with the hypothesis that echolocation evolved once in bats and was secondarily lost in Pteropodidae, but inconsistent with the alternative hypothesis that echolocation evolved twice independently within bats.

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2.24 Non-Gaussian models with long range temporal correlations - understanding the statistics of precipitation

KATJA POLOTZEK AND HOLGER KANTZ

Long range temporal correlations Recorded time series data from very many natural sources exhibit long range temporal correlations (LRC). This phenomenon was first observed in the fluctuations of the Nile river by hydrologist Harold Hurst in 1956 [1]. Today, there are well established mathematical models such as fractional Gaussian noise [2] in continuous time and ARFIMA-models [3] in discrete time, where the power law decay of the auto-correlation function (ACF) can be adjusted as a free parameter. As a consequence of this much slower than exponential decay of the ACF the auto-correlation time diverges and the phenomenon lacks a typical time scale. Detrended fluctuation analysis and a method based on the wavelet transform [4] can detect such type of behavior in data. Long range temporal correlations and hence memory in time series has been found in surface temperatures and water run-offs, heart beats and EEG data sets, as well as in DNA strands, just to name a few. In time series of daily precipitation, LRC phenomena can explain the enhanced probability of long lasting draughts and extended periods of rainfall, among other things. Since the distribution of daily precipitation amounts is highly non-Gaussian and non-symmetric, the above mentioned ARFIMA models cannot be used, while, e.g., for the purpose of modeling flooding or agricultural risks, stochastic precipitation generators would be highly useful. Here we summarize our work on non-Gaussian models with adjustable long range temporal correlations, and implications of such correlations for statistical estimates of mean values, variances, and extremes, with application to precipitation data.

Meta Gaussian models and auto-correlation function after transformation We aim at setting up a time series model for non-Gaussian data with long range temporal correlations with a Hurst exponent $H > 1/2$, i.e., the fluctuations show persistence. If the marginal distribution of the data were Gaussian, an ARFIMA(0,d,0)-model with $d = H - 1/2$ would be suitable, and if we wanted to include short-range temporal correlations as superimposed exponential decay, one could use an ARFIMA(1,d,0)-model: in addition to the memory-parameter d, it has an auto-regressive parameter a to be fitted to the data. The model equation then reads:

$$x_{n+1} = ax_n + \sum_{i=1}^{\infty} c_i \xi_{n+1-i} \text{ with } c_i = \frac{\Gamma(d+i)}{\Gamma(1+i)\Gamma(d)} \quad (1)$$

where x_n is the observable at time n and ξ_i are white Gaussian noises with zero mean and unit variance, and Γ is the Γ-function. This is a data model, not a physical model, since the memory is included "by hand" through the weighted sum over all past noises. Data produced by iteration of this model will show $H = d + 1/2$ in good numerical accuracy. To reproduce the non-Gaussian distribution of the original empirical data, we apply a suitable nonlinear transformation to x_n, $y_n = f(x_n)$. However, such a transformation will inevitably render the ACF of y to be different from x. Since the model distribution is Gaussian, an expansion of $f(x) = \sum_{i=1}^{\infty} a_i H_i(x)$ in Hermite-polynomials $H_i(x)$ enables us to rewrite the ACF of y in terms of the ACF of x in the following way:

$$c_y(\tau) = \frac{1}{\sigma_y^2} \sum_{i=1}^{\infty} \frac{a_i^2}{\sigma_x^{2i} i!} c_x(\tau)^i \quad (2)$$

The ACF of the ARFIMA(1,d,0)-process x decays to zero for large lags τ. The transformed ACF of y is then dominated by the smallest power i for which a_i is non-zero, asymptotically. If this "Hermite rank" of the transformation f is unity, then c_y decays with the same power as c_x. Only if f is symmetric does it have Hermite rank 2 or larger and can change the asymptotic power law decay. Hence, if the non-Gaussian distribution of our empirical data is not symmetric with respect to its mean, the empirical Hurst exponent H of these data tells us to choose $d = H - 1/2$. Also the short range part of the ACF can be suitably translated into the auto-regressive parameter a of the ARFIMA model. For details see [5]. In summary, we end up with the parameters of an ARFIMA model, which under transformation $y = f(x)$ yields a time series model for the observed data, reproducing their auto-correlation function and their marginal distribution.

Precipitation data We apply this procedure to precipitation data measured at mid-latitude meteorological stations. As an example, a histogram of the data set of the Fichtelberg in Germany is shown in Fig.1, with a large peak at 0, representing the dry days, and a long tail towards large precipitation events. A probability density which can fit this histogram very well is obtained by a *truncated Gaussian power* (tGp): $y = f(x) = max(0, x + \mu)^{\beta}$. So all values $x < \mu$ of the Gaussian ARFIMA-process will be mapped to 0 and hence model the dry days, while the others will be stretched out. After fitting μ and β by a method which emphasizes agreements in the tails rather than the bulk our tGp distribution passes strict statistical tests as a model for the empirical distribution. Together with the

value $d \approx 0.1$ which characterizes the LRC, a value a adjusted to also describe the short range correlations, and the measured variance σ_y^2 of the data we have a 5-parameter time series model for these data. In Fig.2 it is shown that, e.g., the non-Poissonian statistics of drought lengths can be well reproduced by our LRC model.

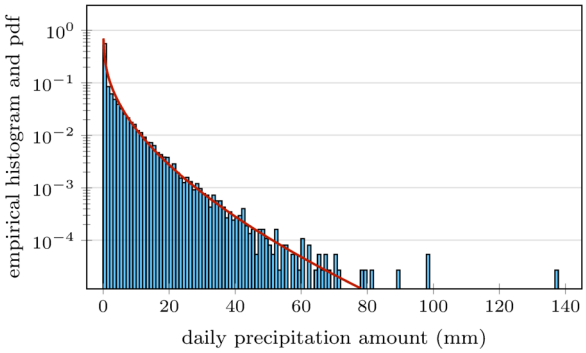

Figure 1: A histogram of the daily precipitation amounts of Fichtelberg station, accumulated over 100 years, together with a fit of the truncated Gaussian power distribution.

Consequences Long range temporal correlations have several implications: First, the probabilities that the signal shows exceptionally low or exceptionally high values over a longer time interval are enhanced in comparison to a short range correlated signal. In precipitation, this can explain in particular the observation of longer lasting droughts with higher probability than naively expected, but also the clustering of extreme precipitation events [7]. Also time averages are affected: Even on large but finite time intervals, time averages might be far from the ensemble mean, and large deviation probabilities do not decay exponentially in the length of the averaging interval, but as stretched exponentials [8]. This explains why we observe "wet" years and "dry" years: a single year as interval for a time average does not grant that this average is close to the long-year climatological mean value.

This latter fact can also be rephrased by the notion of an effective sample size N_{eff} [6, 8]: Given a time series of length N, and performing statistical estimates of its distribution such as mean value or variance, the statistical uncertainty of these will depend on N and decrease as $N \to \infty$. However, a correlated signal contains redundancies, since successive values share part of their information. For short range correlations, it can be shown that the "true" information, carried by independent observations, is N/τ, where τ is the autocorrelation time. For signals with long range correlations such as precipitation data, the scaling in N is sub-linear, i.e., the effective sample size is proportional to N^{2-2H}. So, e.g., doubling the observation time will not double the amount of independent information about the phenomenon.

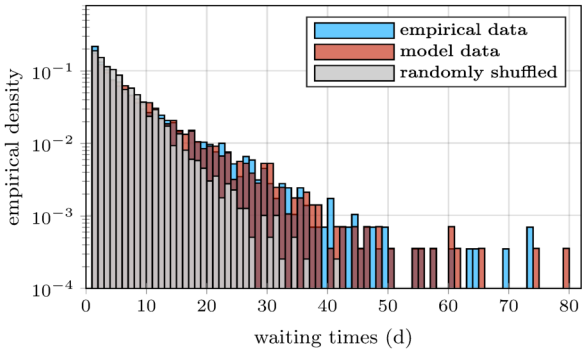

Figure 2: Drought length distribution of Bordeaux for observed and model data.

Another important result concerns the probabilities for extreme precipitin events. Extreme precipitation causes disastrous flooding with huge damages and even human casualties. The relevant issue for flood protection is how strong a precipitation event can be which occurs with a given probability, e.g., once in 100 years on average. Since recorded time series are too short to estimate that directly from the empirical marginal distribution, and also since this probability might have changed in the course of climate change over the past 30 years, the answer to this question requires an extrapolation using the mathematical concept of Extreme Value Theory. A dramatic improvement for the estimate of the 100 year return level, i.e., the value Q_{100} (of precipitation amount) which is overcome on average once in 100 years, can be obtained when knowing the marginal distribution of the observable. Our results that the mid-latitude daily precipitation amounts can be well modeled by a truncated Gaussian power, together with some novel way to calculate Q_{100} can be used to find much more accurate estimates of Q_{100} than before [6].

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2.25 A network analysis of the evolution of astrophysical knowledge

MARYAM ZAMANI, ALEJANDRO TEJEDOR, AND HOLGER KANTZ

Introduction In early modern times, text books for students were of a quite different character than nowadays. A classical book which has been in use for more than two centuries is based on the hand-written text by Johannes di Sacrobosco entitled "tractatus de sphaera" or also "de sphaera mundi" (treatise on the sphere of the world), written around the year 1230. This formed the basis for a compilation of many more texts and commentaries whose first printed editions were published in 1472 in Ferrara and in Venice [1]. The texts cover concepts about the geocentric view of the universe, instructions of how to use astronomical observation instruments and how to perform calculations, as well as tables containing astronomical information. They were designed as teaching material for high school and university students. This stock of knowledge was so overly well received and successful that over 180 years at least 359 printed editions appeared, the last one in 1650, many of them in Latin, but also translated into Italian, German, French, produced by publishers in 41 different European places [1]. Colleagues from the Max Planck Institute for the History of Science in Berlin, under the guidance of Matteo Valleriani and Florian Kräutli, organized the compilation of this corpus of books. They formed a database where, among other data, the contents of the books were atomized into pieces of text and equipped with a network structure [2]. This material allows to study the acquisition of knowledge, its diversification and consolidation, and the process of knowledge spreading and scientific influence inside Europe in the early modern times. In collaboration with Matteo Valleriano and his colleagues from the MPI-WG, we performed a network analysis to gain some understanding and quantification of the above mentioned processes in the evolution of knowledge.

The multiplex network of books The 359 books of the corpus are considered as nodes of a network. There are 563 different text parts contained in the union of all books, from which only 239 are re-printed at least once. Only these will be considered, and by re-printing, these form a set of 1653 parts. A single such unit can be an original text by some specific author, it can be the translation of such a text, it can be an annotation made to a given original text, or an adaptation [3].

The layers of the network represent different semantic categories. One layer is naturally formed by the exact re-print of a text, others are its translation, or annotation, or adaptation. If a later book of the corpus contains a unit of text, which is based on a text which is part of an earlier book, a link is set between these two books in the respective layer of the network. In total, 6 such layers are used to represent the relationships among books through their text parts. In this way, a book enters as a node in the specific network layer if it has a link inside this layer. The resulting network is a directed weighted multiplex network, i.e., a network where each node can have multiple links to other nodes in different categories, but not every node appears in every layer. This structure of semantic layers together with additional socio-economic layers is inherent to the database [2] and defines the network of this study.

Link statistics To illustrate the size of the network, we report here some statistical results. The layer Se16, which means "annotated same original part", has the largest number of links (15326), while layer Se13 (same original part) has the largest number of nodes (321). When aggregating all layers, we arrive at the aggregated graph with 356 nodes and 23586 links. Since links link more recent books to earlier ones, a natural statistics is the average age of the links. Depending on the layer, this average age is between 20 and 45 years. This means that more recent books have the tendency to "forget" about the really old text parts. Nonetheless, there are up to 10% of links with ages larger than 90 years.

Layer name	Number of nodes	Number of links
Se13	321	5681
Se14	199	2173
Se15	43	341
Se16	183	15326
Se17	8	15
Se18	85	3312
aggregated	356	23586

Table 1: Table of nodes and links for all semantic layers.

Network analysis, families of books, and communities We intend to achieve some understanding about the processes of knowledge acquisition and consolidation by a statistical analysis of this network. A good insight can be gained from the aggregated graph: one forms the union of all nodes, and accumulates the links from all layers in a single network. The influence of a book on the subsequent development is then related to its out-degree: the number of links to more recent books. However, the later in time a book is published, the less books will follow and the lower is an evident upper bound to the out-degree. Therefore, we normalize the out-degree of every book by the number of all younger books. The result is shown in Fig.1. The plot

shows several branches, which correspond to families of books with similar content. A simple null-model helps in interpretation: Let us have two different versions of the Sphaera. Let version 1 be reproduced identically with a share of 2/3 of all later books, and version 2 with 1/3. Then every book of version 1 will have twice as many outgoing links as every book of version 2, and after normalization we will see two values of the out-degree: one family at the value 2/3, and one family at the value 1/3. So the family to which a book belongs can be identified by its normalized out-degree. In reality, the situation is more complicated, since books are not exact reproductions of their ancestors, and since books of different families contain different numbers of text parts and hence differ in their out degrees.

An alternative approach to detecting families of books is community detection in networks [5]: One decomposes a network into different components, where the connectivity inside each component should be much larger than the connectivity between the components. This is a special kind of clustering. We use the Louvain community detection algorithm for this purpose and find out that the branches in Fig.1 are mostly formed by books from a single community. In [4] we also show results for the decomposition of the graphs formed by single layers into connected components which allows us to learn more details about the different semantic layers.

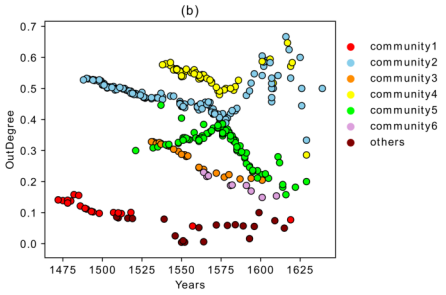

Figure 1: Normalized book out-degree as a function of publication time for the aggregated graph. Color coding shows the largest 6 communities from the Louvain community detection algorithm.

Most influential books, innovations, and great transmitters Of specific interest are innovations in science, and the formation of new ways of thinking. A successful book is innovative, if it is the beginning of a new family as shown in Fig.1: if many later books have many references to this particular one, but not as many to even earlier books. The only possible interpretation is then that some relevant content of this book cannot be found in earlier books, hence, an innovation has been made. The concept of disruption quantifies a slightly different property: Not only shall a book contain some innovation, but at the same time it should break with traditions from the past. The disruptive book itself should not have many links to the past, but, in order to be a successful book, have many links into the future, i.e., a strong imbalance of in- and out-degree.

With these two concepts our analysis revealed several books as being particularly important for the evolution of knowledge. The *enduring innovations* are indeed visible in Fig.1 as those which are at the beginning of a given family. Being highlighted in this way, our colleagues at MPI-WG then analyzed which part of the contents makes them so outstanding [3]. When studying disruption, the converse was also detected: books that incorporate quite old knowledge and at the same time are linked to very recent books. A set of about 15 such books was produced between 1549 and 1562, predominantly in Wittenberg, called *great transmitters*. Our network analysis is also able to detect *sleeping beauties*, i.e., text parts which where not recognized for many years after publication and only much later became very popular and hence frequently reprinted.

Conclusions Quantitative network analysis is able to highlight certain books of the corpus or certain text parts. Historians can then employ their immense knowledge and interprete these findings in the right context. Apart from many more specific results, our team hence could draw two conclusions of broader interest: First, the most relevant text part among all is a rather mathematical text on astronomy and shows the increasing relevance of mathematics in the natural sciences. Second, the most impactful texts are more of practical nature, which can be explained by the much larger audience for such issues than for questions of purely scientific interest. This reflects the relevance of economic factors in science.

Joint project with M. Valleriani, F. Kräutli, M. Vogl and other colleagues at the MPI-WG in Berlin.

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[2] https://sphaera.mpiwg-berlin.mpg.de/database/

[3] M. Valleriani, F. Kräutli, M. Zamani, A. Tejedor, C. Sander, M. Vogl, S. Bertram, G. Funke, H. Kantz, The Emergence of Epistemic Communities in the Sphaera Corpus: Mechanisms of Knowledge Evolution, J. hist. Network Res. **3** 50-91 (2019).

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[5] Leicht, E. A. & Newman, M. E. J. Community structure in directed networks. Phys. Rev. Lett. 100, 118703 (2008).

2.26 Extracting higher-order nonlinear electronic response in solids using high harmonic generation

ALEXANDRA LANDSMAN

Key findings Nonlinear susceptibilities are key to ultrafast lightwave driven optoelectronics, allowing petahertz scaling manipulation of the signal. Recent experiments retrieved a 3rd order nonlinear susceptibility by comparing the nonlinear response induced by a strong laser field to a linear response induced by the otherwise identical weak field. The highly nonlinear nature of high harmonic generation (HHG) has the potential to extract even higher order nonlinear susceptibility terms. However, up till now, such characterization has been elusive due to a lack of direct correspondence between high harmonics and nonlinear susceptibilities. In our recent work [2], we demonstrate a regime where such correspondence can be clearly made, extracting nonlinear susceptibilities (7th, 9th, and 11th) from sapphire of the same order as the measured high harmonics. The extracted high order susceptibilities show angular-resolved periodicities arising from variation in the band structure with crystal orientation. Our results open a door to multi-channel signal processing, controlled by laser polarization.

Background The development of strong ultrafast optical fields opened a possibility to induce and observe the nonlinear dynamics of electrons without damaging the material. High harmonic generation in solids is a nonlinear frequency conversion phenomenon, whose mechanism is still a subject of intense investigation. The process was first observed in atomic gas, where it is well-described by the three-step recollision model. However, in solids, in addition to the above-mentioned recollision scenario (described within non-perturbative interband HHG framework), intraband transitions and Wannier-Stark localization have been found to make important contributions, depending on the material and laser parameters.

Prior experimental extraction of nonlinear susceptibility in attosecond experiments relied on other, non-HHG, mechanisms, such as comparing the linear to the nonlinear polarization response using attosecond streak camera [1]. This allowed the extraction of the third order Kerr nonlinearity, showing the potential of petahertz scaling manipulation by relying on the change of the effective refractive index in optoelectronics. However, extracting higher order nonlinear susceptibilities using this method requires broader spectral coverage.

Discussion In our work, published in Nature Communications [2], we show how to use HHG in suitable regimes to cleanly extract much higher order susceptibilities and therefore achieve unprecedented characterization of nonlinear electronic response directly based on experimental measurements. Figure 1 illustrates different possible mechanisms of HHG in solids, which may be due to either interband transitions (resulting from multi-photon absorption or tunneling) or intraband transitions. Both interband and intraband HHG have been previously observed in solids, with recollision being directly analogous to HHG in atomic gas, while intraband oscillations being unique to solids and determined by the shape of the conduction band.

Figure 2 shows experimentally measured harmonic yield obtained by sweeping over crystal directions in the C-plane (a) and A-plane (b) for various intensities. Figure 2c shows high harmonic yield as a function of intensity for 7th, 9th and 11th harmonics, from which we then extracted 7th, 9th, and 11th order susceptibilities, respectively. As can be seen from Figure 2c (plotted on the log-log scale), the dashed lines follow AI^N fit, where A is a constant, I is the intensity of laser light and N is the order of the harmonic. This type of scaling is typical of multi-photon excitations.

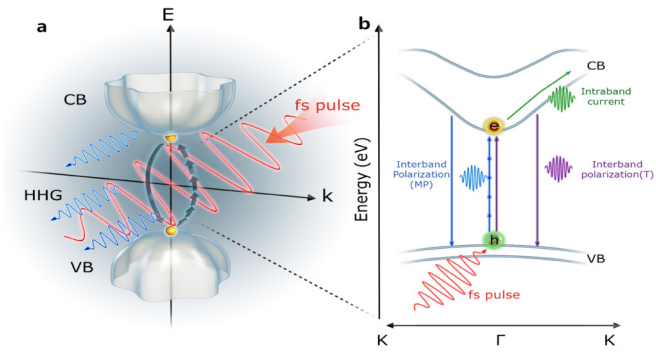

Figure 1: Schematic sketch of the interband and intraband mechanism. (a) Sketch of the 3D band structure with the valence band (VB) at the bottom and the conduction band (CB) at the top. The red wiggle represents the input laser field, and the blue wiggles the high harmonic radiation. (b) The 1D band structure with tunnel (T) transition and multiphoton (MP) transition as possible transition paths from the valence to the conduction band. Intraband HHG is due to the electron's oscillation in the conduction band, whereas interband HHG depends on the electron recombining with its hole.

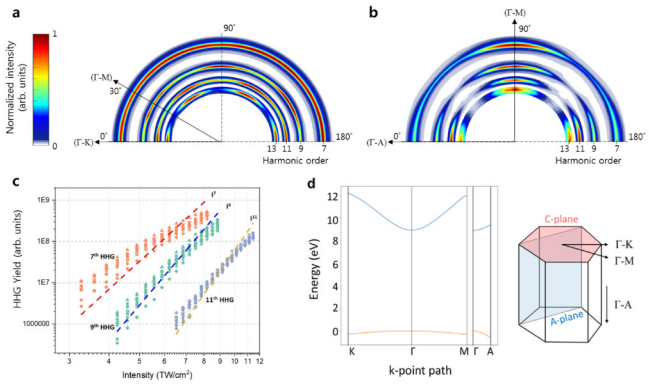

Figure 2: (a) Experimentally measured high harmonic spectra obtained by rotating the laser polarization direction in the C-plane, leading to the expected six-fold symmetry; (b) Measured high harmonic spectra from rotating laser polarization in the A-plane; c) Experimental high harmonic yield plotted on a log-log scale for 7th (red), 9th (blue) and 11th (orange) order harmonics; d) Sketch of the band structure of a sapphire crystal with the highest valence band and the lowest conduction band.

[1] A. Sommer, et al, Nature **534** (2016) 86.

[2] S. Han, et al, Nature Communications **10** (2019) 1-6.

In summary, we investigated nonlinear electronic response in wide bandgap material by measuring angular-dependent high harmonic emission. Having established that the high harmonics are due to interband transitions in the multi-photon regime, we were able to extract orientation-dependent high-order nonlinear susceptibilities of the material. This greatly expands on prior findings, which extracted the 3rd order Kerr susceptibility induced by strong optical fields. Higher order nonlinearities are believed to be crucial to signal manipulation in optoelectronics by affecting the electron response time and refractive index. The susceptibilities obtained in our study have a periodicity that depends on crystal orientation, suggesting a possibility of multichannel signal processing at PHz frequencies by controlling the electron response time and refractive index using laser polarization.

2.27 Many-body delocalization via emergent symmetry

N. S. SRIVATSA, RODERICH MOESSNER, AND ANNE E. B. NIELSEN

Introduction Quantum many-body systems typically follow the eigenstate thermalization hypothesis, which explains how quantum systems can thermalize. There are, however, examples of quantum systems that do not thermalize, but instead retain information stored in them [1]. For many-body localized systems, all states in the spectrum are nonthermal, and for quantum many-body scars only a few states in the spectrum are nonthermal. Here, we show that one can also have a different type of nonthermal system, namely a weak violation of many-body localization, in which most states in the spectrum are many-body localized, but a few states are not. We propose emergent symmetry in eigenstates as a general mechanism to obtain this phenomenon. The results reported here have been published in [2].

General idea If a Hamiltonian H has the symmetry that it commutes with a Hermitian operator X, one can find simultaneous eigenstates for H and X. It is, however, possible that an eigenstate has a higher symmetry than required by the Hamiltonian, and we call this emergent symmetry. Many-body localization is obtained in certain systems when disorder is introduced. It has been argued [3] that some symmetries are incompatible with many-body localization. We hence propose the following general mechanism to obtain weak violation of many-body localization: Construct a Hamiltonian with disorder that is expected to be many-body localized, but ensure that selected eigenstates in the spectrum have an emergent symmetry that is incompatible with many-body localization. Below, we give a concrete example.

Model We consider N spin-$1/2$ particles described by the Hamiltonian

$$H = \sum_{i\neq j} F^A_{ij}(S^x_i S^x_j + S^y_i S^y_j) + \sum_{i\neq j} F^B_{ij} S^z_i S^z_j + F^C \quad (1)$$

where $S^a_i = \sigma^a_i/2$, $a \in \{x, y, z\}$, and σ^a_i are the Pauli matrices. The coefficients

$$\begin{aligned} F^A_{ij} &= -2w^2_{ij}, \qquad w_{jk} = -i\cot[(\phi_j - \phi_k)/2], \quad (2)\\ F^B_{ij} &= -2w^2_{ij} + 2w_{ij}\Big(\sum_{k(\neq i)} w_{ik} - \sum_{k(\neq j)} w_{jk}\Big),\\ F^C &= \frac{N(N-2)}{2} - \frac{1}{2}\sum_{i\neq j} w^2_{ij}, \end{aligned}$$

are defined in terms of N phases ϕ_j, and disorder is introduced into the model by choosing

$$\phi_{f(j)} = \mathrm{mod}_{2\pi}(2\pi(j + \alpha_j)/N), \quad (3)$$

where α_j are random numbers uniformly distributed in the interval $[-\frac{\delta}{2}, \frac{\delta}{2}]$ and $\delta \in [0, N]$ is the disorder strength. The expression $\mathrm{mod}_{2\pi}(\ldots)$ is the modulus after division by 2π, and the function $f(j)$ orders the indices, so that the phases are numbered in increasing order.

The Hamiltonian H conserves the total magnetization $\sum_i S^z_i$, and we shall here focus on the sector with magnetization zero. Within this sector, $H = -2\sum_k \Lambda^\dagger_k S^z_k \Lambda_k$, and it was shown in [4] that $\Lambda_k = \sum_{j(\neq k)} w_{kj}[S^x_j - iS^y_j - 2(S^x_k - iS^y_k)S^z_j]$ annihilates the state

$$|\psi_0\rangle \propto \sum_{s_1,\ldots,s_N} \delta_s \prod_{i<j} \{\sin[(\phi_i - \phi_j)/2]\}^{(s_i s_j - 1)/2} \times \prod_k e^{i\pi(k-1)(s_k+1)/2} |s_1, \ldots, s_N\rangle, \quad (4)$$

where $s_j = \pm 1$ is twice the z-component of the jth spin and δ_s is 1 for $\sum_j s_j = 0$ and 0 otherwise. This state is hence an exact eigenstate of H with energy zero.

The Hamiltonian has only a global Z_2 spin flip symmetry generated by the operator $\prod_{i=1}^N \sigma^x_i$, and this is compatible with many-body localization. The state $|\psi_0\rangle$ instead has a full SU(2) symmetry, which is incompatible with many-body localization.

Many-body localization and glassiness We first show that the system undergoes a transition from a thermal phase at weak disorder into a glassy many-body localized phase at strong disorder.

Figure 1(a) shows the half chain von Neumann entanglement entropy, $S = -\mathrm{Tr}(\rho_{N/2}\ln(\rho_{N/2}))$, where $\rho_{N/2}$ is the reduced density operator of the first $N/2$ spins. At weak disorder, S is close to the value expected for a thermal system (horizontal lines), and at strong disorder, S is much smaller. The inset shows that S scales linearly with system size at weak disorder as expected for thermal systems and is independent of system size for strong disorder as expected for many-body localized systems.

Figure 1(b) shows the adjacent gap ratio r, which is the average of $\min(\Delta_n, \Delta_{n+1})/\max(\Delta_n, \Delta_{n+1})$ over the spectrum restricted to one of the two Z_2 sectors. Here, $\Delta_n = E_{n+1} - E_n$ and E_n is the energy of the nth eigenstate within the considered sector. The expected value in the thermal (many-body localized) phase is marked GOE (Poisson), and also here one sees the transition.

Finally, figure 1(c) shows the spin glass order parameter $\chi^{\mathrm{SG}} = \frac{1}{N}\sum_{i\neq j}\langle\psi_n|\sigma^z_i\sigma^z_j|\psi_n\rangle^2$, where $|\psi_n\rangle$ is an

eigenstate of the Hamiltonian. The low value of χ^{SG} at low disorder means no glassiness, and the linear scaling of χ^{SG} with system size seen at strong disorder means that the system is glassy.

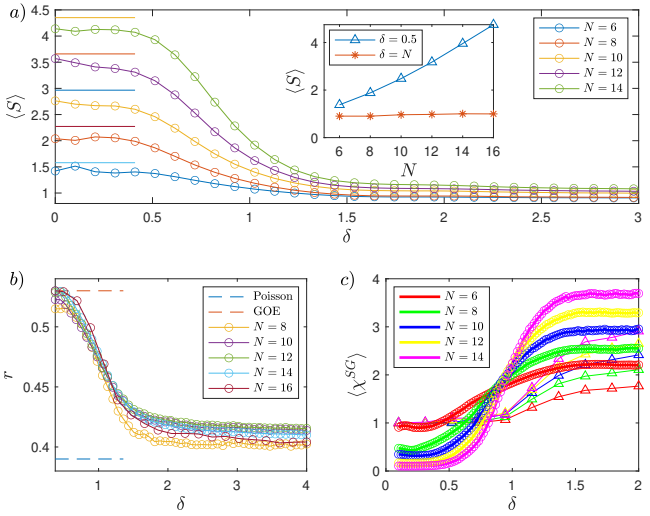

Figure 1: The transition from a thermal phase at weak disorder to a many-body localized phase at strong disorder is seen both in (a) the half chain von Neumann entanglement entropy for states in the middle of the spectrum averaged over 10^5 disorder realizations, (b) the adjacent gap ratio, and (c) the spin glass order parameter for states in the middle of the spectrum (circles) and states at low energy density (triangles) averaged over 10^4 disorder realizations. In all cases the transition happens around $\delta \approx 1$. See text for details. The results shown here have been obtained from exact diagonalization.

Properties of the special state At zero disorder strength, the special state coincides with the ground state of the Haldane-Shastry model, and the low energy physics of this model is described by Luttinger liquid theory. Despite the transition observed above, we now show that the special eigenstate (4) remains critical and non-glassy at strong disorder instead of transforming into, e.g., a glassy phase or a random singlet phase. The critical behavior is seen in the Renyi entanglement entropy, which grows logarithmically with the subsystem size, even when disorder is present, as shown in figure 2(a). We find that the spin glass order parameter χ^{SG} is always 1 for the special state for all disorder realizations, independent of the disorder strength and independent of the system size. This shows that the state is not glassy. Finally, we study the second cumulant $C_2(N/2) = \langle M^2 \rangle - \langle M \rangle^2$ of the half chain magnetization $M \equiv \sum_{i=1}^{N/2} S_i^z$. The second cumulant is known to scale logarithmically with the system size, $C_2(N/2) \sim \xi \ln(N/2) + \text{const}$ for large N, with different coefficients for the Luttinger liquid ($\xi = 1/(2\pi^2)$) and for the random singlet phase ($\xi = 1/12$). We plot $[C_2(N) - C_2(N/2)]/\ln(2) \approx \xi$ in figure 2(b) with and without disorder and observe that the result approaches the value for the Luttinger liquid in both cases.

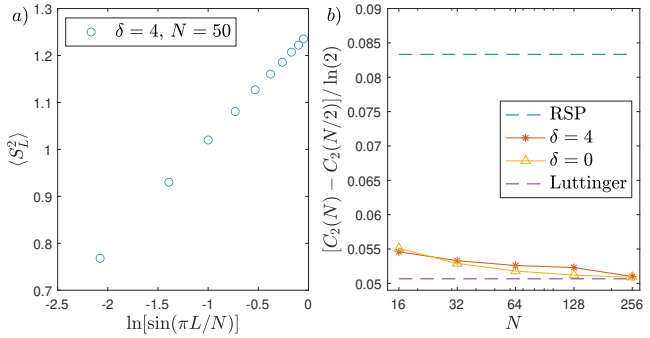

Figure 2: (a) The Renyi entanglement entropy $S_L^2 = -\ln(\mathrm{Tr}(\rho_L^2))$ of the reduced density operator ρ_L of L adjacent spins of the state (4) averaged over disorder realizations grows linearly with $\ln(\sin(\pi L/N))$. (b) The disorder averaged log coefficient of the second cumulant of the half chain magnetization approaches the value expected for a Luttinger liquid and is far from the value expected for a random singlet phase (RSP) both with ($\delta = 4$) and without ($\delta = 0$) disorder. The results shown here have been obtained from Monte Carlo simulations.

Discussion We have proposed and demonstrated the existence of a different type of nonthermal system, in which most of the states in the spectrum are many-body localized but a few states are not. We have also proposed emergent symmetry in eigenstates as a general mechanism to achieve this phenomenon.

For the particular model studied, we find numerically that the special state is the ground state, but one can move it into the bulk of the spectrum without changing the eigenstates of the model, e.g. by considering the Hamiltonian $\tilde{H} = (H - \beta)^2$, where β is a suitably chosen constant.

To further demonstrate the significance of the emergent symmetry, we have observed that the special state localizes and becomes glassy, when a perturbation that removes the emergent symmetry is added to the Hamiltonian.

The studies suggest that several variations of nonthermal systems exist and motivate further investigations.

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[3] A. C. Potter, R. Vasseur, Phys. Rev. B **94** (2016) 224206.

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2.28 2D layered delafossites: Exploring metal-insulator hybrid-Flatlands

TAKASHI OKA

Materials Two dimensional (2D) delafossites form a natural heterostructure (Fig. 1) consisting of layers of metals and insulators [1]. Transport in the metallic layer is strongly two dimensional and the triangular lattice electrons have a hexagonal Fermi surface. The insulator layer can be either band insulating (CoO_2) or Mott insulating (CrO_2), where the latter hosts an antiferromagnetic order at low temperatures. In the band insulating case (CoO_2), the adjacent metallic layer becomes ultrapure and it is known to have the highest conductivity per volume at room temperature [1]. On the other hand, in the Mott insulating case (CrO_2), the spins start to talk with the electrons in the metallic layer.

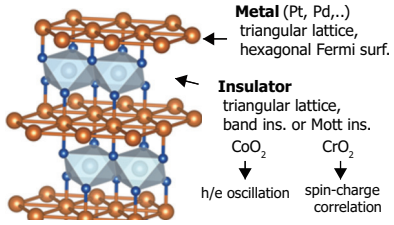

Figure 1: Layered crystal structure of 2D delafossites.

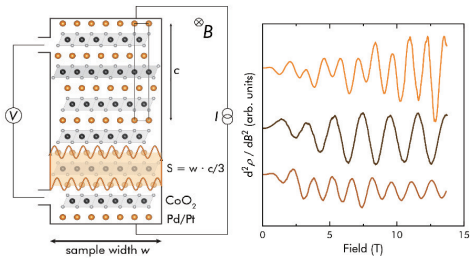

Figure 2: Out-of-plane magnetoresistance in the layered delafossites PdCoO2 and PtCoO2 [2].

h/e oscillations in metal-band insulator heterostructure [2] In the band insulating version of the 2D delafossites ($PdCoO_2$ and $PtCoO_2$), metallic electrons have strong coherence in the in-plane direction, while motion in the inter-layer direction is blocked by the insulating layer. This leads to realization of a new phase-coherent oscillation in the out-of-plane magnetoresistance [2]. This experiment was performed in the groups of A. Mackenzie (MPI-CPfS) and Philip Moll (Institute of Materials, EPFL, Switzerland). The oscillation period is equivalent to that determined by the magnetic flux quantum, h/e, threading an area defined by the atomic interlayer separation and the sample width, where h is Planck's constant and e is the charge of an electron (Fig. 2). The phase of the electron wave function appears robust over length scales exceeding 10 micrometers and persisting up to temperatures of T $>$ 50 K.

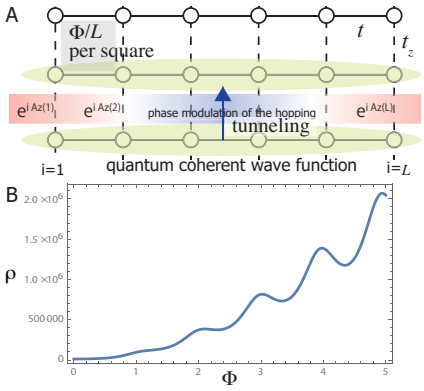

Figure 3: A. Anisotropic Hofstadter model. The z-direction transport is governed by a hopping process between the standing wave solutions in the neighboring layers. In the presence of a magnetic field, the hopping acquires a phase that slowly modulates, and results in a cancellation and reduction of the hopping amplitude. The reduction factor shows an $\Phi \sim \Phi + 1$ oscillation. B. Plot of resistivity obtained by the Kubo formula Eq. (1).

We studied this problem using the anisotropic Hofstadter model with $t_z/t \sim 0.01 \ll 1$ (Fig. 3). A magnetic flux Φ per unit layer of size L is inserted into the system. We stay in the weak-field limit $\Phi \sim \phi_0/L$ with L the length of the ab layer. The out-of-plane conductivity is evaluated using the Kubo formula

$$\sigma_{\alpha\beta} = \frac{i\hbar e^2}{V} \sum_{mn} \left(\frac{f_n - f_m}{\varepsilon_m - \varepsilon_n} \right) \frac{\langle |j_\alpha| m \rangle \langle m | j_\beta | n \rangle}{\varepsilon_n - \varepsilon_m + i\hbar\eta}. \quad (1)$$

The result shows oscillations with striking resemblance with the experimental results.

The origin of this oscillation can be intuitively understood as follows. The wave function of the electron has full phase coherence across the length of the ab plane. In our picture, a phase-coherent wave in the ab plane is transmitted to an adjacent plane with tunneling matrix elements $t_z (\ll t)$ in each unit cell of the lattice. The phase of the tunneling matrix elements at site $j = 1 \ldots L$ is modulated by a factor $e^{i2\pi\Phi j/L}$ due to the magnetic field in the Landau gauge. This results in a periodic array of tunneling paths between the layers. One can imagine this as an L-slit extension of the famous double-slit interference experiment. Summing the resulting series yields the amplitude

$$A(\phi) = \sum_{j=1}^{L} e^{i2\pi\Phi/Lj} = \frac{1 - e^{i2\pi\Phi}}{e^{-i2\pi\Phi/L} - 1}, \quad (2)$$

which shows approximate $\Delta\Phi = \phi_0$ oscillations due to the term in the numerator. The ultrapure nature of the 2D delafossites led to this surprising quantum interference phenomena that is rarely observed in bulk crystals at relatively high temperature.

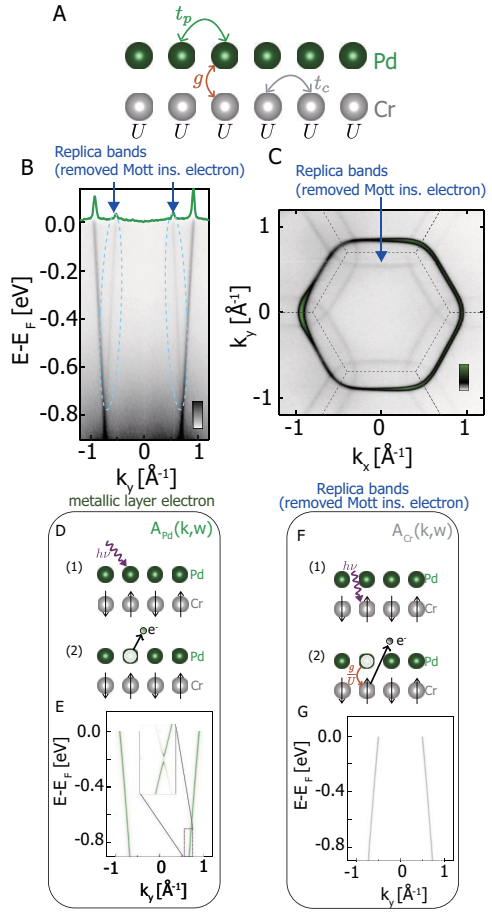

Figure 4: (A) Model system, and (B,C): ARPES spectrum. (D-G): Schematic illustration. (D) The hole feels the AF order. (E) The corresponding spectral function is equivalent to that by a 'band folding' model. (F) Photoemission of a Cr electron involves tunneling of the Cr hole to the Pd layer. (G) This 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 [3].

Spin-charge intertwine physics in metal-Mott insulator heterostructure [3,4] In the Mott insulating 2D delafossites ($PdCrO_2$ and $PtCrO_2$), electrons in the metallic layers interact with the spins in the adjacent Mott insulating layers (Fig. 4 A.). Intertwined spin-charge physics is of central interest in strongly correlated electron systems, and 2D delafossites provide an idealistic testbed since the electronic structure is simple. By performing strong coupling expansion, we obtained an effective Heisenberg-Kondo lattice model

$$H_{\rm eff} = -\sum_{ij\sigma} t^p_{ij} p^\dagger_{i\sigma} p_{j\sigma} + \sum_{ij} (J_{ij}/2) \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \sum_{ijk\sigma\sigma'} K_{ijk} p^\dagger_{i\sigma} (\boldsymbol{S}_j \cdot \boldsymbol{\sigma}_{\sigma\sigma'}) p_{k\sigma'}. \quad (3)$$

The generalized Kondo coupling K_{ijk} and the Heisenberg coupling J_{ij} are of the same order.

We used this picture to explain the mysterious replica band found in the ARPES spectrum obtained in A. Mackenzie's group in collaboration with P. King at St. Andrews [3]. Figure 4 (B, C) depicts the dispersion measured by ARPES along the $\Gamma - K$ 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. The conventional band folding picture does not explain this replica bands since (i) the spectrum weight was energy independent, and (ii) the removed electron was in the Mott insulator layer. We developed a theory to explain the replica band formation as a intertwined state of spin-charge excitations (Fig. 4 F, G).

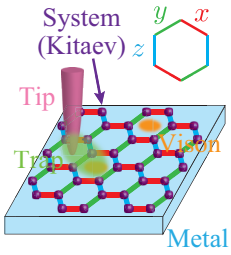

Figure 5: Detection scheme of Majoranas in Kitaev's spin liquid [4].

One lesson from the ARPES experiment is that *non-magnetic spectral methods can detect spin excitations.* As a spinoff, we started a project with M. Udagawa (Gakushuin Univ.) on sabbatical at mpi**pks**. The objective is to find a scheme to detect and control Majoranas in Kitaev's spin liquid using non-magnetic STMs (Fig. 5). The model (3) can be used in this study, where the Heisenberg model (J_{ij}) is replaced by the Kitaev Hamiltonian and the metal by the STM tip [4]. Further progress in this direction is underway.

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2.29 Controlling Cavity-Mediated Superconductivity and Criticality by Engineering Quantum States of Light

AHANA CHAKRABORTY AND FRANCESCO PIAZZA

Introduction The recent success in coupling electrons in two-dimensional materials to the quantum electromagnetic field of optical cavities has opened up many exciting but yet unexplored avenues of quantum electrodynamics. Among these, one promising idea is to use the photons in a cavity to mediate pairing between electrons, inducing superconducting states with novel properties [1]. Cavity photons, as mediators of interactions between electrons, are very different from the phonons in the standard Bardeen-Cooper-Schrieffer (BCS) paradigm. Unlike phonons, which can transfer a large momentum (Debye momentum) to electrons, photons have instead a much steeper dispersion and can only transfer very small momenta. Hence the cavity-mediated electron-electron interactions are very long range, and this changes the rules of pairing between electrons drastically.

In a recent work [2], we have shown that photon-mediated pairing is dominated by novel, non-BCS-type processes mediated by on-shell, non-adiabatic photon fluctuations. As we will discuss below, this new pairing mechanism is completely different from the standard BCS mechanism and for realistic parameters, also including photon loss, this enhances the superconducting critical temperature by more than one order of magnitude with respect to the BCS prediction.

A further exciting prospect is to exploit state-of-the-art engineering of the quantum states of light to control pairing and superconductivity. This new playground for quantum many-body physics is at the same time exciting and theoretically challenging to describe, requiring us to develop new approaches merging quantum optics, condensed matter, and quantum-field-theory. We discuss below our recent results in these directions obtained within a real-time field theoretic formulation.

Model We consider a generic electron system with dispersion ϵ_k (measured from the Fermi surface E_F) coupled to a Terahertz cavity where the cavity field couples to the electron density. The phenomenology discussed here relies crucially on the long-range nature of the cavity-mediated interaction where the momentum transferred by the photon is a fixed vector $\vec{q}_0$ ($q_0 \ll k_F$, the Fermi momentum of the electrons) corresponding to the cavity resonance frequency δ_c. The light-matter coupling Hamiltonian reads [1],

$$H_{\text{light}-\text{matter}} = \sum_{\vec{k},\sigma} \sum_{\vec{q}=\pm q_0 \hat{x}} g_0 \, c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} (b + b^\dagger), \quad (1)$$

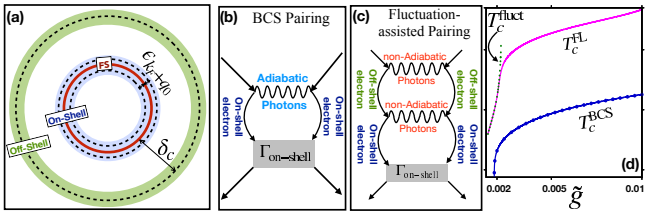

Figure 1: (a)-(c) Energy structure of the standard BCS vs new non-BCS pairing. (d) Enhancement of T_c by the non-BCS pairing mechanism induced by long-range photon fluctuations.

where $c^\dagger$ and $b^\dagger$ are the creation operators of electrons and cavity photons, respectively, and g_0 is the coupling strength.

We compute the superconducting critical temperature T_c via the pairing instability of the scattering vertex function in the Cooper channel. The vertex function, formulated on the real-time Keldysh contour, has two separate contributions. One comes from the retarded (or advanced) response of the mediator and thus depends only on the dispersion (and life-time) of the photons, but not on their energy-momentum distribution (or more generally their quantum state). The other contribution comes instead from scattering processes mediated by photon fluctuations, and hence depends on their distribution. As we will see below, the former contribution corresponds to the standard BCS paring, while the latter is responsible for a new non-BCS pairing mechanism.

Energy structure of the pairing Let us first define the two separate electronic energy scales which are important here. On-shell electrons have frequencies $\sim \epsilon_{k_F \pm q_0}$, where $\epsilon_{k_F \pm q_0} \ll E_F$ as well as $\epsilon_{k_F \pm q_0} \ll \delta_c$. These low energy electrons, highlighted by the blue shell in Fig. 1(a), are the ones that eventually form the Cooper pairs for $T < T_c$. On the other hand, off-shell electrons (highlighted by the green shell in Fig. 1(b)) have frequencies close to the photon resonance frequency $\sim \delta_c$ i.e. far away from the FS. Off-shell electrons are not the ones actually building the pair, but can play a crucial role in intermediate scattering processes, as we shall see is the case when the long-range photon fluctuations mediate the pairing.

In the standard BCS pairing, as illustrated in Fig. 1(b), an adiabatic (off-shell) photon scatters an on-shell electron close to the Fermi surface and leads to an attractive interaction between low-energy electrons, which depends on their thermal occupation. However, differently from the standard phonon case, the long-range

nature of the photon-mediated interaction results in a polynomial dependence of T_c on the light-matter coupling strength, given by $T_c^{\rm BCS} \sim 2\tilde{g}\delta_c$ (see solid line with circles in Fig. 1(d)) .

On the other hand, the new non-BCS pairing depends on the occupation of the photons, which is concentrated around the cavity resonance frequency. These non-adiabatic photons thus scatter electrons far off the Fermi surface, as illustrated in Fig. 1(c). These high frequency electrons then undergo a further scattering process where a second non-adiabatic photon brings them back on-shell close to the Fermi surface. This fluctuation-mediated pairing can enhance superconductivity significantly, with

$$T_c^{\rm fluct} \sim \frac{2\tilde{g}\delta_c}{[1-32(\tilde{g}\delta_c)^2/(3\epsilon^2_{k_F+q_0})]} \tag{2}$$

shown by the green dotted line in Fig. 1(d). Differently from the BCS pairing which is limited by the thermal broadening of the electron distribution, this non-BCS pairing is only limited by the electron lifetime. Considering a Fermi-liquid-type electron lifetime set by the screened Coulomb interaction, the critical temperature $T_c^{\rm FL}$ can be more than one order of magnitude larger than the BCS prediction, as shown by solid magenta line in Fig. 1(d).

	Pure Fock State	Thermal	Engineered
$\hat{\rho}_0$	$\lvert n_0\rangle\langle n_0\rvert$	$\frac{\sum_{n=0}^{\infty} e^{-n\beta\omega_0}\lvert n\rangle\langle n\rvert}{\sum_{n=0}^{\infty} e^{-n\beta\omega_0}}$	$\frac{\sum_{n=n_0}^{\infty} e^{-(n-n_0)\kappa}\lvert n\rangle\langle n\rvert}{\sum_{n=n_0}^{\infty} e^{-(n-n_0)\kappa}}$
$\langle\hat{n}\rangle$	n_0	$n_B(\beta)$	$n_B(\kappa)+n_0$
T_c	$T_c^{\rm vac}=\frac{2\tilde{g}\delta_c}{1-c\left(\frac{\tilde{g}\delta_c}{\epsilon_{k_F+q_0}}\right)^2}$	$T_c^{\rm th}=\frac{2\tilde{g}\delta_c}{1-c\left(\frac{\tilde{g}\delta_c}{\epsilon_{k_F+q_0}}\right)^2(1+2n_B(\beta))^2}$	$T_c^{\rm en}=\frac{2\tilde{g}\delta_c}{1-c\left(\frac{\tilde{g}\delta_c}{\epsilon_{k_F+q_0}}\right)^2(1+2n_B(\kappa))^2}$, In limit $\kappa\to\infty, T_c^{\rm en}\to T_c^{\rm vac}$
$\gamma=$	n_0+1	1	1, In limit $\kappa\to\infty, \gamma\to n_0+1$
$\nu=$	$1/2$	$1/2$	$1/2$

Table 1: Manipulating T_c and critical exponents by engineering initial density matrices of the photons.

As anticipated, this novel non-BCS pairing depends in general on the quantum state of light in the cavity, and hence opens up the exciting prospect of manipulating superconductivity by engineering the density matrices of the photons. We recently developed a non-equilibrium field-theory approach that allows to tackle this issue in Ref. [3]. We found that photons initially prepared in pure Fock states $\hat{\rho}_0 = |n_0\rangle\langle n_0|$, while giving rise to the same superconducting critical temperature as that of the electromagnetic vacuum case, surprisingly result in a strong divergence of the vertex function $\Gamma = (T_c/(T-T_c))^\gamma$, with a susceptibility exponent γ growing linearly with n_0, as opposed to $\gamma = 1$ for thermal states. Moreover, the correlation length also grows as $\sqrt{n_0+1}$, while its divergence at the critical point is governed by the thermal exponent $\nu = 1/2$. We summarize these results in Table 1. The latter also includes an engineered density matrix $\hat{\rho}_0 = \left[\sum_{n=n_0}^{\infty} e^{-(n-n_0)\kappa}|n\rangle\langle n|\right] \Big/ \left[\sum_{n=n_0}^{\infty} e^{-(n-n_0)\kappa}\right]$, which encompasses both the thermal case and the pure Fock state in the limit $\kappa \to \beta = 1/T$ and $\kappa \to \infty$, respectively.

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2.30 Fermi polarons in non-equilibrium driven-dissipative systems

TOMASZ WASAK, FALKO PIENTKA, RICHARD SCHMIDT, AND FRANCESCO PIAZZA

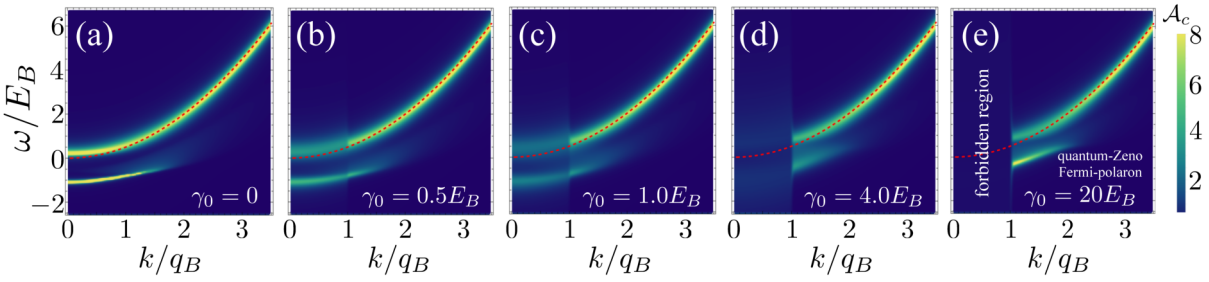

Figure 1: The impurity spectral function $\mathcal{A}_c(k,\omega)$ in units of impurity-fermion binding energy E_B; the momenta are in $q_B = \sqrt{m_f E_B}$. The Fermi wave vector $k_F = 0.7q_B$, and the cutoff momentum of the loss $k_\gamma = q_B$. The dashed curve is the free dispersion relation $\omega = \varepsilon_c(k) \equiv k^2/2m_c$.

Introduction. Atomically thin semiconductors like monolayer transition metal dichalcogenides (TMDs) exhibit interesting optical properties and provide promising platforms for the development of photonic devices. An essential feature for optical control are tightly bound excitons that can be dressed by electrically injected electrons such that the optical response is dominated by the attractive and repulsive Fermi-polaron branches [1, 2]. Besides its relevance for nonlinear optics, polaron formation can induce intriguing collective phenomena both in and out of equilibrium.

Motivated by recent experimental progress, in Ref. [3] we studied the impact of strong dissipation on Fermi polaron physics, and in Ref. [4] we investigated nonlinear relaxation dynamics of Fermi-polarons. In the fist work, we merged the Zeno-paradigm of quantum measurement theory with the concept of polarons in condensed-matter physics. The resulting quantum-Zeno Fermi-polaron is a quasi-particle which emerges for lossy impurities interacting with a quantum-degenerate bath of fermions. We showed that in the strongly dissipative regime of large loss rates a long-lived polaron branch re-emerges. This quantum-Zeno Fermi-polaron originates from the nontrivial interplay between the Fermi-surface and the surface of the momentum region forbidden by the quantum Zeno projection due to strong loss. The situation we considered is realized naturally for polaritonic impurities in charge-tuneable semiconductors and can be also implemented using dressed atomic states in ultracold gases.

In the second work, we studied the case when the higher-energy polarons (repulsive polaron branch) excited around zero momentum quickly decay to the attractive branch at high momentum. Collisions with the fermionic bath (electrons) subsequently lead to a slower relaxation of attractive polarons, which accumulate at the edge of the light-cone around zero momentum where the radiative loss dominates. The bosonic nature of exciton polarons enables stimulated scattering, which results in a lasing transition at higher pump power. The latter is characterized by a superlinear increase of light emission as well as extended spatiotemporal coherence. The many-body dressing of excitons can reduce the emission linewidth below the bare exciton linewidth set by nonradiative loss, indicating an extended temporal coherence.

Driven-dissipative impurity in a Fermi bath. We consider a system composed of a bath of fermions (electrons) interacting with impurity particles (excitons). The system Hamiltonian consists of three parts: $\hat{H} = \hat{H}_c + \hat{H}_f + \hat{H}_{\rm int}$, where $\hat{H}_c = \sum_{\mathbf{k}} \varepsilon_c(\mathbf{k}) \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}}$ and $\hat{H}_f = \sum_{\mathbf{k}} \varepsilon_f(\mathbf{k}) \hat{f}^\dagger_{\mathbf{k}} \hat{f}_{\mathbf{k}}$ are free-particle Hamiltonians with kinetic energies $\varepsilon_c(\mathbf{k}) = \mathbf{k}^2/2m_c$ and $\varepsilon_f(\mathbf{k}) = \mathbf{k}^2/2m_f$ of impurities and fermions, respectively. We assume a contact interaction potential with a coupling strength U, $\hat{H}_{\rm int} = U \int d\mathbf{r}\, \hat{c}^\dagger(\mathbf{r}) \hat{c}(\mathbf{r}) \hat{f}^\dagger(\mathbf{r}) \hat{f}(\mathbf{r})$. To model the action of dissipation and pump, we employ the master equation $\partial_t \hat{\varrho}(t) = -i[\hat{H}, \hat{\varrho}(t)] + \mathcal{L}_d \hat{\varrho}(t)$. The Lindblad operator $\mathcal{L}_d$, acting on the density matrix of the whole system $\hat{\varrho}(t)$, splits into two parts $\mathcal{L}_d \hat{\varrho} = \sum_{\mathbf{k}} \{\gamma(\mathbf{k}) D[\hat{c}_{\mathbf{k}}] + \Omega(\mathbf{k}) P[\hat{c}_{\mathbf{k}}]\} \hat{\varrho}$, which describe loss of particles with rate $\gamma(\mathbf{k})$ and their reinjection with rate $\Omega(\mathbf{k})$, and $D[\hat{c}]\hat{\varrho} \equiv \hat{c}^\dagger \hat{\varrho} \hat{c} - \frac{1}{2}\{\hat{c}^\dagger \hat{c}, \hat{\varrho}\}$ and $P[\hat{c}] \equiv D[\hat{c}] + D[\hat{c}^\dagger]$.

In Refs. [3, 4] we developed a diagrammatic approach based on non-equilibrium Green's functions (GFs), and extended the non-self-consistent T-matrix approach, known in the literature, to driven-dissipative systems. We employed a path-integral formulation of our problem on the Keldysh real-time contour, which allowed for a straightforward inclusion of the Lindblad terms of the master equation [5, 6]. Within our formalism, diagrammatic approaches are applicable in a way analogous to the equilibrium Matsubara formalism.

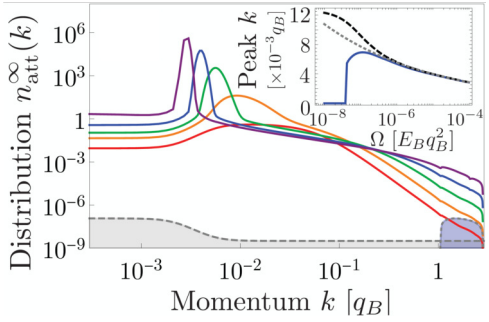

Figure 2: Late-time distribution function $n_{\rm att}^{\infty} = n_{\rm att}(k, t \to \infty)$ in log-log scale for various pump strengths: $\Omega = 10^{-8}, 10^{-7}, 10^{-6}, 10^{-5}, 10^{-4}\ E_B q_B^2$ (from bottom to top at $k = 0$). The loss profile $\gamma(\mathbf{k})$ (gray shaded region) and the effective pump profile $P_{\rm att}$ for attractive polarons (blue shaded region on the right) are displayed at the bottom (shifted vertically and not to scale). Inset: Momentum-space peak position of the polaron distribution (black dashed line) and emitted light distribution (blue solid line) as a function of Ω along with the power-law $\Omega^{-1/7}$ (grey dotted line).

Impurity response function in the quantum-Zeno regime. We consider the loss function $\gamma(\mathbf{k}) = \gamma_0$ if $|\mathbf{k}| < k_\gamma$ and zero otherwise. The spectral response of the system is encoded in the retarded impurity GF, given by $G_c^R(\mathbf{k}, \omega) = [\omega - \varepsilon_c(\mathbf{k}) + i\frac{\gamma(\mathbf{k})}{2} - \Sigma_c^R(p)]^{-1}$, where $\Sigma_c^R(p)$ is the retarded self-energy of the impurity, see [3]. The impurity spectral function, given by $\mathcal{A}_c(\mathbf{k}, \omega) = -2\mathrm{Im}[G_c^R(\mathbf{k}, \omega)]$, for gradually increasing γ_0 is presented in Fig. 1. For small γ_0, two quasiparticle resonances are visible. The lower one in energy is the so-called attractive polaron. It corresponds to a state where the impurity attracts a cloud of surrounding fermions. The second resonance is higher in energy and corresponds to a repulsive polaron state where the surrounding cloud is repelled by the impurity.

Remarkably, for large losses $\gamma_0 \gg E_B$, a resonance reappears below the repulsive polaron just outside the Dissipative Subspace (DS), where $k < k_\gamma$. This resonance has a width which does not depend anymore on the loss rate γ_0 and is rather given only by the coupling to the molecule-hole continuum, as would be the case without losses. At the same time, the DS does not contain any spectral weight and is fully forbidden for the excitations. This phenomenology can be understood within the paradigm of the quantum-Zeno effect. Indeed, when the impurity occupies a state with $\mathbf{k} \in$ DS it is lost immediately, which is equivalent to a frequent measurement performed within the DS. As a result, the dynamics of the particle is confined to the orthogonal subspace, i.e. $\mathbf{k} \notin$ DS. We note that for infinite dissipation strength, the equation for the pole of the impurity Green's function can be reproduced by a trial wave function in which the momenta from DS are excluded.

Polaron kinetic equation. The dynamics of the polaron population can be described by a kinetic equation [4] for the bosonic distribution function $n_\alpha(\mathbf{k}, t)$, $\partial_t n_\alpha(\mathbf{k}, t) = -\gamma_\alpha(\mathbf{k}) n_\alpha(\mathbf{k}, t) + \Omega_\alpha(\mathbf{k}) + I_\alpha(\mathbf{k}, t)$, where the index $\alpha \in \{\mathrm{att}, \mathrm{rep}\}$ labels the polaron branches. As the polaron is a composite particle, its decay rate $\gamma_\alpha(\mathbf{k}) = Z_\alpha(\mathbf{k})\gamma(\mathbf{k})$ is suppressed by the quasiparticle weight, which measures its impurity (in our case excitonic) content. A similar suppression applies to the drive $\Omega_{\rm rep}(\mathbf{k}) = Z_{\rm rep}(\mathbf{k})\Omega(2\pi)^2\delta^2(\mathbf{k})$ modeled as continuous pumping of the repulsive polaron at $\mathbf{k} = 0$ with strength Ω. Here, $\gamma(\mathbf{k}) = \gamma_{\rm exc} + \gamma_{\rm rad}(\mathbf{k})$, where $\gamma_{\rm exc}$ is a momentum independent nonradiative decay rate and $\gamma_{\rm rad}(\mathbf{k})$ is the momentum dependent rate for radiative decay due to coupling to photons, see Fig. 2.

We solved the equations numerically for realistic values of parameters. The development of a strongly peaked occupation number for small $\mathbf{k}$ is shown in Fig. 2 during the late time dynamics. Once the populated attractive polarons reach the light cone, they can decay rapidly by creating a photon, hence, suppressing the polaron occupation in the immediate vicinity of $k = 0$. At later times the occupation number at the edge of the light cone grows above one and stimulated scattering, for pump strengths beyond a certain threshold, leads to the formation of a relatively narrow peak in the steady state. In the inset we show the position of the peak in the momentum distribution and emitted light. Beyond the pump threshold, we also found an extended spatial and temporal coherence of the low-energy photons similar to what happens in a lasing transition.

Conclusions. We developed a formalism capable of describing the collective dynamics of impurities under driven-dissipative conditions. It allowed to discover novel scenarios in the many-body physics of polarons in open systems, with applications both in solid-state materials and ultracold atomic gases.

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2.31 Rabi Regime of Current Rectification in Solids

OLES MATSYSHYN, FRANCESCO PIAZZA, RODERICH MOESSNER, AND INTI SODEMANN

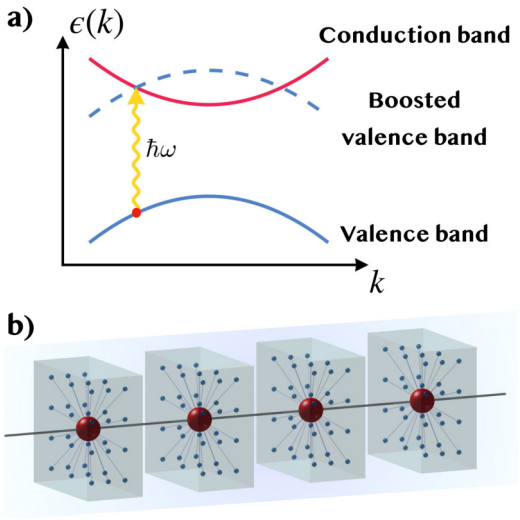

Figure 1: a) Energy crossing between boosted valence and conduction bands in Floquet representation. b) Depiction of underlying tight binding model with physical sites (red balls) which are tunnel coupled (solid lines) among themselves and with their own identical fermionic bath (blue balls).

Abstract. This report summarizes results from Ref. [1], where we investigated rectified currents in band structures lacking inversion symmetry. Perturbatively, these currents are inversely proportional to the relaxation rate, and, therefore, naively diverge in the clean limit. Employing Keldysh and Floquet theories, we showed that this is an artifact of perturbation theory, and that there is a well-defined periodic steady-state of Rabi oscillations leading to finite rectified currents.

Introduction. Our study is motivated by understanding the fate of current rectification in Bloch bands in the limit where relaxation times are very large. As we will demonstrate, there is a well defined steady state in such limit, that we refer to as the "Rabi regime", leading to a finite rectified current. A useful starting point is to analyze the problem perturbatively in the electric field, $\mathbf{E}$. The current is expected to scale as $\mathbf{j} \propto |\mathbf{E}|^2$. Such perturbative "bulk-photogalvanic effects" (BPVE) are often separated into the shift and the injection current effects [2, 3]. Perturbatively, the shift current has a finite value in the limit of vanishing relaxation rate, $\Gamma \to 0$, while the injection current appears to diverge in such limit as $1/\Gamma$. However, recently a non-perturbative semiclassical study in Weyl semimetals [4] demonstrated that the current saturates to a finite value in the limit of $\Gamma \to 0$. Motivated by this, we develop a microscopic description of the currents that captures the perturbative and the non-perturbative regimes on equal footing, employing the Keldysh-Floquet formalism from the work of Ref. [5]. As we will see, in the Rabi regime ($\Gamma \to 0$), the current approaches a finite value that instead scales linearly with the magnitude of the electric field $\mathbf{j} \propto |\mathbf{E}|$.

Problem setting. We consider a two-band model (Fig. 1). The current is: $\hat{\mathbf{j}} = e\hat{\mathbf{v}}/\hbar = \partial \hat{H}_0(\mathbf{k} + e\mathbf{A}(t)/\hbar)/\partial \mathbf{A}(t)$, where $\hat{H}_0(\mathbf{k})$ is the 2x2 matrix Bloch Hamiltonian, and $\mathbf{A}(t) = ie^{i\omega t}\mathbf{E}/\omega + c.c.$, is the vector potential from an oscillating electric field with frequency ω. To model relaxations we couple the system to a bath and apply the Keldysh formalism (see Fig.1(b)). Following the simplifications that lead to a truncated two-band Floquet model from Ref. [5], we obtained that the rectified injection current can be expressed as follows:

$$J_3^\alpha = \pi \frac{e}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} (f_2 - f_1)(v_1^\alpha - v_2^\alpha) \times \\ \times \frac{\left| \frac{e\mathbf{E}}{\hbar\omega} \cdot \left(\frac{\partial H_0(\mathbf{k})}{\partial \mathbf{k}} \right)_{12} \right|^2}{\sqrt{\left| \frac{e\mathbf{E}}{\hbar\omega} \cdot \left(\frac{\partial H_0(\mathbf{k})}{\partial \mathbf{k}} \right)_{12} \right|^2 + \frac{\Gamma^2}{4}}} \delta(\epsilon_1 - \epsilon_2 + \hbar\omega), \quad (1)$$

Here $1, 2$ labels conduction and valence bands, $f_{1,2}$ are Fermi Dirac functions, $\epsilon_{1,2}$ are the band energy dispersions, $v_{1,2}^\alpha = \partial_{k_\alpha} \epsilon_{1,2}$ are the group velocities along $\alpha \in \{x, y, z\}$, and Γ is the relaxation rate. Remarkably, in the clean limit ($\Gamma \to 0$), the above formula predicts a finite current, in contrast to the naive extrapolation of perturbative result. Therefore in the clean limit, the injection current scales as the absolute value of the electric field, $\mathbf{J}_3 \propto |\mathbf{E}|$.

Synchronization of Rabi oscillators. While the Keldysh formalism allows for a description with arbitrary Γ, there is a simpler way to understand the behavior in the limit of $\Gamma \to 0$. In this limit the electrons can be viewed as a collection of synchronized Rabi oscillators driven by the oscillating field. This system is in fact an example of a Periodic Gibbs Ensemble (PGE) [6,7] describing thermalized steady states of Floquet systems.

Let us describe this PGE in more detail. The density matrix of the system can be generally written as:

$$\rho(t) = \sum_{\alpha\beta} \rho_{\alpha\beta} \psi_\alpha(t) \psi_\beta^\dagger(t), \quad (2)$$

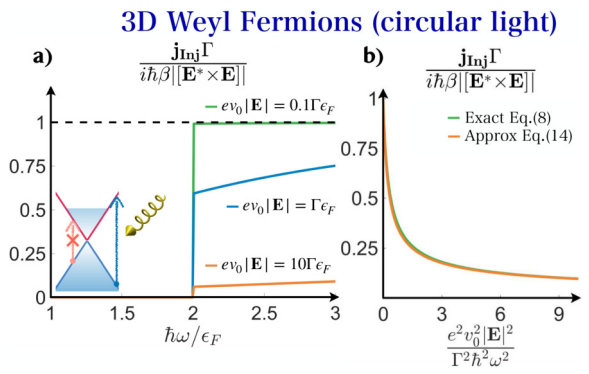

Figure 2: a) Rectified current dependence on frequency, and (b) on electric field amplitude for 3D Weyl fermion.

where $\psi_{\alpha,\beta}(t)$ are the solutions of the time-dependent Schrödinger equation of the isolated system. Now, the Floquet theorem implies that, barring accidental degeneracies, $\psi_\alpha(t)\psi_\beta(t)^\dagger$ are periodic only when $\alpha = \beta$. The synchronization associated with the PGE is a process in which these off-diagonal amplitudes disappear in a thermalization process, leading to a steady state that is periodic and synchronized with the drive:

$$\rho_{\mathbf{PGE}} = \sum_\alpha \rho_{\alpha\alpha}\psi_\alpha(t)\psi_\alpha^\dagger(t). \tag{3}$$

The values of the $\rho_{\alpha\alpha}$ can be found via an entropy maximization principle subject to the constrains of the conservation laws of the problem. In our case these constraints are simply that the average number of particles in the PGE matrix equals the number of particles of a standard equilibrium Gibbs density matrix in the absence of the electric field drive, with the chemical potential μ given by the bath. It is easy to show that also the resulting density matrix has the expected behavior for a collection of Rabi oscillators [1]. Moreover it is possible to show that in the limit of $\Gamma \to 0$, the density matrix obtained from the Keldysh-Floquet formalism, $\rho_{\mathbf{K-F}}(t)$, agrees exactly with the above PGE density matrix:

$$\lim_{\Gamma\to 0} \rho_{\mathbf{K-F}}(t) = \rho_{\mathbf{PGE}}(t). \tag{4}$$

Photocurrents for Weyl semimetals. The rectified current obtained from circularly polarized light, or circular-photogalvanic-effect (CPGE), has interesting manifestations in Weyl semimetals [8, 9]. As an application of our formalism, we will analyze the non-perturbative modifications to this effect specially in the clean limit ($\Gamma \to 0$). We consider an ideal 3D Weyl Hamiltonian of the form:

$$\hat{H}_0 = v_0 \sum_{\alpha=x,y,z} k_\alpha \cdot \hat{\sigma}_\alpha. \tag{5}$$

Light absorption occurs above a threshold frequency $\hbar\omega > 2\epsilon_F$ (see Fig.2(a)). By using the formula from Eq.(1), one obtains the following:

$$\mathbf{J}_3 \approx \frac{i\pi^2 e^2\omega}{v_0(2\pi)^3}\frac{[\mathbf{E}^*\times\mathbf{E}]}{60\sqrt{|\mathbf{E}|^2+\frac{\Gamma^2\hbar^2\omega^2}{4v_0^2e^2}}}\frac{12|\mathbf{E}|^2+5\frac{\Gamma^2\hbar^2\omega^2}{v_0^2e^2}}{|\mathbf{E}|^2+\frac{\Gamma^2\hbar^2\omega^2}{4v_0^2e^2}}, \tag{6}$$

In the perturbative regime we recover the result [8, 9] $\mathbf{J}_3 \approx \hbar(i\pi e^3/(3h^2))[\mathbf{E}^*\times\mathbf{E}]/\Gamma$. However, in the Rabi regime ($\Gamma \to 0$), the current approaches a value independent of the relaxation rate, given by:

$$\mathbf{J}_3 \approx 0.3\frac{\beta\hbar^2\omega}{ev_0|\mathbf{E}|}[\mathbf{E}^*\times\mathbf{E}]. \tag{7}$$

The behavior across these regimes is shown in Fig.2(a,b).

Summary and outlook. We developed a formalism which captures on equal footing the perturbative regime and the non-perturbative regimes of light driven current rectification for inter-band transitions. In the perturbative regime (large Γ), we recover the well-known divergence of the rectification currents scaling as $1/\Gamma$. Interestingly in the opposite limit ($\Gamma \to 0$), the current approaches a finite value that scales as the square root of the radiation intensity, which can guide its identification in experiments. We have shown that this non-perturbative clean limit can be understood as synchronized optical Rabi oscillations realizing a generalized periodic Gibbs ensemble.

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2.32 The universal shear conductivity of Fermi liquids and spinon Fermi surface states and its detection via spin qubit noise magnetometry

JUN YONG KHOO, FALKO PIENTKA, AND INTI SODEMANN

Abstract. This report summarizes results from Ref. [1], where we demonstrated that the transverse conductivity of 2D metals assumes a highly universal value of $(e^2/h)\mathcal{R}_{\rm FS}/q$ in the quasi-static ($\omega \to 0$) and collision-less long wavelength regime. Here $\mathcal{R}_{\rm FS}$ is the radius of curvature of the Fermi surface, and therefore, this response is only determined by the geometric shape of the Fermi surface and remains unchanged by interactions. This leads to a universal low-frequency magnetic noise that can be probed via a nitrogen-vacancy (NV) center, given by $C\omega\mathcal{P}_{\rm FS}/z$, where $\mathcal{P}_{\rm FS}$ is the perimeter of the Fermi surface in momentum space and C is a combination of fundamental constants of nature. U(1) spin liquids with a spinon Fermi surface have a closely related transverse conductivity and magnetic noise in such limit.

Quasi-static transverse conductivity of metals. There are relatively few measurable properties of systems with a Fermi surface (FS) that remain unchanged by details of interactions and dispersion. One notable example is the invariance of the period of the quantum oscillations [2], which serves as tool to measure the area of the FS. In this work we demonstrated that a different quantity enjoys a similar degree of universality. This quantity is the quasi-static transverse or shear conductivity, denoted by $\sigma_{\perp,0}(\vec{q})$ that measures the net current in response to a nearly static but spatially oscillating transverse or shear force (or a transverse electric field when the Fermi liquid is charged) with wavevector $\mathbf{q}$, as depicted in Fig. 1(a). As detailed in Ref. [1], in the low temperature collision-less regime of Landau Fermi liquids (also referred to as "ballistic" regime) where the wavevector of the applied force satisfies $p_{\rm F} \gg q \gg l_{\rm mfp}^{-1}$, where $p_{\rm F}$ is the Fermi radius and $l_{\rm mfp}$ the mean free path, and in the low-frequency quasi-static regime ($\omega \to 0$), the transverse conductivity takes the following universal form in two dimensions:

$$\sigma_{\perp,0}(\vec{q}) \quad = \quad (2S+1)\frac{e^2}{2hq}\sum_i \mathcal{R}_i. \qquad (1)$$

Here e is the electron charge, h Planck's constant, $(2S+1)$ is the spin degeneracy factor, and $\mathcal{R}_i$ is the absolute value of the local radius of curvature of the FS at points i on the FS at which the Fermi velocity is orthogonal to the direction of the wavevector $\vec{q}$, as depicted in Fig. 1(c). Therefore, this limit is universal in the sense that it is independent of the quasi-particle mass and interactions, and only controlled by the local geometric shape of the FS.

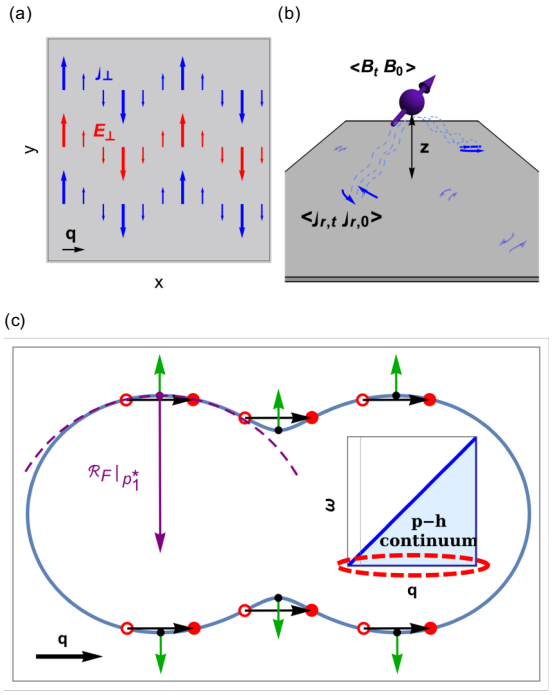

Figure 1: (a) Transverse currents (blue arrows) and electric fields (red arrows) with wavevector $\vec{q}$. (b) Schematic of a spin qubit located at a distance z above a 2D sample detecting the magnetic noise $\langle B_t B_0\rangle$ induced by current fluctuations $\langle j_{\vec{r},t} j_{\vec{r},0}\rangle$ in the sample. (c) Depiction of the particle-hole excitations with small wavevector $\vec{q}$ that are tangential to the FS (solid blue line) and dominate the dissipative transverse conductivity. For a given $\vec{q}$ these excitations are located near certain points, $\{\vec{p}_i\}$, where the Fermi velocity is orthogonal to $\vec{q}$, and their contribution to the universal transverse conductivity depends only on the local radius of curvature $R_{i=1}$, which we show explicitly in purple for one of these points $\vec{p}_{i=1}$. The inset shows the region of the particle-hole continuum containing these $(\vec{q}, \omega \to 0)$ excitations.

Quasi-static transverse conductivity of spinon Fermi surface. Remarkably, we have found that a similar limit of Eq. (1) is also approached by the transverse electric conductivity of a strongly correlated fractionalized state, namely, the U(1) spin liquid with a spinon FS [3], which has been a "holy grail" of condensed matter research since the pioneering ideas of Anderson [4]. This state features a form of spin-charge separation above one-dimension, in which the electron fractionalizes into a spinful fermion (the spinon) and a spinless boson (the chargon or holon). The chargon is gapped and the spinon remains in a gapless FS state, but both particles remain strongly coupled via an emergent U(1) photon field. This state displays electromagnetic responses that are a sort of blend of insulating and metallic behavior. On the one hand, while it has a vanishing electrical conductivity at $q = 0$ in the DC zero temperature limit just like insulators, it also displays power-law

subgap optical conductivity [5], quantum oscillations under magnetic fields [6,7] and cyclotron resonance [8].

The results in Ref. [1] for the spinon FS are valid in the limit in which the spinon diamagnetic susceptibility, χ_s, is much smaller than the chargon diamagnetic susceptibility, χ_b. In this case, the electric transverse conductivity of the spinon FS approaches the same universal limit at low frequencies given in Eq. (1). More generally, however, a correction to the results in Ref. [1] appears, and the spinon Fermi surface approaches a limit equal to that in Eq. (1) but multiplied by the ratio $\chi_c^2/(\chi_s+\chi_c)^2$ [9].

Universal noise and its NV center detection. While the universality of this limit of the transverse conductivity in ordinary Fermi liquids has been known since the early days of Landau Fermi liquid theory, to our knowledge, its precise form for anisotropic FSs has not been derived previously in two-dimensions, although a related dependence of the quasi-static conductivity at finite wavevector on the FS curvature has also been discussed in the context of the anomalous skin effect in 3D metals [10]. More importantly, to this date there is no report of the experimental observation of this remarkable universal regime of the transverse conductivity even in ordinary two-dimensional Fermi liquids or metals. This is largely because it is experimentally challenging to probe the linear response regime, where Eq. (1) holds, by controllably applying external transverse electric fields (shear forces) with a finite wavevector that is not too small ($q \gg l_{\rm mfp}^{-1}$) and at very low frequencies. There is, however, an alternative way to probe linear response functions that does not require actively applying external perturbations on the system, but instead to monitor its fluctuations since the fluctuation-dissipation theorem dictates that these are governed by the dissipative part of the same linear response susceptibilities. This is the key idea behind the technique of magnetic noise spectroscopy of nitrogen-vacancy center spin qubits, which is emerging as a powerful tool to study current and spin correlations of diverse condensed matter systems [11].

In the above regime, the transverse conductivity gives rise to a universal regime of the magnetic field noise when it is probed at a distance z above the 2D sample (see Fig. 1(b)) within the range $p_{\rm F}^{-1} \gg z \gg l_{\rm mfp}$, and at low temperatures and low frequencies. In this regime, the magnetic field autocorrelation function at a single point, takes the following universal form for metals:

$$\chi''_{B_zB_z}(z,\omega\to 0) \simeq \frac{e^2\mu_0^2}{16\pi h}\frac{\omega}{z}\frac{(2S+1)}{2\pi}\mathcal{P}_{\rm FS}+\mathcal{O}(\omega^3). \quad (2)$$

Here $\mathcal{P}_{\rm FS}$ is the perimeter of the FS in momentum space, and μ_0 the permeability of free space. In the case of spinon FS the above result is again multiplied by the ratio $\chi_c^2/(\chi_s+\chi_c)^2$ [9].

Summary and outlook. We have shown that the quasi-static transverse conductivity of 2D metals in the quantum (or ballistic) limit takes a universal form, given in Eq. (1), which is only controlled by the FS geometry and is independent of kinematic details or interactions. We have demonstrated that this leads to a universal low-frequency magnetic noise, given by Eq. (2), which can be directly measured by spin qubit noise spectroscopy. In experiments, the dependence of the noise on the qubit-sample distance can be used to identify the quantum regime, in which the noise is fully determined by the FS perimeter.

This noise, which arises from orbital current fluctuations, dominates over the noise from spin fluctuations in both the spinon FS state and metals. We estimate in Ref. [1] that the required frequencies are of the order of MHz in organic spin liquid candidates and of order of GHz in transition-metal-dichalcogenide spin liquid candidates, placing them within experimental reach of current nitrogen-vacancy noise spectroscopic techniques [11]. Therefore, the correlation function described in Eq. (2) is not only of conceptual interest due to its dependence on the pure geometry of the FS, but it is also of great significance as an experimental probe to characterize correlated states with a FS.

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2.33 Relaxation dynamics of an open Wannier-Stark system

LING-NA WU AND ANDRÉ ECKARDT

Introduction Many-body localization (MBL) [1], which describes the failing of an interacting system with quenched disorder to thermalize, has attracted widespread attentions in recent years. It is a very intriguing question, whether MBL can be achieved also without disorder. Recent studies [2, 3] show that an interacting Wannier-Stark system can exhibit non-ergodic behavior analogous to disorder-induced many-body localization (MBL) [1]. Understanding both the differences and similarities between such disorder-free and conventional MBL constitutes a fundamental question, which currently attracts a lot of attention.

While the possibility of disorder-free MBL is an important result addressing the fundamental problem of ergodicity (i.e. whether and how an isolated many-body system can thermalize), realistic systems will always suffer from the coupling to an environment, which eventually will lead to a relaxation to thermal equilibrium. Hence, it is also crucial to understand in how far this relaxation will be influenced by disorder-free MBL.

Model In the following, we consider an open chain of interacting spinless fermions subject to a strong electric field, with Hamiltonian

$$H = J\sum_{i=1}^{M-1}\left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right) + \sum_{i=1}^{M} W_i n_i + V\sum_{i=1}^{M-1} n_i n_{i+1}.$$

Here the operator $c_i^\dagger$ creates a fermion on lattice site i, and $n_i = c_i^\dagger c_i$ is the associated number operator. The first term denotes tunneling between nearest neighbor sites with rate J. The second term is the on-site potential describing the applied static gradient, $W_i = -ri$. The last term describes the nearest-neighbor interactions with strength V. The non-interacting system (in the thermodynamic limit) exhibits the well-known Wannier-Stark effect [4], where the particles are localized due to the linear potential. When interactions are turned on, the system is shown to remain localized above a critical potential gradient r and exhibit non-ergodic behavior analogous to conventional MBL [2,3], such as logarithmic growth of entanglement entropy, Poissonian level statistics, etc.

Bath-induced decay of Stark localization In Ref. [5], we investigate the relaxation dynamics of the system when it is coupled to a dephasing bath. The full dynamics of the system can be described by a master equation of Lindblad form [6],

$$\frac{d\rho}{dt} = -i\,[H,\rho] + \gamma\sum_{i=1}^{M}\left(n_i\rho n_i - \frac{1}{2}n_i^2\rho - \frac{1}{2}\rho n_i^2\right), \quad (1)$$

where ρ is the system's density matrix and $\gamma > 0$ sets the coupling to the bath. To study ergodicity breaking in the open system, we investigate the dynamics of population imbalance between even and odd sites, $I(t) = (N_{\rm even}(t) - N_{\rm odd}(t))/N$. For the isolated system in the MBL phase, the imbalance approaches a finite value in the steady state [2, 3]. Such a memory of the initial condition can no longer be maintained in the presence of dissipation.

Figure 1(a) shows I for the non-interacting system with different field gradients r. The imbalances (solid lines) oscillate at short times $t < 1/\gamma$ and then decay to zero at a rate that is found to depend on the field gradient r. We show $-\log(I)$ for large r in a logarithmic plot as a function of the scaled time $\tilde{t} = t/\tau$ with $\tau = \gamma^{-1}(r/J)^2$ in Fig. 1(b). The results collapse onto each other from the time where decay sets in. The decay is found to be approximately exponential, which is different from the behavior that was found for disorder-induced localization [7]. There the population imbalance exhibits a stretched exponential decay under dephasing noise and it is attributed to the different decay rates at distinct parts of the system due to fluctuations in the disorder strength, which is absent in our model.

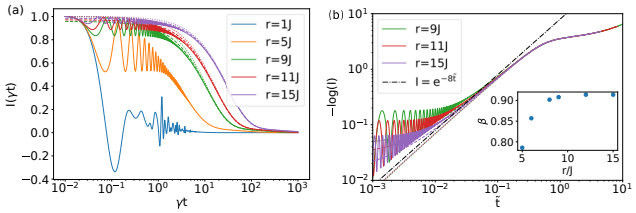

Figure 1: Dynamics of the population imbalance between even and odd sites, I, for non-interacting systems from the initial charge-density wave state. (a) shows I as a function of γt. (b) shows $-\log(I)$ as a function of the scaled time $\tilde{t} = \gamma t(J/r)^2$. The inset shows the stretching exponent β of the fitting curve $I = I_0 e^{-(t/t_0)^\beta}$ as a function of field gradient r. The dashed lines in (a), (b) are the approximated results given by the classical rate equation [5]. The system size is $M = 8$. The dissipation rate is $\gamma = 0.1J$.

Prethermal memory loss and universal dynamics In Ref. [8], we investigate the relaxation dynamics of the system when it is weakly coupled to a thermal bath. The dynamics of the system is then described by a Redfield master equation [6],

$$\frac{d\rho}{dt} = -i\,[H,\rho] + \eta\sum_{k,q,p,l=1}^{M}\Big[R_{kqlp}\left(L_{kq}\rho L_{pl}^\dagger - L_{pl}^\dagger L_{kq}\rho\right) + R_{plqk}\left(L_{kq}\rho L_{pl}^\dagger - \rho L_{pl}^\dagger L_{kq}\right)\Big], \quad (2)$$

with jump operators $L_{kq} = |k\rangle\langle q|$ between many-body eigenstates $|k\rangle$ of energy ε_k [9, 10]. The corresponding transition rates read $R_{kqpl} = \pi v_{kqpl}\, g(\varepsilon_k - \varepsilon_q)$, with

$v_{kqpl} = \sum_{i=1}^{M} \langle k|n_i|q\rangle\langle p|n_i|l\rangle$ and bath correlation function $g(E) = J(E)/(e^{E/T} - 1)$, where we assume an Ohmic spectral density $J(E) = E$.

Figure 2(b) shows the evolution of the von Neumann entropy of the total system, $S(t) = -\mathrm{Tr}\{\rho(t)\log[\rho(t)]\}$, for an initial state with one fermion on each site in the left half of the system. It is found to approach its equilibrium value rather differently for negative and positive field gradient r. Remarkably, we can observe that for large positive gradients r, the peak entropy almost reaches the largest possible entropy S_∞ (dotted line), which uniquely corresponds to the maximally mixed state $\rho_\infty \equiv \rho_{T=\infty} = \mathcal{D}^{-1}\sum_k |k\rangle\langle k|$. This effect can be observed for a wide range of initial conditions [see Fig. 2(c)]. Since the maximally mixed state is unique, reaching an entropy peak with $S_{\mathrm{peak}} \approx S_\infty$ indicates that we can expect the system dynamics to become (approximately) independent of the initial conditions near and after approaching the peak entropy. Such a behavior is confirmed in Fig. 2(d), where we plot the evolution of the site occupation $\langle n_{i=3}\rangle$ relative to the time t_{peak} at which the entropy peak is reached. The different curves, which correspond to different initial states, clearly converge near $\eta(t - t_{\mathrm{peak}}) = 0$ and subsequently show almost identical behavior. Thus, the system undergoes an effective prethermal memory loss, long before it reaches thermal equilibrium. This prethermal memory loss is attributed to a *dissipative* form of prethermalization, where the system rapidly approaches a negative temperature Gibbs state, whose effective temperature then slowly relaxes to the equilibrium temperature [see Fig. 2(e)].

By comparing the system's dynamics to that of a simplified model [8], the underlying mechanism is found to be related to the localization property of the Wannier-Stark system, which favors dissipative coupling between eigenstates that are close in energy. For a disorder-localized Fermi-Hubbard chain without this spatio-energetic correlation we find no prethermal memory loss. This constitutes an even more drastic difference between the relaxation dynamics of Stark and disorder-induced MBL than the one observed for dephasing noise [5].

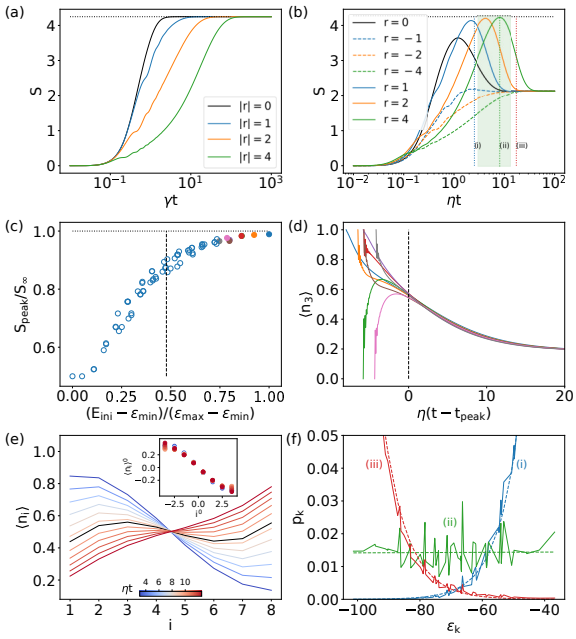

Figure 2: (a), (b) Time evolution of the von Neumann entropy for the tilted ladder initialized in a Fock state with the left half of the chain occupied and coupled to (a) a dephasing bath [Eq. (1)] or (b) a thermal bath [Eq. (2)]. The dotted line marks the largest possible entropy S_∞. (c) Normalized peak entropy for initial Fock states of various energies E_{ini}. The vertical dashed line marks E_∞. (d) Evolution of the mean occupation of the third lattice site relative to the time t_{peak}, where the entropy peak is reached. The line colors mark different initial Fock states corresponding to colored bullets in (c). (e) Density profile $\langle n_i \rangle$ at equidistant times during the time window marked by the shaded area in (b). The black line marks $t = t_{\mathrm{peak}}$. The inset shows the collapse of all the curves by rotating them by an angle proportional to the corresponding time. (f) Diagonal elements of the density matrix p_k at three points in time [marked by (i)-(iii) in (b)] (solid lines) compared to effective thermal states of identical average energy (dashed lines). The parameters are $M = 8$, $J = 1$, $V = 1$, $\gamma = \eta = 0.1$, and T so that $S_T = S_\infty/2$. The field gradient for (c)-(f) is $r = 4$.

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2.34 Advanced Study Group 2018/2019: Forecasting with Lyapunov Vectors

CONVENOR: PROF. MARCUS W BEIMS

Scientific Context Forecasting has become one of the most required researches in actual days. The ability to predict the future based on past and present data is highly relevant in distinct areas, like climate changes, stock markets, critical transitions, extreme and rare events, including giant ocean waves, extreme weathers, and laser peaks, among others. The dynamics in such realistic problems is typical of highly nontrivial high-dimensional complex systems. There is no model which can fully describe such realistic complex systems, making the prediction a difficult task. More specifically, achieving the fundamental principles behind the mechanism of predicting chaotic time series and rare and extreme events was of particular interest in the present ASG. One of such fundamental principles is the alignment of covariant Lyapunov vectors preceding significant peaks in chaotic time series. The alignment of covariant Lyapunov vectors occurs due to tangencies between curves that live in the tangent space of such systems and, astonishingly, occur short times before significant peaks appear in a chaotic time series. Combining results of the alignment of the covariant Lyapunov vectors, machine learning and classification techniques, we performed improved predictions of the time spent inside regimes (attractors) in the Lorenz system and Rikitake's geomagnetic dynamo model. Although the method of Lyapunov vectors is restricted to a linear analysis around trajectories, signatures of the alignment should be observed at larger scales. This can be done by studying bred vectors, which capture the fast-growing dynamical instabilities of solutions and were used in the context of breeding ensembles for the weather forecast. However, bred vectors did not furnish information about angles between distinct stable and unstable directions.

Furthermore, a distinct but related line of research is the decomposition of nonlinear time series. An interesting method extensively used during the past decades is the so-called empirical mode decomposition, which, along with its many variants, has gained popularity in several fields, especially in analyzing geophysical records, biomedical signals, coupled chaotic systems, economic and market data, and in other complex scenarios. While traditional methods do not well perform the decomposition of nonstationary, nonlinear, noisy signals, empirical mode decomposition provides a general tool for an adaptive signal decomposition into a finite number of narrowband intrinsic mode functions. The local extrema of the signal determine the intrinsic mode functions generated by the empirical mode decomposition algorithm, and traditional empirical mode decomposition uses a cubic spline for upper and lower envelope interpolation. Notably, the empirical mode decomposition algorithm works as a dyadic filter bank, that is, the mean frequency of a given intrinsic mode function is approximately half of the previous one. For this reason, the basic problem of all top-to-bottom decompositions is the interpretation: how to distinguish relevant intrinsic mode functions and irrelevant intrinsic mode functions efficiently. The ASG proposed an alternative procedure providing a bottom-to-top decomposition. Similarly to empirical mode decomposition, this empirical method is purely data-driven and uses cubic spline fits.

The ASG brought together experts from relatively distinct areas to explore the proposal in a more general perspective, emphasising time series analysis and the alignment of covariant Lyapunov vectors.

Structure, calendar, summary of activities The ASG Forecasting with Lyapunov Vectors took place over four months, beginning on November 1st, 2018. An additional month extension was granted and took place in February 2019. Its convener was Marcus Werner (UFPR, Brazil) and the invited long-term members were Imre Jánosi (University of Public Service, Faculty of Water Science, Hungary) and Jason Gallas (UFPB, Brazil). A mini-workshop in Jan 22-23th provided an opportunity to present several ideas and have a brainstorming session among participants and members of the mpi**pks**, specially Prof. H. Kantz and his PhD student J. Brisch.

The ASG has also benefited from the visits of other scientists, which typically resulted in new collaborations and/or the invigorating/extension of existing ones: G. M. Ramírez-Ávila (UMSA, Bolivia), P. Lind (OMU, Norway), B. Hunt (UM, USA), T. Tel (LEU, Hungary), D.Weingaertner (UFPR, Brazil), H. Varela (USP, Brazil), J-C Garreau (UL, France) and PhD student E. L. Brugnago (UFPR, Brazil). Collaborations between ASG members and/or ASG invitees and/or the mpi**pks** researchers have started at the occasion of the ASG activity periods. Several of them have already led to publications. Below we summarize the most notable results achieved related to time series analysis.

- *Alignment of covariant Lyapunov vectors, bred vectors, machine learning and classification techniques.* In chaotic systems containing two-wing (Lorenz's case) or multiple-wing chaotic attractors, we combined the Lyapunov vector alignment with maxima observed in the local expansion of bred

vectors to significantly decrease errors in predicting the time spent inside the wings (attractors), thereby providing competitive predictions for the onset of large and possibly catastrophic events. The alignments of Lyapunov vectors were used to train multi-layer perceptron to predict regime durations in chaotic time series of Rikitake's geomagnetic dynamo model.

- *Alignment of covariant Lyapunov vectors, machine learning and classification techniques.* The strategy was to transform the problem of the determination of time intervals into a classification problem by associating time duration inside the wings (attractors) with the number of maxima (or minima) observed inside each wing. High accuracy is obtained for the predictions, even for the most prolonged regimes that include 17.5 Lyapunov times. Machine learning allowed us to identify the most relevant pairs of aligned covariant Lyapunov vectors needed for a successful prediction.
- *Decomposition of nonlinear time series.* A bottom-to-top procedure for the decomposition of time series was proposed by smoothness-controlled cubic splines. We have successfully validated the procedure on a series of synthetically constructed composite signals. We illustrated the method's capability by reconstructing a synthetic signal composed of a chirp, a strong nonlinear background, and a large-amplitude additive noise, where all empirical mode decomposition-based algorithms fail spectacularly. Specifically, we demonstrated the efficiency of the method on two real signals: daily sea ice extent over the Arctic and over the Antarctic as determined by satellite image processing. In this way, we uncover distinct freezing-melting dynamics between the Arctic and the Antarctic.

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2.35 Advanced Study Group 2019/2022

CONVENOR: PETER HÄNGGI, SERGEY DENYSOV

Results *Signatures of Dissipative Quantum Chaos.* Similar to the conventional Quantum Chaos, foundation of Dissipative QC (DQC) could be based on spectral properties of generators of evolution, in this case open. There is a strong need for establishing universalities, i.e., for figuring out spectral features which are typical to properly defined ensembles of generators.

The importance of universal spectral properties was realized recently by several independent groups which led to a strong boost of research on the DQC topics. A paper on the notion of an ensemble of random Lindblad operators was published by the group's members in October 2019 [S. Denisov, T. Laptyeva, W. Tarnowski, D. Chruściński, and K. Życzkowski, Phys. Rev. Lett. 123, 140403 (2019).]. Since then, a number of other works on spectral aspects of random Lindblad operators (with different types of randomness) where published. Very recently, spectral properties of random Lindbladians, on which some additional constrains were imposed, were studied experimentally on the IBM Quantum Experience platform [O. E. Sommer, F. Piazza, and D. J. Luitz, Phys. Rev. Research 3, 023190 (2021)].

In our work [1], we generalized the idea of random Lindbladians further. We present the concept of super-decoherence, i.e., a decoherence acting on the level of generators of dissipative quantum evolutions. We demonstrated that super-decoherence bridges, in a continuous way, Lindblad operators (generators of quantum open evolution) and their classical counterparts, Kolmogorov operators (generators of time-continuous Markovian evolution). We addressed random ensembles of generators, both quantum and classical, evaluated their spectral properties [see in the figure, depicting the complex-valued spectral distribution of random Lindbladians], and demonstrated that the two ensembles are related by superdecoherence. We also defined a procedure of "coherefication" which allows crossing the bridge in the opposite directions, i.e. to obtain a Lindblad operator from a Kolmogorov one. Finally, we addressed the so-called Complex Spacing Ratio measure, which is generalization of a measure used to quantify the degree of chaos in Hamiltonian systems.

In Ref. [2] we consider another quantifier of DQC. By unraveling Lindblad equation describing an open quantum Kerr-nonlinear cavity, periodically modulated in time by coherent pumping of the intracavity photonic mode, into an ensemble of quantum trajectories and employing the recently proposed quantum Lyapunov exponents [I. I. Yusipov et al., Chaos 29, 063130 (2019)], we identify "chaotic" and "regular" regimes. In particular, we show that chaotic regimes manifest themselves in intermediate power-law asymptotics in the distribution of photon waiting times. This distribution can be measured by monitoring photon emission with a single-photon detector.

Open Floquet systems. Here we moved along two directions.

Are there Floquet Lindbladians? We consider open quantum systems that are modulated periodically in time; in other words, the corresponding Hamiltonian is a time-periodic Hermitian operator. In the weak- coupling limit, the dynamics of such a system is governed with a Lindblad equation, possessing a time-periodic generator. Would it be possible to construct time-independent Lindblad generator (which we termed "Floquet Lindbladian") yielding at stroboscopic instants of times, T, 2T, 3T, ... , the same states of the system as in the case of original time-dependent generator? The answer is always "yes" in the Hamiltonian limit but. It is no longer holds true when the system is open. In fact, as we demonstrated [3] with a simple qubit model, the Floquet Lindbladian does not exist in the most interesting case when the driving is neither diabatic nor adiabatic.

With the consecutive work [4] we advanced further along this line and explicitly demonstrated that different high-frequency expansions, used in recent works as a tool to construct effective Floquet-Lindbladians are, in fact, ill-suited for this task and the outcomes of the corresponding analysis should not be used as a basis to judge the existence of the effective stroboscopic generator. We demonstrated that a proper Floquet Lindbladian can still be obtained from a high-frequency expansion when treating the problem in a suitably chosen rotating frame.

Spectral characteristics of Dissipative Quantum Chaos in Floquet-Markov systems. Universal features were fund and some new concept, like the "Complex Spacing Ration", have been put forward by using the Lindblad framework (as discussed in the first section). However, stationary Lindblad generators do not provide a straightforward way to model the semi-classical chaotic regime; therefore, it is seemingly difficult to relate an open quantum dynamics to a dissipative classical dynamics exhibiting chaotic dynamics.

We considered another type of generator of dissipative quantum evolution, the so-called Redfield generators, which emerge in the Floquet-Markov theory and allows for a semiclassical transition [5]. We used a quantum version of the driven Duffing oscillator as a model

to illustrate spectral properties of Redfield generators. Our two main findings here are the following: First, the notion of a random generator can also be extended to Redfield ones. Second, Complex Spacing Ratios (CSR) of the generator exhibits Poisson statistics (typical to integrable Lindblad generators) in the chaotic regime whereas for the regular regime it yields the horseshoe structure (typical to 'chaotic' Lindbladians). In other words, the behaviour is reversed as compared to the case of Lindbladians. We attributed this to the fact that chaotic behaviour of Floquet-Markov systems is encoded within coherent Floquet states of the corresponding Hamiltonians.

Transport in open many-body systems far from equilibrium. Combinations of many-body effects, openness, and strong deviation from equilibrium can lead to transport regimes, which, however, are not accessible in the near-equilibrium limit.

In Ref. [6], we explored spin transport in an open XXZ chain with strong interaction strength and demonstrated that the transport in this system becomes suppressed significantly when the bias of the dissipative driving becomes large enough. We also detected the regime of negative differential conductance caused by the formation of two oppositely polarized ferromagnetic domains at the edges of the chain. Thus, we demonstrated that this many-body effect, combined with a non-uniform magnetic field, allows for a high degree of control of the spin current.

Workshop "Openness as a Resource"

The workshop "Openness as a Resource: Accessing New Quantum States with Dissipation" (mpi**pks** 31 Jan. - 04 Feb., 2022), is planned to crown the work of the ASG and to provide a forum to exchange and discuss ideas related to the topics addressed by the ASG. The workshop participants will represent three scientific communities: Researchers working on mathematical aspects of open quantum systems that make use of Lindblad generators, semi-groups, and quantum Monte-Carlo methods, their colleagues from the field of quantum thermodynamics. Last but not least, theoreticians and experimentalists dealing with circuit-QED and solid-state based quantum systems will attend as well.

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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 mpi**pks**. 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 mpi**pks**: PhD positions funded through external grants are advertised in scientific journals and on the internet pages of the institute. Applications for PhD positions funded through the Visitors Program are accepted at all times and invited via the internet pages of the institute, workshop announcements and print publications.

In 2019, a total of 82 PhD students were working at the mpi**pks**, thereof 54 students from abroad (also counting those who finished or started their studies during that year). The respective numbers for 2020 were 81 PhD students working at the mpi**pks** (58 from abroad), and in 2021 up until 30. September we had 81 PhD students (61 from abroad). We note that, while the overall number of PhD students at the institute at any given time remains basically constant since 2017 (between 80 and 85), the number of international students has 0 increased, from 50 in 2017 to 61 in 2021. We counted 8 successful final PhD exams for the year 2019, 6 for the year 2020, and 4 for the year 2021 (up until September).

In addition to the scientific training by their supervisors, PhD students at the mpi**pks** benefit from a variety of opportunities to develop their expertise, skills, and career: The students are admitted to the lecture courses offered by the TU Dresden and the mpi**pks** (p. 153). 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. 154). Students from foreign countries receive financial and logistic support for joining German language courses.

The majority of the PhD students at the mpi**pks** receive their degree from the TU Dresden (p. 155). 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.15.

PhD students – There are currently 62 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 5 students from the Americas (one each from Argentina, Colombia, Ecuador, Mexico and Venezuela), 9 from India, 1 from Iran, 5 from China and one each from Taiwan, Thailand and Vietnam. The rest

are from across Europe (Belgium 1, Croatia 1, Czech Republic 10, Germany 12, Greece 2, Hungary 1, Italy 3, The Netherlands 1, Poland 4, Slovakia 1, Spain 2, Ukraine 1). Ten of the students are women. The distribution across partner institutions is mpi**pks** 25, TUD 14, IFW 2, IOCB 9, UCT 5, University of Wrocław 1, ILTSR 2, Charles University 2, TU Berlin 2 (formerly mpi**pks**).

Annual Events – The IMPRS organizes various meetings for the students of the graduate school. Under non-pandemic circumstances there would be an annual retreat and a summer school cycling between Germany, the Czech Republic and Poland. The retreat is typically a three-day meeting framed around student talks and discussions that is partly intended to introduce new students to the activities of the school and especially to give students experience in communicating their research to others working in adjacent areas of the physical sciences. The summer school is themed around topics of considerable contemporary interest within the general areas covered by the graduate school.

In 2019 the summer school and retreat took place during the six days from September 2nd to 7th in Karpacz in Poland – a town historically important as the host of meetings between scientists from both sides of the Iron Curtain. This event was also attended by some guest PhD students of the Universidade Federal do Parana, Curitiba in Brazil – the beginning of a planned initiative to invite PhD students from Brazil and India to selected IMPRS events. The summer school covered diverse topics including strongly interacting metals, non-equilibrium quantum systems and open quantum systems.

The COVID-19 pandemic led the graduate school to move regular events online in 2020 and to the postponement of the annual summer school and retreat. Admissions to the graduate school continued as normal, however, so a Kickoff Meeting was held in April 2021 primarily to introduce these students to the wide-ranging research carried out by the various partner groups and, in turn, for those students to introduce themselves. The format was a two-day online meeting with plenary talks from new students and from representatives of the partner groups with breakout sessions for more senior students to discuss with the relatively new arrivals.

Late in the summer of 2021 it became possible once more to hold in-person events with measures taken to safeguard against new cases arising. As a result, the IMPRS held a summer school from September 1st to 3rd as a hybrid event with the in-person talks broadcast from a pole marquee on the grounds of mpi**pks** that also hosted an audience of students including participants from Prague and Wrocław. There has been considerable progress in the development of general purpose quantum computation in recent years, so one set of lectures was focused on the opportunities to study quantum many-body dynamics on existing machines. Other lecture topics included modern developments in topological materials and novel experimental techniques in magnetism.

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 regular IMPRS seminar is the main vehicle for students and partners of the graduate school to hear about the research activities of the affiliated groups. These seminars are opened with a colloquium-style talk from an external invited speaker who has the task of introducing the broader context of the work carried out by one of the students. This student then gives a seminar based on their own research. Every doctoral student gives such a seminar usually during the final year of the PhD.

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 mpi**pks**. Of the courses offered by the university, the IMPRS selects English language lectures in the topics 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 IMPRS are invited back to share their experiences of work and life beyond academia. Our focus in organizing such talks has been on sectors of industry where a background in theoretical physics may be attractive to employers, including 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 first-hand accounts of career possibilities where their unique skills and interests have proven valuable beyond academic research.

The IMPRS also runs a series of journal club talks framed around classic results in many-particle quantum physics. The purpose of these talks is to provide a forum for learning and discussing important concepts

that form the fabric of the topic, but may not be covered directly in lectures. Students themselves choose and present the topics in an informal setting at the blackboard or on a tablet computer with plenty of opportunity to raise questions and discuss.

The day-to-day coordination 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 mpi**pks**.

3.3 Workshop and Visitors Program

The Visitors Program of the mpi**pks** hosts guest scientists for a period of up to two years. Excellent working conditions are offered to highly qualified, mostly young, scientists. In close collaboration with the other service departments of the mpi**pks**, the Visitors Program is dedicated to support the scientists in every possible way to allow them to focus on their research. This also includes logistic help, e.g., for finding suitable accommodation, 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 "Microscale Motion and Light", July 22 - 26, 2019

During the past three years, the numbers of guest scientists including predocs with contracts for at least three months hosted by the mpi**pks** were 240, 217 and 196 (in 2019, 2020 and between January and September 2021, respectively). The number for 2019 is practically identical to the one for 2017 and 2018, while in 2020 and 2021 we notice the effects of the pandemic. One characteristic, which is not visible from the cumulative number for the entire year but requires a finer resolution in time, is that the pandemic has led to strong inhomogeneities within the year regarding the question when long-term guest scientists commence their position. The pattern we have witnessed in 2020 and 2021 is that during winter and spring, most processes which are required for the arrival preparation, such as visa appointments at German consulates, were often frozen or significantly delayed. They became operational again in summer, leading to a strong peak of new arrivals in the months September-November. This also explains the rather low number given for the period January-September 2021, since a large cohort is scheduled to arrive in October and November, so that in the end, the expected cumulative number for the year 2021 should be comparable to 2020.

In addition to the long-term guest scientist positions, the Visitors Program hosts many short-term visits for up to three months. These visits are usually related to collaborations between the mpi**pks** research groups and other institutes. In this category, the detrimental effect of the pandemic is much more

pronounced than for long-term guests. The usual number of short-term guests per year in recent years was about 300, e.g. 325 in 2019. This number dropped to 63 in 2020 and 49 in 2021 (up until September). Moreover, out of the 63 short-term guests in 2020, 55 arrived at the institute between January and the first half of March, with a few more during the summer months, and all but one short term visitors of 2021 came to mpi**pks** in May or later. In other words, the flux of short-term visitors basically came to an almost complete halt in the period April 2020 - April 2021.

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. 130).

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 January 2019 and September 2021, we had seven PKS Fellows working at the mpi**pks**: *Dr. Aline Ramires* (until March 2020), *Dr. Falko Pientka* (until July 2020), *Dr. Felix Mackenroth* (until September 2020), *Dr. Matthew Eiles* (until December 2020), *Dr. Stefano Bo* (since June 2019), *Dr. Nazmi Burak Budanur* (since May 2021), and *Dr. Suzy Zhang* (since September 2021).

To strengthen the transfer of knowledge and experience at the mpi**pks**, the institute annually awards the Martin Gutzwiller Fellowship to a senior scientist who made exceptional contributions in the area of the Physics of Complex Systems. Gutzwiller Fellows spend up to one academic year at the mpi**pks** and can nominate a young guest scientist for the Visitors Program. Between 2019 and 2021, our institute had the honor to host two Gutzwiller Fellows: *Prof. John Toner* (University of Oregon) and *Prof. Benoît Douçot* (Sorbonne University & CNRS).

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. The core of an Advanced Study Group attracts further short-term visitors, who contribute to seminars and discussions. While we are usually able to host up to two Advanced Study Groups per year, the outbreak of the pandemic has disrupted the rhythm. The Advanced Study Group *Forecasting with Lyapunov Vectors*, convened by Prof. Marcus Werner Beims, successfully conducted the planned scientific activities in 2018 and 2019. The Advanced Study Group *Open Quantum Systems Far from Equilibrium* under the convenor Prof. Peter Hänggi commenced its work in December 2019, shortly before the global outbreak, and was originally scheduled to be concluded during 2020. As several phases of the intended activities could not be carried out as planned due to travel bans and lockdowns, the Advanced Study Group had to be re-scheduled and is now envisaged to conclude by January 2022 (see reports on p. 48).

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-Fellow

Gutzwiller Fellowship 2019/20
(Prof. John Toner)

Overview:

I have had a very productive time as Martin Gutzwiller Fellow. I have had extremely productive collaborations with Abhik Basu of the Saha Institute, Kolkata, who made two visits here to collaborate with me during my stay. I have also finished one major project, and started (and finished!) another, in collaboration with Chiu Fan Lee and Leiming Chen, both of whom also visited mpi**pks** during my stay to collaborate with me. And finally, I have worked with Frank Jülicher and Jacques Prost on a study of dislocations in active smectics. In addition, I have completed an investigation of the "Mpemba effect", which I first learned about in a talk given here by Marija Vucelja.

I will now describe the projects I have worked on during my fellowship.

Ordered active fluids on a surface in contact with a bulk fluid

This project, motivated by experiments by Andreas Bausch of TU Munich in which microtubules bound to a surface by active motors form ordered "flocks", and by experiments by Denis Bartolo on "Quinke rotators", which are dielectric spheres spontaneously rolling along the bottom of a chamber filled in an electrically conducting fluid, addresses the effect of hydrodynamic interactions mediated by a passive bulk fluid on an active system that lives on a surface.

We have constructed the hydrodynamic theory for this system. This describes the coupled dynamics of the polarization of the active agents and their concentration for a planar quasi two-dimensional polar-ordered flock at the interface of passive, isotropic bulk fluid and a solid surface. These equations imply that for such a polar-ordered flock, the interplay between the friction and hydrodynamic interactions, respectively due to the solid surface and bulk fluid in contact, either (i) leads to large fluctuations of the active particle concentration in stable polar-ordered states with a standard deviation proportional to the 3/4th power of the mean, and distinct long-time tails $\sim 1/t$ and $1/t^3$ in the autocorrelation of tagged particle velocities transverse and longitudinal to the reference order, or (ii) destabilizes the flock. We also predict anomalous super-diffusion of tracer particles either floating in, or sedimenting through, the bulk fluid.

Dislocations in active smectics

There has been a considerable amount of work over the past few years on active smectics. However, whether or not these phases are actually stable against activity generated dislocations in the smectic layer structure, remains an open question. Stimulated by discussions I had with them during a previous visit here, Jülicher and Prost developed a model for the dynamics of dislocations in active smectics that was quite different from the one I had originally proposed. I believe my earlier model of those dynamics was incorrect, and that their model is correct. We now believe (contrary to statements made in my short scientific report last year!) that this correct model implies that dislocations will always be unbound in two dimensions, which implies that there is no active smectic phase in $d = 2$, unless there is an externally applied symmetric breaking "field" of some sort.

In my work on this problem during my visit here this year, I have shown that, even in the presence of such a symmetry breaking field, it is, surprisingly, *more* difficult to order an active smectic than an equilibrium one. That is, a stronger symmetry breaking field is required to bind dislocations in an active smectic than in an equilibrium smectic with the same noise. As a result, the active smectic melts through an active "Kosterlitz-Thouless" transition that does *not* exhibit a universal order parameter exponent η at the transition. Rather, this exponent becomes a function of the ratio $\gamma \equiv g/\alpha$, where g is the strength of the symmetry breaking field, and α is the activity. As $\gamma \to 0$, $\eta(\mathrm{melting}) \to 0$, while for $\gamma \to \infty$, $\eta(\mathrm{melting})$ approaches the equilibrium result $\eta(\mathrm{melting}) = 1/4$.

Active polar suspensions

This project, done in collaboration with Leiming Chen of the China University of Mining and Technology, Chiu Fan Lee of Imperial College, London, and Ananyo Maitra of Universite Pierre et Marie Curie, Paris, is a study of the effect of quenched disorder on active polar particles moving through an incompressible fluid either permeating a bulk, three dimensional disordered network, or between two narrowly spaced plates. In the three dimensional case, we have been able to obtain exact scaling exponents, which prove to be anomalous (that is, different from those that one would predict from a simple linear theory). In the two-dimensional case, we can find exact exponents when the system is "clean", and very good approximate exponents when the system is disordered.

A simple realization of the Mpemba effect which also exhibits an apparent violation of the zeroth law of thermodynamics

The Mpemba effect, which is almost certainly the most important phenomenon ever discovered by a thirteen-year-old, is the term applied to the counterintuitive fact that sometimes it can take *longer* to cool a hot system to a given temperature than a cooler system, even when both are brought onto contact with the same cooler heat bath. After learning about this topic for the first time in a talk given here by Marija Vucelja, I found a simpler realization in a suitably prepared system obeying a simple thermal diffusion equation. It turns out that such a system can not only display the Mpemba effect, but can actually, when brought into contact with a cooler heat bath, first drop to a temperature *lower* than that of the bath, and then warm up to the temperature of the bath. This requires that, for some of the time, heat is actually flowing from an initially cooler system (the bath) to the initially hotter system.

3.3.1.2 PKS-Fellow

(Dr. Stefano Bo)

I have joined the research activities at **mpipks** on diverse topics, ranging from the physics of phase separation and its applications to biology, to the irreversible-thermodynamic description of odd viscoelasticity. I have also worked with external collaborators. In the next paragraphs I will provide a short summary of the main research findings.

Single molecules in phase-separated media. There is increasing evidence that living cells exploit the physics of phase separation to form compartments that do not require a membrane to segregate from the cytoplasm, named membraneless organelles. Over the past few years, these compartments have been proposed to provide a mechanism for a variety of tasks including noise suppression, localization of specific proteins, and rapid sensing of changes. The biological function of such liquid-like droplets relies on the flux of molecules across phase boundaries. At the microscopic level, the stochastic movement of single molecules across phase boundaries can be observed by modern experimental techniques. This experimental progress raises the question of how to relate the dynamics of molecules that enter and leave droplets to the physics of droplets that emerges at larger scales.

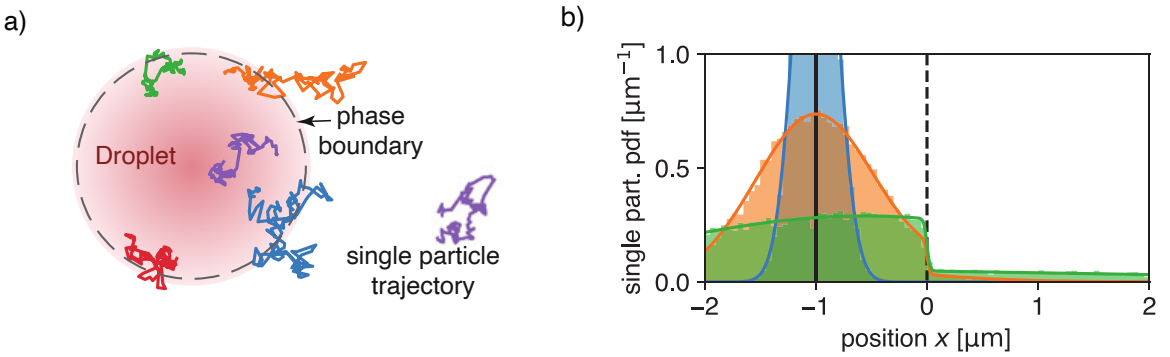

Figure 1: Single-molecule dynamics at phase boundaries. (a) Schematic illustration of single-molecule trajectories in a phase-separated medium. (b) Examples of single-molecule propagators for a molecule starting in the dense phase at different times.

Within a collaboration involving members of the biological physics division we derived the stochastic equation for single-molecule trajectories [1]. We started from the coarse-grained dynamics of concentration fields in phase separation and explicitly considered the labeling of certain molecules. We found that molecular trajectories can be described as diffusion in an effective potential due to interactions with the other molecules. This potential has a steep gradient at the interface, which induces a drift, allowing the concentrations to be different in the two phases. When the system is out of equilibrium there can be concentration gradients also away from the interface. In these cases, single molecules are subject to an additional non-equilibrium drift.
Deriving the single-molecule dynamics allowed us to characterize quantitatively the displacement statistics of molecules across phase boundaries, and to relate them to the physical properties of coexisting phases. At equilibrium, microscopic reversibility imposes symmetries and constraints on single-molecule statistics,

which we investigated. When these symmetries are violated, our theory can reveal the non-equilibrium nature of droplet-like condensates from single-molecule trajectories. We are currently quantitatively investigating how the breaking of these symmetries relates to the dissipation associated with non equilibrium. Our work, bridging different levels of description, revealed how information obtained from single-molecule trajectories can be used to obtain insights into the physics of liquid-like droplets.
In parallel, I have contributed to the theory behind the development of an experimental technique for the measurement of diffusion coefficients and partition factors for phase-separated media based on the fluorescent labeling and unlabeling of molecules [2].

Odd viscoelastic materials. Viscoelastic materials that exhibit solid-like properties on short time scales and relax towards a fluid behavior on longer time scales are abundant in nature and encompass polymer systems, metamaterials and many biological systems, including the cytoskeleton. Two-dimensional materials with chiral properties that break parity invariance called odd viscoelastic materials have recently been studied. It is known that materials which are purely odd elastic can perform work on their environment and therefore cannot be passive. This has motivated the study of odd elastic and viscoelastic models in the context of active matter. A material is called active when it is composed of a large number of energy-consuming agents constantly driving the system out of equilibrium. In a collaboration between members of the biological physics and the condensed matter division, we characterized odd viscoelastic systems within the framework of linear irreversible thermodynamics [3]. We found that there is a wide range of viscoelastic models that are passive and odd. We therefore complemented the current viewpoint on odd elasticity, by showing that passive materials can be transiently odd elastic. The precise understanding of the circumstances under which odd viscoelasticity can be passive is crucial for characterizing odd materials. By showing that active ingredients are not a requirement, our results extend the range of systems where odd properties could be observed experimentally.

Heterogeneity in epidemic models. When an epidemic wave passes through a population, a fundamental question is to understand when a peak on infections is reached and what fraction of the population will become infected. We considered the importance of population heterogeneity in shaping epidemic waves [4]. We found that population heterogeneity has a governing effect, which is particularly relevant when power-law distributions are involved. Extending the classic SIR model, our analytic results highlighted that, for epidemic waves characterized by the same initial development, heterogeneous populations are characterized by less severe epidemics, which become self-limited earlier than for homogeneous populations. In combination with modeling, we also analyzed data for the first wave of SARS-CoV2 contagions in Germany.

Machine learning for inference and classification of stochastic time series. Machine learning has become the standard approach for a large numbers of tasks such as natural language translation, image recognition and other artificial intelligence problems. It is also establishing itself as new key tool for the study of physical systems. Together with collaborators from the University of Gothenburg and Leipzig University we have worked on the application of machine learning techniques (recurrent neural networks) to the study single stochastic trajectories. In [5] we considered anomalous diffusion dynamics. These dynamics are defined by a nonlinear growth of the mean squared displacement with time, which follows a power law characterized by the anomalous exponent. We applied recurrent neural networks to infer the anomalous exponent and identify the most likely model giving rise to the dynamics from individual stochastic trajectories. In [6] we reconstructed the force fields acting on microscopic particles under various non-equilibrium drivings. In both studies, the use of recurrent neural networks allowed us to extract information in scenarios that are overwhelmingly challenging for traditional algorithmic methods such as short and irregularly sampled time series which could be corrupted by measurement noise and other disturbances.
We have also taken part in the Anomalous Diffusion challenge (AnDi) [7], a competition comparing methods for the inference and classification of short trajectories following anomalous diffusion dynamics and subject to additional noise. I enjoyed pleasant and fruitful interactions with members of the Nonlinear Time Series Analysis group at MPI-PKS who also took part in the competition. Our method proved to be the most successful in most tasks and outperformed the competitors using traditional approaches such as Bayesian techniques and other time series analysis approaches.

Irreversibility in active matter systems. In parallel with my research with members of the MPI-PKS I have worked on a project with collaborators from Nordita and Bielefeld University investigating the relations between the breaking of time-reversal symmetry and dissipation in simple models of active

matter systems [8]. Focusing on active Ornstein–Uhlenbeck particles in confining potentials we found that, despite the active nature of the system, stationary trajectories in harmonic potentials obey pathwise time-reversal symmetry exactly. Anharmonic potentials are typically required to observe the breaking of time reversal symmetry.

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3.3.2 Conferences, Workshops and Symposia

Up until February 2020, all events were held at the institute regularly as on-site events. After the outbreak of the Covid-19 pandemic, the scheduled events in 2020 and the first half of 2021 had to be either postponed or carried out on-line. Moreover, a number of purely virtual events were proposed on shorter notice and included into the program. For some of the events which were re-scheduled, the scientific organizers decided to hold short virtual meetings (1-2 days) in order to generate input for the full meeting and ensure a continuous connection to the relevant communities (so called virtual stay-in-touch meetings). Some of these meetings were organized autonomously and some under the umbrella and with the help of the visitors program. Beyond fully virtual workshops, the situation during the pandemic also gave rise to two new formats at the institute: scientific open air camps and hybrid workshops. The former is particularly suited for the summer months, with the talks taking place in a large tent with open sidewalls and the discussions and social program in the open. The hybrid format allows to combine a small on-site audience with a large virtual audience, and one of the seminar rooms at the institute has been technically equipped for this purpose. The workshops which were scheduled for autumn 2021 could be carried out in this format, with the very first one taking place in September 2021. In the long run, the technical setup will also enable the institute to hold workshops delocalized over two hubs on different continents, thus reducing the necessity of intercontinental travel for a short period and thus improving the environmental footprint of the visitors program, which has been the initial thought behind the equipment even before the outbreak.

Events on-site before the outbreak of the Covid-19 pandemic:

1. *Anyons in Quantum Many-Body Systems*
   Workshop: January 21 - 25, 2019 — 52 participants
   Scientific coordinators: A. Bernevig, A. E. B. Nielsen, N. Regnault
2. *Phase Transitions in Polymeric and Protein Systems*
   Focus Workshop: February 14 - 15, 2019 — 60 participants
   Scientific coordinators: A. Hyman, F. Jülicher, J.-U. Sommer
3. *Atomic Tunneling Systems and Fluctuating Spins Interacting with Superconducting Qubits*
   Workshop: February 25 - March 1, 2019 — 47 participants
   Scientific coordinators: C. Enss, M. Schechter, A. Shnirman
4. *Image-based Modeling and Simulation of Morphogenesis*
   Focus Workshop: March 13 - 15, 2019 — 35 participants
   Scientific coordinators: K. Harrington, I. Sbalzarini
5. *Constrained Many-body Dynamics*
   Workshop: March 26 - 30, 2019 — 68 participants
   Scientific coordinators: M. Heyl, R. Moessner, F. Pollmann
6. *Bound States in Superconductors and Interfaces*
   Focus Workshop: April 8 - 10, 2019 — 66 participants
   Scientific coordinators: T. Domanski, K. Franke, R. Zitko

7. *BiGmax Workshop on Big-data-driven Materials Science*
   Workshop: April 15 - 18, 2019 — 50 participants
   Scientific coordinators: T. Bereau, J.-M. Rost
8. *Quantum Ferromagnetism and Related Phenomena*
   Workshop: May 6 - 10, 2019 — 69 participants
   Scientific coordinators: D. Belitz, M. Brando, A. Huxley
9. *Synthetic Topological Matter*
   Workshop: May 20 - 24, 2019 — 53 participants
   Scientific coordinators: J. Meyer, G. Refael, K. Shtengel
10. *Engineering Nonequilibrium Dynamics of Open Quantum Systems*
    Workshop: June 17 - 21, 2019 — 47 participants
    Scientific coordinators: A. del Campo, M. Plenio, A. Rahmani
11. *Bio-inspired Optics and Photonics - From Metamaterials to Applications*
    Focus Workshop: June 24 - 27, 2019 — 47 participants
    Scientific coordinators: H. Hölscher, M. Kolle
12. *Granular and Particulate Networks*
    Focus Workshop: July 8 - 10, 2019 — 42 participants
    Scientific coordinators: D. S. Bassett, K. E. Daniels, M. A. Porter
13. *Microscale Motion and Light*
    Workshop: July 22 - 26, 2019 — 60 participants
    Scientific coordinators: T. E. Mallouk, R. Marschall, J. Simmchen
14. *Quantum Criticality and Topology in Correlated Electron Systems*
    Seminar and Workshop: August 5 - 16, 2019 — 80 participants
    Scientific coordinators: A. V. Chubukov, D. L. Maslov, O. Vafek
15. *Challenges in Nanoscale Physics of Wetting Phenomena*
    Workshop: August 26 - 30, 2019 — 44 participants
    Scientific coordinators: S. Afkhami, T. Gambaryan-Roisman, L. Pismen
16. *Korrelationstage 2019*
    Workshop: September 16 - 20, 2019 — 109 participants
    Scientific coordinators: T. Giamarchi, C. Kollath, D. Luitz
17. *Dynamical Methods in Data-based Exploration of Complex Systems*
    Workshop: October 7 - 11, 2019 — 65 participants
    Scientific coordinators: H. Kantz, U. Parlitz, A. Pikovsky
18. *Fluid Physics of Life*
    Workshop: October 21 - 25, 2019 — 62 participants
    Scientific coordinators: K. Alim, E. Bodenschatz, G. Gompper
19. *Atomic Physics 2019*
    Workshop: November 19 - 22, 2019 — 76 participants
    Scientific coordinators: J.-M. Rost, O. Smirnova
20. *Gapless Fermions - from Fermi Liquids to Strange Metals*
    School: February 17 - 28, 2020 — 60 participants
    Scientific coordinators: S. Bhattacharjee, R. Moessner, A. Ramires

Virtual, hybrid, and open-air events following the outbreak of the Covid-19 pandemic:

1. *Real-time Dynamics in Strongly Correlated Quantum Matter*
   Virtual Workshop: April 8 - 9, 2020 — 270 participants
   Scientific coordinators: M. Dalmonte, M. Heyl, F. Piazza

2. *Mesoscopic Cold Atom Systems in and out of Equilibrium*
   Virtual Workshop: September 7 - 11, 2020 — 150 participants
   Scientific coordinators: D. Blume, T. Busch, A. Widera

3. *Dynamics, Criticality, and Universality in Random Quantum Circuits*
   Virtual Workshop: September 30 - October 2, 2020 — 197 participants
   Scientific coordinators: M. Gullans, J. Pixley, R. Vasseur, J. Wilson

4. *Winter School on Strongly Correlated Quantum Matter*
   Virtual School: November 30 - December 18, 2020 — 164 participants
   Scientific coordinators: M. Collura, M. Dalmonte, M. Heyl, D. Luitz

5. *Waiting for the Conference on Highly Frustrated Magnetism*
   Virtual School and Workshop: January 21 - 27, 2021 — 228 participants
   Scientific coordinators: C. Castelnovo, G. Chen, R. Moessner, R. Singh, F. Zhang

6. *Tensor Product Methods for Strongly Correlated Molecular Systems*
   Virtual Workshop: March 8 - 11, 2021 — 87 participants
   Scientific coordinators: Ö. Legeza, M. Reiher, R. Schneider

7. *Korrelationstage 2021*
   Virtual Workshop: April 15 - 20, 2021 — 253 participants
   Scientific coordinators: K. Everschor-Sitte, R. Moessner, F. Piazza, R. Valenti

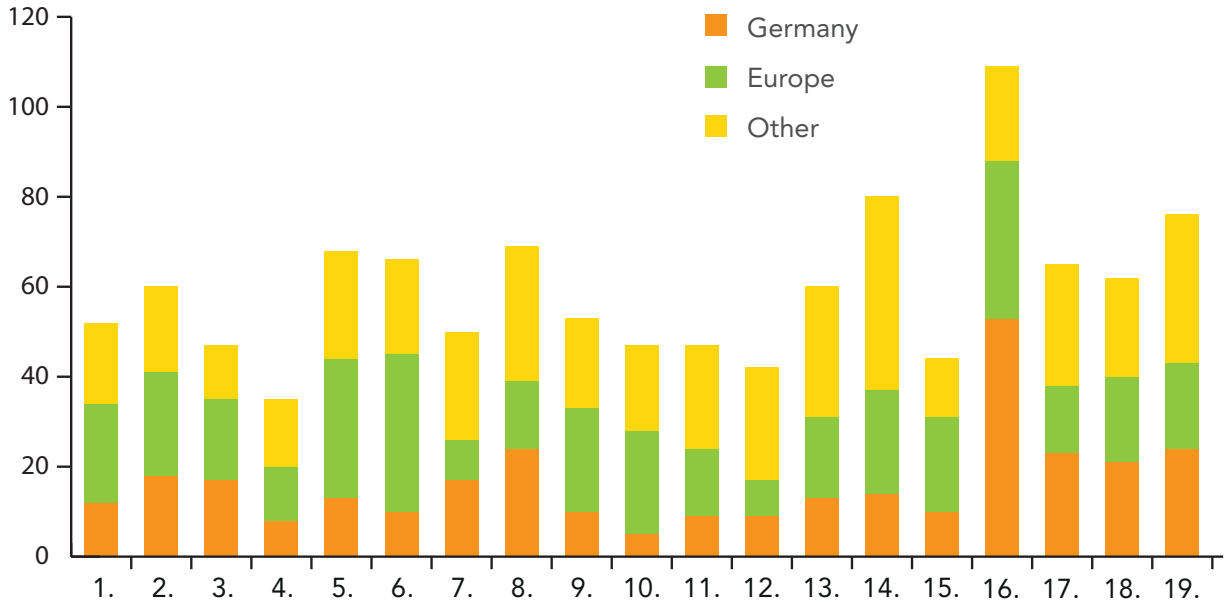
8. *Random Matrix Theory and Networks*
   Virtual Workshop: June 7 - 18, 2021 — 115 participants
   Scientific coordinators: F. L. Metz, I. Neri, I. Pérez Castillo

9. *Atomic Summer Camp 2021*
   Open Air Scientific Camp: July 26 - 30, 2021 — 42 participants
   Scientific coordinators: A. Buchleitner, T. Pfeifer, J.-M. Rost

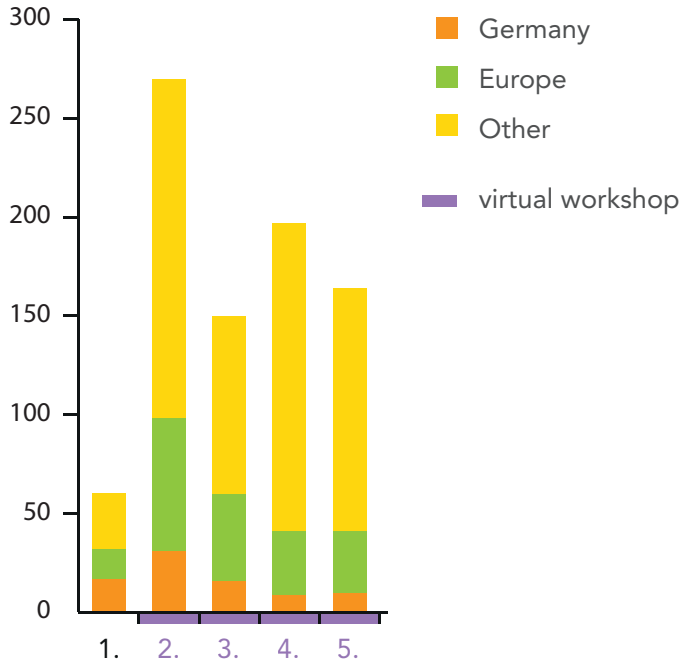
10. *Topological Materials: From Weak to Strong Correlations*
    Virtual Stay-in-Touch meeting: August 4 - 6, 2021 — 233 participants
    Scientific coordinators: S. Bühler-Paschen, T. Neupert, Q. Si

11. *Physical Biology Circle Meeting*
    Hybrid Workshop: September 13 - 15, 2021 — 133 participants
    Scientific coordinators: F. Jülicher, S. Rulands

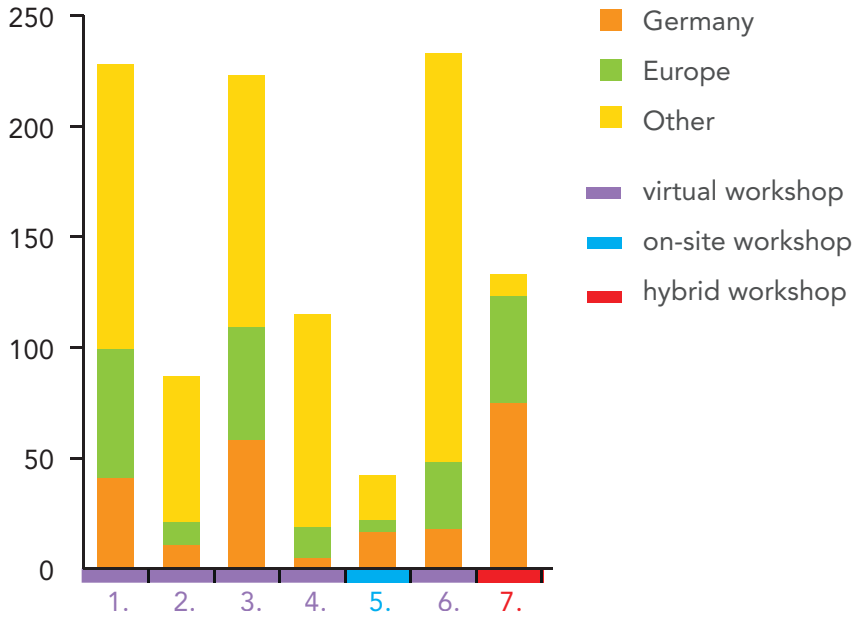
3.3.3 Workshop Participation



Number of Workshop/Seminar participants in the year 2019.



Number of Workshop/Seminar participants in the year 2020.



Number of Workshop/Seminar participants in the year 2021.

3.3.4 Workshop Reports

Anyons in Quantum Many-Body Systems, Workshop
Scientific coordinators: A. Bernevig, A. E. B. Nielsen, N. Regnault

The workshop Anyons in Quantum Many-Body Systems took place during the period January 21 - 25, 2019, and hosted about 50 participants from 14 different countries. The purpose of the workshop was to discuss opportunities and current challenges in the field of anyon research.
Anyons are a type of quasiparticles that can exist in two-dimensional systems. They are neither bosons, nor fermions, and they can have a charge which is only a fraction of the elementary charge. The fractional charge has already been observed in experiments, and theoretical studies show that different types of anyons can exist in a variety of models. The study of anyons requires new tools to be developed, and there is still much we do not know about them.
During the workshop there were several talks that covered a broad range of topics within anyon research. The talks were given by a mixture of researchers from different career stages and backgrounds. A portion of the invited talks were given by younger scientists who had recently obtained faculty positions. Most of the talks covered theoretical aspects, but there were also talks discussing recent experimental progress. The younger participants had the opportunity to present their work in two poster sessions, which gave rise to lively discussions. The program also included time slots for discussions among the participants to support the formation of new collaborations and further development of existing collaborations. On Monday afternoon Charles Kane gave a colloquium on "Symmetry, topology and electronic phases of matter". The talk was attended by a large number of people, including conference participants, institute members, and members from the neighboring institutes, and it was necessary to expand the seminar room to its largest possible size.
Anyon research is currently a very active research field. In the last decades, it has led to several discoveries of new types of behavior that quantum many-body systems can exhibit, and this series of discoveries is likely to continue in the years to come. There is also a lot of work to be done to understand fully these behaviors and what is needed for them to arise. The workshop contributed to the exchange and generation of ideas in this lively research field.

Atomic Tunneling Systems and Fluctuating Spins Interacting with Superconducting Qubits, Workshop
Scientific coordinators: C. Enss, M. Schechter, A. Shnirman

The workshop Atomic Tunneling Systems and Fluctuating Spins Interacting with Superconducting Qubits welcomed about 50 participants from 12 different countries to the Max Planck Institute for the Physics of Complex Systems. The purpose of the workshop was to discuss the physics of two-level tunneling systems and paramagnetic spin impurities, which are nowadays one of the major sources of decoherence in superconducting quantum circuits.
The workshop brought together experts in the fields of superconducting qubits, of two-level tunneling systems in amorphous solids, and of spin-glass physics. It aimed to enhance the exchange of ideas, to advance fundamental understanding, and to promote progress towards future applications in quantum computation and material science. Highlights of the workshop were several experimental and theoretical talks, which provided new and exciting results on the physics of two-level tunneling systems and paramagnetic spins in conjunction with superconducting quantum circuits. Beside oral presentations the workshop program included ample time for thorough discussions of particular aspects like the microscopic structure of the two-level systems in amorphous solids and their coupling to the microwaves. In addition, a very lively poster session enhanced the in-depth exchange of ideas and gave in particular the younger participants the opportunity to present their work.
On Monday afternoon John Martinis gave a colloquium on Fluctuations of Energy-Relaxation Times in Superconducting Qubits in which he showed convincingly the telegraphic time dependence of the energy relaxation of qubits due to the interaction with neighboring systems and discussed possible practical solutions like recalibrating large registers of qubits in the presence of jumps. The talk was attended by a large number of people, including conference participants and institute members.
In addition to the scientific program the participants of the workshop enjoyed a very nice guided tour in the Royal Castle and in the city of Dresden.
Overall the workshop contributed to the scientific exchange and generation of ideas in this lively research field and the participants expressed repeatedly that they found this workshop useful and enjoyable.

Image-based Modeling and Simulation of Morphogenesis, Focus Workshop
Scientific coordinators: K. Harrington, I. Sbalzarini

The inaugural workshop on Image-based Modeling and Simulation of Morphogenesis brought together some of the leading minds from diverse fields to discuss how computer modeling and bioimage analysis can contribute to understanding biological morphogenesis. Participants were researchers working at the molecular, cellular, tissue, and whole-organism scales using both theoretical and experimental approaches. Robert F. Murphy (Carnegie Mellon) presented a generative model of the cell. He drew upon graphical models as a representation for spatial relationships within the cell. He showed how multiple classes of generative models can be combined to reproduce cellular morphology in the computer both statically and dynamically. Alexis Pietak (Tufts) used computational modeling to reveal a simple and elegant mechanistic hypothesis to explain the spatial organization of regeneration in Planaria, highlighting a hitherto overlooked role of the nervous system. James Sharpe (EMBL Barcelona) presented a combination of theoretical and experimental work to explain mechanistically limb bud morphogenesis in mice. Throughout his presentation he drew upon the coupling of molecular-scale control, cellular coordination, and tissue mechanics. He emphasized the need to establish a morphological ordering of developmental stages that may not align with precise developmental times. Nicole Theodosiou (Union College) gave an experimentalist perspective on the exciting question: what is the morphological event that triggers the chirality of gut formation in skates? This left participants with a sense of curiosity about which biological questions can be answered with computational models, and which questions are only now beginning to be asked. On the final day, Henrik Jönsson (Cambridge, UK) presented an impressive body of work on computational morphodynamics in plants. He focused on the interplay between genetic regulation of stem cells, hormones, and mechanics of growth, highlighting key differences between animal and plant morphogenesis.
The workshop also saw impressive presentations by graduate students and junior scientists that were selected from the submitted abstracts. These included: A. Asadullah (IIT Bombay), M. Marin-Riera (EMBL), G. Dalmasso (EMBL), U. Günther (CSBD), K. Ishihara (mpi**pks**), K. Soans (MPI-CBG), L. Epstein (U Idaho), and A. Matyjaszkiewicz (EMBL).
It was particularly rewarding for participants from theoretical, computational, and experimental backgrounds to be able to discuss and exchange ideas in the time between the presentations. All participants

actively engaged in discussions often continuing in the evenings, which was an important part of the workshop concept. The modest size of the workshop greatly facilitated discussions by promoting a sense of community that enabled all participants, from graduate students to keynote speakers, to approach one another and to be involved actively.
At the conclusion of the meeting, we received very positive feedback and throughout the meeting new collaborations were established. Multiple attendees expressed interest in hosting the next iteration of the IMSM meeting in 2021. A number of the speakers also plan to write a perspectives paper that presents the next steps towards a mechanistic understanding of the centuries-old mystery of morphogenesis. On the whole, the meeting helped unify researchers working across physical scales, scientific disciplines, and methodologies. The collaborations and ideas that were established at IMSM19 will help nucleate a new community for image-based modeling in developmental biology.

Constrained Many-body Dynamics, Workshop
Scientific coordinators: M. Heyl, R. Moessner, F. Pollmann

The mpi**pks** workshop "Constrained Many-body Dynamics" took place March 26 - 30, 2019. Constraints form a constitutive element of many theories of matter, such as in gauge theories in high energy and correlated electron physics, frustrated systems in condensed matter physics, or a range of archetypal models in statistical physics. At present, the dynamics in many-body systems with constraints is seeing rapid progress, driven by developments both in theory and experiment. This workshop aimed to provide a platform for discussing and advancing these developments.
The invited speakers were chosen to cover a wide range of topics across different fields from both junior as well as established scientists. The talks mostly followed the main themes of the workshop including gauge theory and confinement dynamics (Michael Knap, Jürgen Berges, Alexey Gorshkov), quantum scars and fractons (Vedika Khemani, Maksym Serbyn, Michael Pretko, Olexei Motrunich), kinetically constrained systems (Stephen Powell, Mari Carmen Bañuls, Juan Garrahan), many-body localization (Maximilian Schulz, Evert van Nieuwenburg, Fabian Alet), dynamics in spin liquids, spin ice, and quantum magnets (Thomas Bilitewski, Yuan Wan, Elsa Lhotel, Christian Pfleiderer, John Chalker, Satoru Nakatsuji, Martin Mourigal, Shu Zhang, Nic Shannon, Attila Szabo), and nonequilibrium dynamics of quantum many-body systems (Pasquale Calabrese, Asmi Haldar, Anatoli Polkovnikov).
The main topic of the workshop represents an emerging field of research, as reflected also by the age structure of the participants with many PhD students as well as young postdocs. The talks were well attended and discussions among the participants were very lively, which was also stimulated by the extended discussion times and coffee breaks offered by the schedule. The two poster sessions, which in particular gave the young researchers the chance to present their results, were also well attended even though they were scheduled at a later time in the evenings. The discussions in front of the posters lasted until late in the night.

Bound States in Superconductors and Interfaces, Focus Workshop
Scientific coordinators: T. Domanski, K. Franke, R. Zitko

The focus workshop Bound States in Superconductors and Interfaces took place from 8th till 10th April 2019, and hosted 66 participants from 20 countries. Its main purpose was to exchange information on the current realizations, challenges, and future perspectives of electronic bound states inside the superconductor energy gap at impurities, interfaces with superconducting reservoirs, and various hybrid nanostructures. The associated quasiparticles are presently of considerable importance because they enable unique phenomena, such as long-lived qubits, evolution of discrete sub-gap states into topologically non-trivial bands hosting Majorana-type endmodes, and allow for experimentally controllable spectroscopy of correlated many-body states.
The workshop brought together the leading experts, both in experimental and theoretical studies in this field. The talks discussed realizations of the subgap states in various materials and devices, their detection in hybrid quantum dots and/or artificial quantum impurities embedded in Josephson- and Andreev-type junctions, spectroscopy of the bound states in semiconducting nanowires, carbon nanotubes, hybrid superconductor-semiconductor quantum dots, gate-tunable studies of the sub-gap Kondo regime, and many other related issues. Theoretical lectures addressed the correlation effects, nonlocal processes, dynamic phenomena, and properties of exotic mutations of the bound states in topological materials.
A comprehensive overview of the phenomena relating to the existence of defects/impurities in superconductors was delivered by Alexander V. Balatsky (NORDITA), emphasizing the recently discovered Dirac materials and exotic types of electron pairing with an odd symmetry. His colloquium was attended

not only by participants of the workshop but also by members of the Max Planck Institute and other neighboring research institutions. Invited lectures were given by internationally recognized experts in experimental and theoretical studies. Several younger scientists contributed their brief talks on important problems related to the bound states. During the first day of the workshop a poster session with 30 presentations was organized. Individual discussions between participants gave an opportunity to exchange ideas and might stimulate ongoing and establish new collaboration projects, leading to developments in this research field. Overall, the workshop provided a pleasant atmosphere with lively discussions.

BiGmax Workshop on Big-data-driven Materials Science, Workshop
Scientific coordinators: T. Bereau, J.-M. Rost

Scope:
Materials science is entering an era where the growth of data from experiments and calculations is expanding beyond a level that is properly processable by established scientific methods. Dealing with this big data is not just a technical challenge, but much more: it offers great opportunities. Big-data analytics will revolutionize new material discovery and will make the successful search for structure-property relationships among multiple length and time scales possible. This workshop represented the annual meeting of the Max Planck Network on Big-data-driven Materials Science.
Structure and Special events:
Representatives of all projects reported on progress of their research; in addition there was a poster session. Special events included two tutorials on Deep Learning and Compressed Sensing, respectively. There was also a special break-out session with different discussion/question rounds without the PIs (during the PI meeting) which was received very well by the junior participants.
Important participants:
As an internal workshop of the network, there were only two external invited speakers: Prof. Anatole von Lilienfeld (U Basel, CH) and Dr. Alpha Lee (U Cambridge, UK). Both presented impressive accounts of data-driven work on small-molecule chemistry using machine learning techniques, partially far away from the well-known concepts.
Scientific newcomers:
One notable newcomer was present: Markus Kühbach, BiGmax scientific advisor for software engineering. Kühbach stressed the different roles he represents within the network, the help he could provide in terms of clean, well-built software. He also mentioned recent guidelines on FAIR data infrastructure - a timely initiative that is bound to take a larger role within BiGmax.
Summary:
The workshop this year helped bring the experimentalists and the theoreticians closer together. We have seen a lot more interactions between members, as well as a common language and framework shaping up throughout the talks, suggesting more coherence in the network. Smaller discussion rounds focused on technical topics helped students and postdocs exchange ideas more intensively. The invited talks were regarded very positively as inspiring research directions. Overall we have received positive feedback from various members of the network.

Quantum Ferromagnetism and Related Phenomena, Workshop
Scientific coordinators: D. Belitz, M. Brando, A. Huxley

This international workshop was held at the **mpipks** from May 6 to May 10, 2019 and was supported by the Deutsche Forschungsgemeinschaft (DFG). The main purpose of the workshop was to discuss recent advances and open problems in the field of quantum ferromagnetism, with a focus on metallic systems. In addition to the ferromagnetic quantum phase transition proper in both clean and disordered systems, topics covered included competition between different magnetic phases, and the interplay between magnetism and superconductivity.
There were 69 participants - including 44 invited speakers - from 15 European and non-European countries with a balanced mixture of well-established experts in the field and promising young scientists who were chosen to form a diverse group with respect to gender, seniority, and national origin. Specific topics covered included phase diagrams and types of quantum phase transitions (Taufour, Baenitz, Aronson, Friedemann, Kotegawa, Pourret, Wysokinski, von Löhneysen, Stewart), low-dimensional systems (Kliemt, Yuan), the interplay between ferromagnetism and superconductivity (Ishida, Geibel, Braithwaite, Aoki, Butch, de Visser, Knebel, Grosche, Mercaldo), spin dynamics (Janoschek, Niklowitz, Pfleiderer), effects of disorder (T. Vojta, Baumbach, M. Vojta, Sales, Schroeder, Uemura, Fritsch), Lifshitz transitions (Pfau, Betouras), magnetism in exotic fermion systems (Kirkpatrick, Rost, Chubukov), competing mag-

netic orders (Hayden, Krellner, O'Neill, Krüger), anisotropies (Sokolov, Green, Jesche), spin liquids (Perkins). A related topic covered was the quantum antiferromagnetic transition in a two-dimensional metal (Lee). In addition, A. Chubukov delivered a colloquium on superconductivity induced by quantum critical magnetic fluctuations.
The mpi**pks** provided an ideal environment for stimulating scientific discussions and an exchange of ideas between these various fields. Many of the participants commented to us that they found the meeting enjoyable and of benefit for their research and initiating future collaborations. This was also stimulated by alternative activities like the barbecue dinner and the hiking tour in the Saxon Switzerland National Park.
In addition to the talks, 22 posters were presented, mostly by PhD students and postdocs. Both the talks and the poster session were well attended (by more than 80% of the workshop participants) and also by several colleagues from neighbouring institutions (TU Dresden, MPI-CPFS or IFW). This led to lively discussions. Even on Friday, the leaving day of the workshop, more than 60% of the participants attended the last sessions. Feedback from the participants, both during and after the workshop, was very positive.

Synthetic Topological Matter, Workshop
Scientific coordinators: J. Meyer, G. Refael, K. Shtengel

Topological phases of matter have been a focus of much theoretical and experimental attention in recent years. In the usual condensed matter setting, physical realizations of such phases are often constrained by the existence or availability of materials with the desired band structure or desired interactions. While much progress has been made in finding and fabricating new materials and combining them to achieve the desired physics, a new, alternative approach has also recently emerged: namely, to use other systems to mimic the sought-after topological properties. These include cold-atom systems, in which internal degrees of freedom can be manipulated to create synthetic dimensions and synthetic gauge fields, driven Floquet systems, with a multi-frequency space also providing the notion of an extra dimension, multi-terminal Josephson junctions, in which superconducting phases can be used to mimic the Brillouin zone of a topological materials, and many others. In addition, topological phenomena have been discovered in classical systems including coupled mechanical oscillators, judiciously constructed electric circuits, and even in water waves.
The one-week workshop Synthetic Topological Matter gathered a broad range of researchers seeking to expand the reach of topological physics beyond intrinsic material properties to a variety of such new systems. Participants from many leading institutions across the globe gave presentations on their research during the workshop. In addition, Dr. Sebastian Huber (ETH) presented a colloquium on mechanical topological systems. Underscoring the vibrant nature of the field, a significant fraction of the speakers were junior faculty or postdocs. Furthermore, junior participants, including a number of graduate students, presented posters on their work in two well-attended poster sessions.
The workshop brought together experimentalists and theorists working on very different systems, which realize emergent topological properties. While similar sets of underlying principles are at play in these widely different systems, one of the important goals of the workshop was to stimulate exchanges between separate fields, in particular, between the condensed matter, cold atom, and quantum optics communities, broadly defined. After all, different systems allow for different probes to be used, and while addressing some questions may be difficult or even impossible in some settings, it might be quite feasible in others. Furthermore, understanding how topological phenomena could be engineered and probed in a wide variety of systems such as photonic systems, mechanical systems, as well as systems of excitons and cold atoms significantly enhances the range of interesting phenomena one can attempt to observe in this rich variety of settings. Specifically, several talks addressed the utility of driven, optical, and superconductor-based systems for exploring thermalization and many-body localization. The workshop has allowed many researchers seeking to implement topological control in such a rich variety of systems to exchange ideas across and beyond their respective subfields, further stimulating research in this active field.
The young average age of the participants, the large number of prominent researchers that accepted our invitations, the breadth of the topics presented, as well as an excellent support infrastructure provided by mpi**pks** contributed to a successful workshop.

Engineering Nonequilibrium Dynamics of Open Quantum Systems, Workshop
Scientific coordinators: A. del Campo, M. Plenio, A. Rahmani

The international workshop on Engineering Nonequilibrium Dynamics of Open Quantum Systems (DYN-

QOS) took place during the week June 17 - 21, 2019. The focus of the event was on the quantum dynamics of open systems - realistic systems in contact with a surrounding environment - as well as controlled evolution. Fifty senior and junior scientists from sixteen countries participated in the workshop. The scientific program comprised a total of 33 invited and contributed talks, including a colloquium by Susana Huelga on the applications of open quantum systems to metrology and precision sensing.
Several speakers reported significant advances in the field. To name a few, Howard Carmichael presented results on the experimental control of individual trajectories in continuously monitored quantum systems, a milestone in the study of quantum measurements. Eric Lutz reported experiments on the reversal of the arrow of time, and Fedor Jelezko discussed the progress on the use of nitrogen-vacancy centers for precision measurements. On the theory side, Sahar Alipour presented a universal description of the evolution of quantum systems correlated with the environment. Luis Pedro Garcia-Pintos discussed the possibility that an observer controls symmetry breaking by monitoring. Other important results reported include shortcuts to adiabaticity in complex systems, ultimate bounds on decoherence, noisy quantum metrology, and boundary time crystals.
In addition to the oral presentations, numerous informal discussions took place, which helped with generating ideas and starting or renewing collaborations. Finally, the poster sessions included 15 high-quality contributions, stimulating lively discussions.

Bio-inspired Optics and Photonics - From Metamaterials to Applications, Focus Workshop
Scientific coordinators: H. Hölscher, M. Kolle

Workshop Philosophy:
Many of the physical concepts and working principles of technologies that control light are intriguingly similar to nature's light manipulation approaches, while others are extremely different. Long before humans invented lenses, light-guiding fibers, light-emitting active matter, photonic crystals, and various other light management strategies, these concepts had already evolved in many non-related species in nature. Animal vision, the ability of plants to harvest energy from sunlight, the dynamic camouflaging ability of cephalopods and chameleons, and the stunning color displays of butterflies, peacocks, and fruits have evolved to address the organisms' specific light manipulation requirements enabling individual and species survival. Many of the functional criteria and constraints which biological optical systems have evolved to satisfy and comply with are also highly relevant in human needs for light control. Consequently biological optics provides useful inspiration for light manipulation and optical device design.
Workshop scope and community:
The primary focus of the Workshop "Bio-inspired Optics and Photonics: From Metamaterials to Applications" (BioOpt 2019) organized by Hendrik Hölscher (KIT) and Mathias Kolle (MIT) was the question "What can be learned from biological optical materials and systems to guide the design of synthetic or bio-derived optical materials and devices within application and resource-imposed constraints?". Experts from the fields of optics, biology, materials science and engineering, physics, genetics, chemistry, medical engineering, and arts met to discuss the state-of-the-art, update each other on recent achievements and scope out future interdisciplinary projects and collaborations.
Workshop attendance and key contributors:
The workshop featured 22 invited presentations, 15 contributed talks, and 7 poster contributions delivered by renowned leading experts, outstanding early-career research group leaders, and highly-talented PhD students from 15 countries. Silvia Vignolini (University of Cambridge) gave the introductory talk providing a beautiful account of the opportunities arising through successful transfer of fundamental research insights and practical implementations of bio-inspired light manipulation strategies with bio-derived cellulose architectures. A pleasant highlight of the first day was the colloquium talk on "Biological photonics" given by Peter Vukusic (University of Exeter), who presented an informative and captivating review of the field. In addition, Peter demonstrated how well-conceived and entertaining science outreach presentations for children can stimulate and amplify their enthusiasm for natural sciences. Peter's presentation was followed by the talk "From mimesis to biomimetics: towards 'smarter' art" by Franziska Schenk (University of Birmingham), who approached the topic from the viewpoint of the arts. Later in the week, the two organizers presented a review of the topic of the workshop in a public evening talk. It was very well received by a general audience from Dresden and surrounding areas, despite of the hot summer day. During the workshop, young researchers at different stages of their careers (Masters and PhD level to junior faculty) had the opportunity to showcase their studies on the photonics of butterflies, spiders, hummingbirds and on synthetic photonic materials in presentations and posters (many of which were among the highlights of the conference) and to exchange ideas with seasoned experts during

the sessions. Organized social events and spontaneous evening outings to sample the Dresden nightlife allowed for socializing across career levels. Several of the talks were given by researchers who are part of Dresden's vibrant academic landscape, including Andreas Fery (Leibniz Institute for Polymer Research Dresden), Moritz Kreysing (Max Planck Institute of Molecular Cell Biology and Genetics, Dresden) and Igor Zlotnikov (B CUBE, Technische Universität Dresden). The workshop concluded with two invited presentations that focussed on examples of emerging applications for bio-inspired optical materials. Radislav Potyrailo (GE Global Research) presented bio-inspired gas sensors and Raúl Martin-Palma (Universidad Autonóma de Madrid) showed that biophotonics could help with pest control.
Workshop outcomes:
The workshop provided a unique opportunity to review and evaluate the current progress in the highly interdisciplinary field of biological and bio-inspired optics and photonics. Many of the presentations provided a clear account of the conceptual and technological insights that can be gained from a deeper understanding of nature's strategies to control light and to form optical materials. The breadth of emerging engineered bio-inspired optical materials and technologies captured in this workshop provided strong evidence that many lessons can be learned by taking a closer look at nature and - more importantly - provided clear evidence of how such lessons can be translated to technology development. The local organization was perfectly handled by Jenny Kuehne and the other members of the mpi**pks**. All participants truly enjoyed this workshop and are grateful to the mpi**pks** for providing the infrastructure and generous financial and logistical support.

Granular and Particulate Networks, Focus Workshop
Scientific coordinators: D. S. Bassett, K. E. Daniels, M. A. Porter

The emphasis of our focus workshop was to address the key questions in granular and particulate networks through a balance of methods-oriented and application-oriented talks across experiment, computation, and theory. Our speakers (ranging from early-career to established researchers) were Erin Koos, Marc Timme, Silke Henkes, Jonathan Kollmer, Antoinette Tordesillas, Andrea Liu (colloquium), Xiaoming Mao, Michael Engel, Anton Souslov, Dawa Seo, Erin Teich, Carl Dettmann, Eleni Katifori, Konstantin Mischaikow, Kabir Ramola, Katie Newhall, Zackery Benson, Estelle Berthier, Giovanni Petri, Matthias Schröter, and Jürgen Kurths.
By having group-wide discussions roughly every two talks, all newcomers were able to hear (and contribute to) the scientific conversation, rather than being excluded from discussions in small groups. Additionally, having NSF travel funds available led to a significant number of early-career researchers presenting talks and posters. One of the early-career researchers commented on how the long, communal tables further encouraged conversations across disciplinary and career-stage boundaries.
We also held a scientific communication panel - with moderator Karen Daniels and panelists Zoe Budrikis, Mason Porter, and Olga Shishkov - whose wide-ranging topics included pressures that arise from open-access and high-impact publishing, developing writing skills, and opportunities for communicating with non-specialist audiences.
A key scientific outcome is that there are network techniques that are ripe for use, and that participants gained access to information and connections to start new avenues for analysis of computational and experimental data. The final discussion led to a plan to have a second workshop in two years' time, as these new research directions start to bear fruit. We have created a resource page to share some of the key papers and methods that were mentioned during the course of the workshop. We are in touch with the American Physical Society Division on Soft Matter Physics (via organizer Karen Daniels) about plans for a Short Course at the 2021 APS March Meeting on topological data analysis in granular and particulate networks. Mason Porter has volunteered to be lead organizer, and core participant Giovanni Petri has also indicated potential willingness to be a lecturer.

Microscale Motion and Light, Workshop
Scientific coordinators: T. E. Mallouk, R. Marschall, J. Simmchen

The main focus of our workshop "Microscale Motion and Light" was the relationships between light as a driving force for micromotors, the optical influences, and the photocatalytic reactions that dictate the boundary conditions as energy suppliers. Additional value was conveyed to this meeting by discussions of microscopic techniques such as differential dynamic microscopy and super-resolution microscopy, or the use of enhanced learning techniques to improve motion on the microscale.
Participants consisted of an international mixture of physicists, chemists, engineers, and biologists. Organizer Thomas Mallouk and his long term collaborator Ayusman Sen, for the longest time both professors

at Penn State University, are two of the founders of the field of light-driven motors and contributed their experience and knowledge to create truly interdisciplinary discussions. The photochemical expertise was represented among others by Bettina Lotsch, who presented novel materials ranging from covalent organic frameworks to carbonitrides. Insights in particle-based photocatalysis were given by Frank Osterloh, who lectured on the physico-chemical differences in photocatalysis and photosynthetic processes. Alejandro Baeza spoke about light-responsive nanocarriers for anti-tumor drugs, bringing biological insights and applications to the discussion. More entertaining insights on the potential of organic dyes in efficient photocatalytic reactions were given by Burkhard König. Local expertise from Saxonian universities was represented for example by Larysa Baraban from TU Dresden and Frank Cichos from Leipzig University. The beautiful mpi**pks** campus was embraced enthusiastically by several accompanying families who quickly occupied the table tennis table and the kicker. Everybody complimented the canteen on the great culinary delicacies served day after day.
How did scientific newcomers present themselves:
However, the workshop would not have been the lively, active dialogue it was without all the international young participants from different European countries, China, Brazil, Gaza, and Hawaii. Many of the speakers were at the PhD or postdoc levels and gave direct insights into experimental realizations and progress. The youngest speaker, from the University of Northern Arizona, was just about to start his PhD program. During the coffee breaks and on Tuesday evening, 16 PhD students and postdocs presented their work in posters and the best two presentations were awarded prizes from the Royal Society of Chemistry.
The scientific results of the workshop in the broader sense:
Scientifically, the workshop and all the enthusiastic speakers ensured that everybody learned something new. This input of knowledge started many interdisciplinary discussions during the coffee breaks which will hopefully be continued on a frequent basis. The workshop led to enhanced interactions between the two fields, first results had been presented by Prof. Lotsch with a collaboration with the Sitti group, but new connections were also made during the workshop. These will enhance the analytical quality of micromotors papers and offer some new applications for their materials to the photochemists. A strong focus on light and microscopic interactions ranging from Leipzig to Prague was identified and will lead to closer interactions in the future. Additionally, all participants were able to gain an impression of the active exchange that the mpi**pks** workshops can foster and a few of the participants are considering applying for the mpi**pks** guest program. It was not only the well-connected Dresden scientific landscape that contributed to this, but also the natural beauty of the Bastei, the destination of the afternoon excursion.

Quantum Criticality and Topology in Correlated Electron Systems, Seminar and Workshop
Scientific coordinators: A. V. Chubukov, D. L. Maslov, O. Vafek

The main focus of our workshop was on new developments in strongly correlated electron systems and on the interplay between electron correlations and topology. Invited talks were given by world leaders in the field of condensed matter physics, including Andrei Bernevig (Princeton University), Claudia Felser (MPI for Chemical Physics of Solids), Liang Fu (MIT), Aharon Kapitulnik (Stanford University), Andrew Mackenzie (MPI for Chemical Physics of Solids), Yuji Matsuda (Kyoto University), Roderich Moessner (mpi**pks** Dresden), Subir Sachdev (Harvard University), and others.
At the same time, younger participants had ample possibilities to present their work. Several invited and contributed talks during the workshop week were given by postdocs and graduate students, including Eli Fox (a PhD student at Stanford), Jian Kang (a postdoc at Florida State University), Avraham Klein (a post-doc at the University of Minnesota), and Julia Link (a postdoc at Simon Fraser University). There were also two sessions with blackboard talks during the seminar week, in which more students and postdocs gave their presentations. Finally, all junior participants presented posters during the workshop week.
Several new and important results were presented at the workshop, including an observation of ferromagnetism in twisted bilayer graphene, quantization of thermal Hall conductivity in a spin-liquid candidate material, theoretical explanation of the linear T resistivity in $SrRu_2O_4$, new results on time-reversal symmetry under strain in $SrRu_2O_4$ and theoretical scenarios for the observed behavior, an exactly solvable SYK model of a bad metal, a proposal for the mechanism behind a recently discovered giant Hall thermal conductivity in high-T_c cuprates, and others. Each of these results was thoroughly discussed by the participants. We are sure that discussions and collaborations started during this workshop will lead to new important results in the immediate future.

Challenges in Nanoscale Physics of Wetting Phenomena, Workshop
S. Afkhami, T. Gambaryan-Roisman, L. Pismen

The understanding of wetting presents formidable challenges due to the multi-scale nature of the problem in which macroscopic behavior can be directly related to non-trivial microscopic and/or mesoscopic interactions. Probing wetting phenomena down to the nano-scale can help to understand the physical processes involved in the interaction of a liquid with a solid surface. This became therefore the center of recent intense activities with the advent of new nano-materials. This multidisciplinary workshop focused on the challenges and new opportunities in modeling, experimentation, and computation of wetting phenomena on small scales. Building upon new developments in the past decade, this workshop brought together mathematicians, engineers, and physicists to present their state-of-the-art theoretical and experimental techniques. Examples of applications that were discussed during the workshop include wetting phenomena in micro- and nanofluidic systems, the process of ice formation on substrates, heat transfer enhancement, and flows in porous media. New concepts and approaches on superhydrophobic and textured surfaces, electrowetting, drying of suspensions on surfaces, self-assembly of particles at contact lines, evaporation and solidification of liquids on substrates, and spreading and wetting of droplets were extensively discussed. We hope that the above interdisciplinary exchanges will help setting up future directions, providing new priorities for the mathematical modeling and computation as well as physical experiments.
Various groups of scientists from across Europe, the United States, and Asia were present at the workshop, representing 13 countries. There were 42 invited and contributed talks amongst whom were invited speakers at the forefront of research, from modeling and analysis: Jens Eggers (University of Bristol, United Kingdom), Uwe Thiele (University of Münster, Germany), and Stephen Wilson (University of Strathclyde, United Kingdom); from large scale computations: Nikolaus Adams (Technical University Munich, Germany), Gustav Amberg (KTH / Södertörn University, Sweden), and Stéphane Zaleski (Sorbonne Université, France); and from experiments: Daniel Bonn (University of Amsterdam, Netherlands), Paul Steen (Cornell University, USA), Laurent Limat (Sorbonne), and Glen McHale (Northumbria University, United Kingdom). The colloquium seminar was given by the prominent scientist and researcher, David Quéré (ESPCI & École polytechnique, France), on the topic of special dynamics of water pearls.
A number of presentations were given by junior researchers and young assistant professors, such as Roland Knorr, researcher from the Max Planck Institute of Colloids and Interfaces, who reported on intracellular wetting regulating autophagic degradation of fluid cargoes, Ugis Lacis, researcher from the KTH Royal Institute of Technology, who presented phase field simulations matched with molecular dynamics for no-slip substrates, Hyoungsoo Kim, assistant professor from the Korean Advanced Institute of Science and Technology, who discussed solutal Marangoni flows from large to small scales, and Ofer Manor, assistant professor from the Israel Institute of Technology, who talked about deposition patterns of colloidal particles. A number of PhD students also had the opportunity to present their research at the workshop. The workshop provided a platform for the students to further develop a common understanding of the challenges involved in wetting problems.
All the participants expressed their positive view of the workshop and found it to be very interesting; this resulted in many intriguing and instructive discussions. The workshop provided a unique opportunity to foster and encourage synergetic discussions on new modeling, experimental, and computational approaches to wetting phenomena on nanoscales and helped to establish new opportunities in multiscale modeling for bridging the dynamics of the contact line at the mesoscopic length scales to the macroscopic flows. We believe that the workshop was widely successful in allowing stimulating interactions between researchers with various backgrounds, providing a basis for future developments in the direction of nanoscale physics of wetting phenomena. Following the success of the workshop, we will also publish a topical issue as part of the European Physical Journal - Special Topics including some contributions to the workshop.

Korrelationstage 2019, Workshop
Scientific coordinators: T. Giamarchi, C. Kollath, D. Luitz

The international mpi**pks** workshop Korrelationstage 2019 was held from 16 to 20 September 2019. The aim of the workshop was to bring together the international community working on strongly correlated systems in the broader context of condensed matter and ultracold atomic systems. The meeting is a traditional conference organized biannually at mpi**pks** since 1995, and has as one of its central objectives the identification and promotion of the next generation of researchers in the field.
This year's instance put a particularly strong focus on this goal by selecting junior researchers who do not

yet have a permanent faculty position as invited speakers (47 talks). This selection of young speakers was extended by 4 well-established experimental keynote speakers: Claudia Felser (MPI-CPFS), Michael Köhl (U Bonn), Luca Perfetti (École Polytechnique), and Jean-Marc Triscone (U Geneva). The workshop Colloquium on Monday was given by Christian Rüegg (PSI). All other participants including the senior researchers (out of a total of 115) were given the opportunity to present their research in poster form (58 posters in total). In addition several well-established members of the community served as chairs for the sessions.
The selection of the invited speakers was done in a community effort using a new nomination system. A large number of colleagues (consisting in particular of attendants of previous events) were asked to nominate junior researchers for talks. This call was well-received and the organizers tried to make a balanced selection of the most promising candidates.
The somewhat unusually strong spotlight on non-tenured invited speakers was generally well-appreciated by the participants of the conference and due to the competitive selection of the speakers, the quality of the presented talks was very high. In addition, since most senior colleagues presented their work in the form of posters, the poster sessions were well-attended and led to lively and in-depth discussions which continued over dinner.
Further discussions and collaborations in smaller groups were enabled by the reservation of 6 discussion rooms for the participants.
In summary, the conference was a very successful meeting during which many interesting ideas were exchanged, hopefully leading to new connections and collaborations within the community. Several particularly promising new developments in the areas of tensor network methods and artificial neural networks as well as in the area of quantum computing were discussed and sparked strong interest among the participants.
The scientific coordinators are very grateful to the visitors program and in particular to Katrin Lantsch for the outstanding organization of the workshop. Her professional, experienced, and always friendly attitude towards everyone was highly appreciated by all participants and guaranteed a smooth and very successful workshop.

Dynamical Methods in Data-based Exploration of Complex Systems, Workshop
Scientific coordinators: H. Kantz, U. Parlitz, A. Pikovsky

The main focus of the workshop was on inverse problems in the dynamics of complex systems: what can one say about the composition and operation of a complex dynamical system from observations of the system? This is a truly interdisciplinary research field with numerous applications in physics, engineering, environmental and life sciences, and in social systems. Big Data is now becoming a widely used and publicly appreciated concept for dealing with complex systems, and we are experiencing rapid development of novel statistical approaches for the analysis of huge data sets from complex systems of different nature. However, in many applications, complex systems are intrinsically nonlinear, and their complexity comes quite often not from random, noisy inputs, but from dynamical nonlinear interactions. This makes the approaches based on dynamical reconstruction of complex data sets extremely relevant. The main aspects addressed in invited and contributed presentations were: general concepts of machine learning and data assimilation from the viewpoint of statistical physics; discovering complex dynamical networks and partial differential equations from data; concepts of synchronization in data analysis; operator theoretic methods in network identification; applications to particular problems in engineering, neurosciences, physiology, climate research, and the social sciences.
Generally, we believe that there was a good balance between theoretical and experimental talks and that an appreciated aspect of the workshop was the opportunity for each participant to interact with members of different communities: experimentalists, theoretical physicists, and data science specialists.
The mpi**pks** colloquium talk by Prof. Ott, one of the world-leading specialists in nonlinear dynamics, contributed to placing the recently developed methods of reservoir computing in a broader perspective of complex system theory. When arranging the schedule of the workshop, we allocated many oral presentations to young researchers, and these gave a very lively picture of particular developments and applications. Two poster sessions were a place of intensive discussions. Finally, the friendly environment at the mpi**pks** 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 novel directions such as machine learning as well as of advances in more traditional methods 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.
We are grateful to the DFG for the additional financial support which made possible a full support of overseas speakers. Special thanks go to mpi**pks**, its team of secretaries, and especially to Mandy Lochar for her support and a very professional and efficient organization.

Fluid Physics of Life, Workshop
Scientific coordinators: K. Alim, E. Bodenschatz, G. Gompper

Fluid flow-based transport of cargo (dissolved substances, like oxygen, signaling molecules, and waste products, particulates, etc.) is a ubiquitous and essential process in life. Once the length scales exceed a few microns, the time scales for diffusive transport of just about anything become prohibitively long. Yet, flow not only beats the diffusion barrier, but it also allows for directed transport and timed delivery of cargo. Without fluid flow, life as we know it would not exist.
Fluid flow is a key player for the function and behavior of biological systems. The dynamics of blood flow, microbiota, cerebral fluid, but also cytoplasmic streaming, flows in algae and bacterial colonies, and in cells, are challenging problems since fluid flows are inherently coupled over many spatial and temporal scales, and the fluids themselves have suspended particulates (possibly active), are viscoelastic, couple strongly to the walls, or take place in geometrically complex spaces. In biological systems, the dynamics of fluid flow can be very complex as flows impact morphology, biological signaling, and also the dynamics of development. Yet, except for a few very promising glimpses into the role of flows, often our knowledge is limited to the fact that fluid flows are important, but fundamental insights into the principles of how flows interact with living systems are missing.
The workshop was timely because tremendous advances in imaging as by light sheet microscopy, fluorescent nano-tubes and real-time MRI, but also in biology by opto-genetics are emerging. These technical advances in physics and biology open up entirely new possibilities for the development of a theoretical understanding of the complexity of the flows to be understood, from nanoscales to large scales. The workshop aimed and succeeded at forging a new research field by bringing together theoretical physicists (R. Golestanian, F. Jülicher, D. Kelley, M. Wilczek), applied mathematicians (J. Dunkel, M. Roper, M. Shelley), experimental physicists (K. Drescher, R. Goldstein, K. Jensen, M. Kreysing, M. Sano, A. Zidovska), as well as biologists (R. Faubel, N. Jurisch-Yaksi) and physiologists (A. Siekmann). This fostered intense discussions of the fundamental principles of how flows govern living systems.
The small size of the workshop, with about 60 participants, allowed a vivid exchange of ideas, particularly between young and experienced scientists. This exchange of ideas, but also mentoring, was further fueled by very lively poster sessions as well as the three-hour timeslots for discussions in the afternoon each day. Taken together, the workshop succeeded at its ambition to forge a new research field as recognized by all participants, to the delight of the participants and the organizers.

Gapless Fermions - from Fermi liquids to strange metals, School
Scientific coordinators: S. Bhattacharjee, R. Moessner, A. Ramires

This winter school was in some ways a pioneering effort for the organisers, who had thus far mainly been involved in either shorter formats, or more extended versions of schools.
Its aim was to bring students from all over the world up to the cutting edge of research into, essentially, metals of various types. The students, numbering about 45 in total, were selected from a large pool of applicants. We were somewhat, but luckily not massively, oversubscribed.
The first week had two points of emphasis. One was the experimental situation, for which the speakers were asked to give an introduction to their methods as well as their most salient results. These talks turned out very different in character, playing to the various strengths of the speakers. Joe Checkelsky was extremely engaging, Amalia Coldea provided copious experimental results, and Veronika Sunko had prepared an excellent introduction to ARPES specifically for this occasion. The other can be described as the past (R. Shankar), present (I. Herbut), and future (S.-S. Lee) of metallic theories. Again, these talks were all excellent in their own ways, and were attended even by established experts in the field.
The second week again had a number of broad overviews (M. Vojta on Kondo etc.; J. Schmalian on transport), as well as targeted presentations (e.g. W. Metzner on FRG, and an outstanding presentation by A. Georges on DMFT and by T. Giarmarchi on bosonisation).
It was a pleasure to see how various topics were treated by the different speakers in often complementary ways.
On a broader note, we found attendance was an issue initially, and we had to exert some pressure to stop students from disappearing from the talks given by less prominent speakers.

We found that speakers were happy to stay for several days, which made for a wonderful and stimulating atmosphere.

Real-time Dynamics in Strongly Correlated Quantum Matter, Virtual Workshop
Scientific coordinators: M. Dalmonte, M. Heyl, F. Piazza

The mpi**pks** workshop Real-time dynamics in Strongly Correlated Quantum Matter took place from 8 to 9 April 2020. Besides the topical focus on exploring new avenues in characterizing and probing the real-time dynamics of quantum matter far from equilibrium, the virtual format of the workshop was designed to provide a platform for reinforcing scientific exchange during the present times characterized by severe travel constraints.
The short workshop was organized in four two-talks sections in the afternoons, each followed by a longer virtual discussion session. The 30 minute discussion slots were organized so as to provide two types of virtual rooms: A PhD-students-only room where students could discuss with the speakers, and, in parallel, 20 further rooms for free, self-organized discussions. Among those, two were featuring one or two chairpersons guiding and triggering the discussions.
The senior speakers were among the leading scientists performing cutting-edge research within the scope of the workshop. Also a large number of senior and prominent persons joined as participants from all over the world. We had 260 signed-up participants with actual attendance fluctuating around 230 on the first day and 200 on the second day. Half of the speakers were young researchers who gave sharp talks despite the novel format and very large audience.
During the discussions with the speakers in PhD-students-only rooms, students were very active, which resulted in very lively discussions. During this pioneering effort several formats and solutions had to be put to the test. A positive note is surely the large resonance in terms of participant number. A crucial but challenging aspect with virtual workshops is to trigger interactive discussions. We introduced a format for interactive virtual discussions in the present workshop with several features which proved to work, like student-speaker and chaired self-organized rooms. An online survey with many participants has been completed. The overall feedback was extremely positive and several interesting suggestions for the future have been gathered.

Mesoscopic Cold Atom Systems in and out of Equilibrium, Virtual Workshop
Scientific coordinators: D. Blume, T. Busch, A. Widera

This mpi**pks** workshop was held during the period September 7-11, 2020 and was originally planned as a regular in person workshop with about 80 participants. Given the Covid-19 situation worldwide, the scientific organizers decided in May 2020, after a number of informative discussions with the mpi**pks** staff (Mandy Lochar and Dr. Michael Genkin), to change the workshop format to a fully virtual workshop via the Zoom platform. To accommodate the different time zones, the invited talks were shortened to 30 minutes and distributed across three morning sessions (Europe and Asia friendly time) and three afternoon sessions (Europe and North/South America friendly time). In order to maintain the character of a workshop and to foster scientific discussion, the invited talks were complemented by two discussion sessions, which were organized around a few selected topics in separate Zoom sessions. Due to the online nature of the workshop, the poster session had, unfortunately, to be canceled. All invited speakers gave their consent for the talks to be recorded and to be available for registered participants via a password-protected website hosted by the mpi**pks** for 48-hour viewing.
The workshop registration was closed just a few days prior to the start of the workshop and 157 participants from 22 countries were accepted. The talks were attended by a live audience of between 35 and 85 participants and the individual discussion rooms drew up to 10 people each. The Max-Planck colloquium, which was given by MacArthur fellow Ana-Maria Rey, drew an audience close to 150. The recordings of the individual talks were accessed between 457 and 1250 times. Speaker invitations went out between 12 to 18 months ahead of the workshop; most individuals approached accepted the invitation right away. Even after the switch from the in-person to the virtual format only one invited speaker cancelled their participation. The demographics of the invited speakers were diverse in many aspects: 14 were located in Europe, 5 in the US, and one each in China and Australia. Seven of the speakers were female and 14 were male. The career stage of the speakers ranged from postdoctoral researcher (Bienias and Williams) to group leader (Luitz) to senior researcher/faculty. Two of the speakers (Greiner and Rey) are MacArthur fellows.
The key topics and questions addressed during the workshop covered many aspects that are currently driving the field of medium-sized cold atomic systems from experimental and theoretical points of view.

These included how to observe non-classical correlations between constituents such as atoms, molecules, quasi-particles or spins of mesoscopic systems, and how to apply them; how possible deviations from the eigenstate thermalization hypothesis can be observed and studied in mesoscopic systems; how transitions between coherent and incoherent quantum diffusion can be observed; how non-equilibrium descriptions can be effectively benchmarked, theoretically and experimentally, and what the limits of non-adiabatic evolution are. On a sadder note, Bruno Julia-Diaz gave an in-memoriam presentation about Artur Polls, who was a highly-valued member of the community and had passed away unexpectedly just before the workshop in August 2020. Despite this new and unfamiliar workshop format, the feedback received from the speakers and participants confirmed the need for workshops of this kind in times when face-to-face exchanges across borders are not possible.
We would like to sincerely thank the mpi**pks** for supporting this event in its online form. We are particularly grateful to Mandy Lochar and Dr. Michael Genkin who were invaluable in helping us to work out the organizational details and ensured a smooth running of the workshop.

Dynamics, Criticality, and Universality in Random Quantum Circuits, Virtual Workshop
Scientific coordinators: M. Gullans, J. Pixley, R. Vasseur, J. Wilson

The workshop "Dynamics, criticality, and universality in random quantum circuits" was a successful, virtual conference. We chose speakers from condensed matter and quantum information to both foster communication in a rapidly developing field. The focus of the workshop was random quantum circuits, which all speakers spoke on, and in particular, the measurement-driven phase transition. As we learned in the course of this conference, this phase transition draws interest for its critical nature, mappings to statistical mechanics models, relation to quantum error-correcting codes, and experimental applications in quantum simulators and quantum computing systems.
There were very lively discussions throughout the conference. The most important participants were the speakers and discussion session leaders, who actively contributed to all the discussions. We received positive feedback from many participants who enjoyed the ample opportunity for discussions created by the conference format. The discussions tended to be at a high level of expertise and delved into many important issues relevant to the topic.
Scientific newcomers played an important role in the workshop primarily through their posters and questions within discussion sections. The experts and established participants contributed heavily to the virtual discussions, allowing for in-depth and exciting scientific discussions. We encourage mpi**pks** to get feedback from participants if possible, to improve the format of virtual meetings and poster sessions.
In light of the challenges of a virtual format, the workshop was an overall success in our view. The workshop brought together leaders in quantum information science and condensed matter physics, fostering interdisciplinary discussions and activities. The workshop put the study of random quantum circuits into a broader context and helped clarify the scientific motivation for pursuing these problems. Several participants expressed gratitude for the timeliness of this workshop. The opportunity for a larger group to discuss and dissect much of this will undoubtedly lead to new work and collaborations within this field. Some general open questions that came out of the discussions and talks are listed below. We hope that the coming years see continued progress on these questions:
-How do we define universality classes and classify different phases for dynamical phase transitions in random circuit models?
-What are the possible experimental realizations of monitored nonequilibrium quantum many-body systems?
-Can noisy random circuits still have quantum computational advantage in near-term devices?
-Can we prepare volume-law entangled phases of matter in a fault-tolerant manner?

Winter School on Strongly Correlated Quantum Matter, Virtual School
Scientific coordinators: M. Collura, M. Dalmonte, M. Heyl, D. Luitz

The virtual Winter School on Strongly Correlated Quantum Matter, organized jointly with ICTP Trieste, took place from 30 November to 18 December 2020. The Covid-19 pandemic has drastically affected scientific exchange. On the level of seminars and colloquia many virtual activities have been successfully started around the globe to compensate for the lack of real meetings and events. However, a substantial gap has remained when it comes to activities targeted at Masters and PhD students as well as other junior researchers. This has been the key motivation for us to initiate the virtual Winter School with the purpose to provide a modern overview of the field of strongly correlated quantum matter and to provide a platform for reinforcing scientific exchange during the present times characterized by severe

travel constraints.
The winter school extended over three weeks. As the typical attention span in virtual formats is limited compared to in-person formats, we designed the scientific program in a very dilute form. For that purpose, we aimed for at most 3 lecture, tutorial, or colloquium events a day and also left two days free for self-study. Overall, we hosted 8 lectures with accompanying tutorials, 3 colloquia, and 3 poster sessions. The lectures and colloquia were given by leading scientists performing cutting-edge research in the respective fields, while the tutorials were given by junior collaborators. Overall, we admitted roughly 150 external participants. We observed a live attendance of around 90 in the first week, 80 in the second week, and 60 in the third week. Importantly, however, we also recorded and made available the events online for download. From a subsequent survey we learnt that almost 50 % of the participants were also watching the recordings at a later stage, which let us speculate that overall a large fraction of participants were attending the school.
In order to be as inclusive as possible, we decided to use BigBlueButton (BBB) as our video conferencing platform. BBB is an open-source software and was hosted on a dedicated server at mpi**pks**, after initial attempts with a virtual machine were unsuccessful. For users, BBB is web-browser-based and easy to use, although operation is not as smooth as with fine-tuned proprietary software like zoom. After instructing participants to use recent chromium-based browsers and to open only one connection, BBB ran relatively smoothly. We had minor problems with some speakers who had a weak internet connection, and in such cases we used zoom as a fallback option.
It appears that most technical problems with BBB are manageable, and the fact that it is open-source makes it preferable over zoom.
In parallel to the video sessions, we established an independent, asynchronous communication channel among all participants, based on the open-source Matrix platform. We created one chat room per lecture and encouraged participants to ask questions and discuss among themselves on Matrix instead of the built-in BBB chat. There are two advantages with that: The Matrix chat is persistent even after the end of the school and in case of technical problems with BBB, Matrix was still operational, allowing us to solve problems in real time. The discussion on Matrix was generally lively and several initiatives from the participants emerged, such as collaborative writing of lecture notes for some lectures. This helped generating a feeling of a school community, which is very difficult to create in remote events. According to the subsequent survey roughly 25% of the participants utilized matrix for their own interactions, beyond the official channels we had established.

Tensor Product Methods for Strongly Correlated Molecular Systems, Virtual Workshop
Scientific coordinators: Ö. Legeza, M. Reiher, R. Schneider

The computation of the electronic structure is a task of utmost importance for molecular engineering in modern chemistry and material science. The accurate computation of the electron correlation is a fundamental and extremely difficult problem in this context. Due to the enormous developments in the past decade - made from different perspectives for different purposes in distinct communities - tensor network state methods have already matured to provide a variety of tools to attack highly challenging strongly correlated electronic problems in quantum chemistry. Therefore, the treatment of high-dimensional problems, such as the Schrödinger equation, can be approached efficiently by concepts of tensor product approximation. The aim of the 4-day workshop was to bring together the expertise of theoretical chemists in molecular structure theory, condensed matter physicists in many-body physics and mathematicians in numerical analysis to intensify the exploration of this continuously growing new field of research, and to stimulate further developments of tensor network methods.
Unfortunately, the workshop organized originally for 2020 had to be shifted by a year due to the emergence of the Covid pandemic, and finally converted to an online event in 2021. The technical support received from mpi**pks**, however, provided an excellent scientific environment for presenting lectures, contributed talks and posters online, and for discussions as well. Talks were organized into a morning and an evening session, taking into account the different time zones of speakers and participants from Europe, Asia, and the Americas. In addition, talks were recorded and made available to the participants for one month. Altogether there were more than 60 participants, including 16 invited speakers, from three continents (A. Alavi (DE), G. Booth (UK), G. Kin-Lic Chan (US), J. Eisert (DE), E. Fromager (FR), K. Hallberg (AR), S. Knecht (CH), K. Kowalski (US), S. Kvaal (NO), N.J. Mayhall (US), J. Pittner (CZ), C. Schilling (UK), S. Sharma (DE), F. Verstraete (BE), S.R. White (US), T. Yanai (JP)).
The spectrum of the workshop was very broad, covering various subtopics on electronic correlation theory. Among the key questions, the most appropriate existing tensor network state structures, or

variants to be developed for treating strongly correlated molecules were discussed. Furthermore, the state of the art for different multireference generalizations of conventional single-reference methods like CC or DFT, utilization of concepts of quantum information theory, treatment of relativistic effects, consideration of electron dynamics and time-dependent phenomena for molecules via tensor network state methods were also addressed. In addition, different embedding approaches, basis optimization protocols, identification and measurement of entanglement, various approaches based on first and second quantization, and reformulation of the underlying tensor algebra have also been among the main topics. Rigorous mathematical analysis, novel algorithmic developments and applications to model systems, as well as large-scale applications to real materials demonstrated the tremendous progress achieved since the density matrix renormalization group (DMRG) was introduced by Steven R. White. The two poster sessions provided a friendly atmosphere for young colleagues to present their research and results, and the longer breaks between the morning and evening sessions gave the participants a great opportunity for private discussions.
The scientific results of the workshop in the broader sense helped to intensify the communication among the different scientific communities, and are expected to give a new impetus toward new developments in the field.

Korrelationstage 2021, Virtual Workshop
Scientific coordinators: K. Everschor-Sitte, R. Moessner, F. Piazza, R. Valenti

Main focus of our workshop:
For many years, the Korrelationstage have biennially brought together the members of the community studying the correlated electron problem (in an increasingly broad sense, now also comprising cooperative phenomena in cold atomic systems) in Germany and its environs. Given the present pandemic situation, we held a virtual version, specifically aimed at redressing the effective isolation of young members of the community who did not yet have a research network of their own, by providing a platform for presenting their work, meeting colleagues, and becoming known in the community.
Most important participants:
As explained above, the most important participants have been the junior researchers, ranging from PhD students to PostDocs and young PIs, who made up by far the biggest part of the roughly 250 participants. Accompanying each of the 4 sessions, we had also 4 excellent speakers delivering an overview talk. The average attendance was always above 100, reaching its peak during one overview talk, given in the framework of the mpi**pks** colloquium, where the threshold of 200 was broken.
How did scientific newcomers present themselves?
All the talks were exclusively given by junior researchers i.e. researchers without a tenured position. Most of them were not even PIs, and several were PhD students. Nonetheless, the quality of the contributions was very high. Essentially all the remaining participants presented a poster and an associated flash talk during a dedicated session. Each flash talk was allotted only one minute, still basically every speaker managed to find the right compromise between speed and clarity. In addition, we organized two informal gatherings on the platform gather.town, which was also used during the breaks. Finally, during one session, two local speakers gave their talk in hybrid form using a dedicated seminar room at mpi**pks**.
Scientific results of the workshop in the broader sense:
Given the large pool of participants and the high attendance during each session, we believe that the main goal of the workshop has clearly been achieved: A large number of young scientists had the chance to present themselves and their work to each other as well as to a broader community beyond their own specific field. Moreover, the overview talks allowed the more junior participants to get a very useful introduction to 4 different modern subfields, while the regular sessions touched basically all of the current "hot topics" in strongly correlated physics.

Random Matrix Theory and Networks, Virtual Workshop
Scientific coordinators: F. L. Metz, I. Neri, I. Pérez Castillo

On 7-18 June 2021 the mpi**pks** hosted a virtual workshop on random matrices and networks. The workshop counted 112 participants from 19 countries.
The aim of the workshop was to bring together researchers working on applications of random matrix theory to different branches of complex systems theory. Random matrix theory was initiated about 80 years ago as a new mathematical tool to study many-body systems, such as heavy nuclei or atoms. Standard models of random matrix theory rely on independent and identically distributed matrix entries. In recent years, new random matrix models have been developed that incorporate features of real-world

systems, such as network architecture, modularity, and recurrent motifs. These network models appear in the study of complex systems, such as financial markets, signalling networks, neural networks, or ecosystems. Therefore, we thought that it would be a good idea to bring scientists together and discuss the recent progress.
A recurrent theme in the workshop was the linear stability of complex systems, as inspired by the seminal paper of Robert May in 1972. For example, Jean-Phillipe Bouchaud presented novel results on the stability of economies, Giorgio Carugno discussed the stability of complex fluids, Ariel Amir and Srdjan Ostojic examined the stability of gene regulatory networks and neural networks, respectively, and Tim Rogers analysed the fluctuation spectra of stable ecosystems. Novel approaches that go beyond the linear stability analysis were also explored. For instance, Boris Khoruzenko explained how to compute the number of fixed-points in a nonlinear system, and Stefano Allesina discussed the feasibility of equilibria in ecosystems described by Lotka-Volterra equations.
Another central theme of the workshop was the localisation of eigenvectors in random matrices. David Nelson and Grace Zhang discussed localisation of right eigenvectors in one-dimensional chains, Paolo Barucca presented novel results for the eigenvector moments in time series analysis, Ivan Khaymovich discussed the multifractality of eigenvectors in random matrix models, Federico Ricci-Tersenghi presented recent results on the eigenvector localisation of the Hessian matrix of spin-glass models, and Diego Tapias discussed localisation phenomena in trap models on networks.
Applications of random matrix theory are diverse, and this was also apparent from the wide variety of topics covered in the conference. Other topics that were touched upon are the slow relaxation of non-equilibrium driven systems (Peter Sollich), new results on ranking nodes in a complex system (Fabio Caccioli), novel random matrix models for quasi-Hermitian and pseudo-Hermitian systems (Joshua Feinberg), the capacity of neural networks to store low-dimensional manifolds (Rémi Monasson), the applications of random matrix theory to study exploration and search in complex networks (Reimer Kühn), the representation of complex data by simple models (Matteo Marsili), and different types of statistical inference problems on networks (Antoine Maillard, Carlo Lucibello, Andrea de Matino, and Rok Cestnik), and many others. Maciej Nowak concluded the conference with an inspiring talk on the links between random matrix theory and classical mechanics. The conference also hosted a social event, a talk by Giuseppe Mussardo on the enigma of J. Robert Oppenheimer that was joined by several members of the mpi**pks**.
The balance between experts and newcomers was an important characteristic of the event, which stimulated the discussion between the participants on the social media platform gather.town. Taken together, the diversity of topics explored in the event provided a very interesting overview of the most recent applications of random matrix theory to complex systems, which will hopefully inspire new researchers to enter this field.

Atomic Summer Camp 2021, Open Air Scientific Camp
Scientific coordinators: A. Buchleitner, T. Pfeifer, J.-M. Rost

The Atomic Summer Camp 2021 at mpi**pks** successfully (re-)established a new, strictly analog seminar format: A relatively small number of participants (approx. 40), dedicated discussion slots after each talk, most talks given by young scientists between M.Sc. and early PostDoc levels, permanent attendance and contributions by a small group of senior scientists, unstable internet connectivity in the lecture hall tent preventing the audience from working on their emails, and outdoor social events altogether created an informal, curiosity-driven and - under the wide AMO+quantum science umbrella - rather interdisciplinary, vivid and open-minded scientific discourse. The scientific topics covered a broad range of recent experimental and theoretical ideas and results, from light-matter interaction phenomena in solids, over many-particle coherence properties, to the creation of entanglement in molecular degrees of freedom. The open atmosphere seeded scientific interactions between several of the participating groups, with the potential for new collaborations.
The camp format, developed under the boundary conditions of the pandemic with talks in an open tent, and discussions as well as other activities taking place outdoors, prompted enthusiastic reactions and may prove in the future to be a new and additional conference format for mpi**pks**.

Physical Biology Circle Meeting, Hybrid Workshop
Scientific coordinators: F. Jülicher, S. Rulands

The Circle Meeting is an annual series of symposia bringing together researchers from leading European research institutes including the EMBL in Heidelberg, the Institut Curie in Paris, the AMOLF in Ams-

terdam, the University of Saarbrücken, the Francis Crick Institute in London, the IST Austria in Vienna, the IBEC in Barcelona, and the mpi**pks**. The scientific focus of the Circle Meeting is broadly on theoretical and experimental biophysics, including tissue mechanics, molecular biophysics, and stochasticity in biological systems.
The meeting took place in a hybrid format with 55 participants from various European institutions attending on site and 78 participants joining online via Zoom and gather.town. As keynote speakers we invited Nathalie Balaban from the Hebrew University in Jerusalem who gave a virtual talk about self-replicating biological matter and Anne Grapin-Botton from the MPI-CBG who joined in person and spoke about self-organisation in organoids.
All remaining slots were reserved for researchers at the graduate student and postdoc levels. They gave shorter talks of 20 minutes' duration, which were followed by lively discussions among on-site and online participants. In addition to these regular talks we had a poster session in gather.town, which was preceded by a flash-talk session with brief presentations of poster presenters.
For most of the participants, the Physical Biology Circle Meeting facilitated - for the first time since the outbreak of the Covid pandemic - scientific interactions which might lead eventually to future collaborations.

3.4 Collaboration with Experimental Groups

- *Mechanics and patterning of developing fruit fly wing* with N. Dye, Physics of Life, TU Dresden (Dresden, Germany)
- *Left-right symmetry robustness of zebrafish embryo during somitogenesis* with A. Oates, EPFL Lausanne (Switzerland)
- *Genomic changes in bats and moles* with S. Mundlos, MPI Molecular Biology (Berlin, Germany)
- *Genome and brain evolution in snakes* with V. Borrell, Instituto de Neurociencias (Alicante, Spain)
- *Genome analysis of jerboas* with K. Cooper, UCSD (San Diego, USA)
- *Kosterlitz-Thouless Kritikalität in Quantenmagneten* with H. Kuehne, J. Wosnitza, HZ Dresden-Rossendorf, TU Dresden (Dresden, Germany)
- *2d/3d crossover in an XXZ magnet* with H. Kuehne, J. Wosnitza, HZ Dresden-Rossendorf, TU Dresden (Dresden, Germany)
- *Biomechanics of inversion in the green alga Volvox* with R. Goldstein, S. Hoehn, University of Cambridge, (Cambridge, Great Britain)
- *Continuum mechanics of cell intercalation during epiboly in Tribolium* with P. Tomancak, MPICBG, (Dresden, Germany)
- *Mechanics of the formation of the bile canaliculi in the liver* with M. Zerial, MPICBG, (Dresden, Germany)
- *Quantum dynamics of ultracold atoms* with J. Sherson, Aarhus University, (Aarhus, Denmark)
- *Radiative and non-radiative decay of molecules on rare gas clusters* with F. Stienkemeier, University of Freiburg, (Freiburg, Germany)
- *Spectroscopy of molecular monolayers on surface* with J. Hauer, TU Muenchen, (Muenchen, Germany)
- *Floquet prethermalization* with D. Weld, University of California, (Santa Barbara, USA)
- *Quantum metrology* with J. Cai, Huazhong University of Science and Technology, (Wuhan, China)
- *Quantum Kibble-Zurek mechanism* with W. Yi, University of Science and Technology of China, (Hefei, China)
- *Quantum walks* with G.-C. Guo, University of Science and Technology of China, (Hefei, China)
- *Anomalous magnetic dynamics* with A. Tennant, Oak Ridge National Laboratory, (Oak Ridge, USA)
- *Topological metamagnetism* with S. Grigera, CONICET La Plata, (La Plata, Argentina)
- *Non-hermitian quantum dynamics* with P. Xue, Beijing Computational Science Research Center, (Beijing, China)
- *Quantum interference in delafossites* with P. Moll, EPFL, (Lausanne, Switzerland)
- *Quantum computing* with X. Mi, P. Roushan, Google AI, (Kalifornien, USA)
- *Epigenetic processes during liver regeneration* with M. Huch, MPICBG (Dresden, Germany)
- *Epigenetic processes in development and ageing* with W. Reik, The Babraham Institute (Cambridge, UK)
- *Multi-scale fluctuations in the regulation of cell death* with P. Mergenthaler, Charite University Clinic (Berlin, Germany)
- *Machine learning and modelling for personalised medicine in cancer treatment* with D. Stange, Charite University Clinic (Berlin, Germany)
- *Skull morphogenesis* with J. Tabler, MPICBG (Dresden, Germany)
- *Epithelial cell plasticity* with M. P. Alcolea, Stem Cell Institute (Cambridge, UK)
- *Lung tumour tracing* with J.-H. Lee, Stem Cell Institute (Cambridge, UK)
- *Cellular pausing* with A. B. Karslyoglu, MPIMG (Berlin, Germany)
- *Liver homeostasis* with B. Stanger, Rockefeller University (New York, USA)
- *Cavity QED mit ultrakalten Atomen* with T. Donner, ETH Zuerich (Zuerich, Switzerland)
- *Nichtlineare Dynamik von exciton-polaron-polaritons in 2D Halbleitern* with A. Imamoglu, ETH Zuerich (Zuerich, Switzerland)
- *Fermi-Polaron Dynamik in ultrakalten Gasen* with M. Zaccanti, F. Scazza, LENS Florenz (Florenz, Italy)

3.5 Externally Funded Research and Relations to Industry

3.5.1 DFG Projects

- Gottfried Wilhelm Leibniz-Preis 2013, Prof. R. Moessner
- Gottfried Wilhelm Leibniz-Preis 2017, Prof. F. Jülicher
- Collaborative Research Center 1143 *Correlated magnetism: from frustration to topology*, Prof. R. Moessner
- Priority Program 1929 *Schnittstellen-induzierte Kohärenz und Verschränkung von Rydberg Einheiten*, Prof. J.-M. Rost, Dr. A. Eisfeld
- *Kontrolle von Ionisation durch die zeitliche Änderung der Pulsform des Lichts*, Prof. J.-M. Rost, Prof. Dr. U. Saalmann
- Exzellenzcluster *Physics of Life*, Prof. F. Jülicher
- Exzellenzcluster *Complexity and Topology in Quantum Matter*, Prof. R. Moessner, Dr. P. Surowka

Individual Projects

- *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
- *Phasentrennung von membrangebundenen Proteinen als Mechanismus zur Bildung der Zonula Occludens*, Dr. C. Weber
- *Ein vergleichender Ansatz, um die genomischen Faktoren zu entdecken, die zu natürlichen Anpassung an eine zuckerreiche Nahrung in nektartrinkenden Vögeln beitragen*, Dr. M. Hiller
- *Die Entstehung von phasengetrennten Transkriptionszentren und ihre Funktion in der Transkriptionsregulation*, Dr. J. Brugues
- *Prinzipien der räumlichen und zeitlichen Kontrolle der Initiation meiotischer Rekombination in Mäusen*, Dr. S. Rulands
- *Exzitonentransport und optische Eigenschaften von Quantenaggregaten*, Dr. A. Eisfeld

3.5.2 EU Funding

- EU - Horizont 2020 *Climate Advanced Forecasting of Sub-seasonal Extremes (CAFE)*, Prof. Dr. H. Kantz
- EU - ERC STG *Machine learning quantum dynamics*, Dr. M. Heyl
- EU - ERC STG *Understanding collective mechanisms of cell fate regulations using single-cell genomics*, Dr. S. Rulands
- EU - ERC STG *FuelledLife - Selection and Regulation of Compartments by Fuel-driven Phase Separation*, Dr. Ch. Weber

3.5.3 Additional External Funding

- AvH *Programm: Förderung von Institutspartnerschaften*, Prof. F. Jülicher, Dr. A. Basu
- Boehringer-Ingelheim Foundation *Discovering novel genes underlying human eye disorders by comparative genomics in mammals with degenerated eyes*, Dr. M. Hiller
- Leibniz-Gemeinschaft e.V. *Identifying the genomic loci underlying mammalian phenotypic variability using Forward Genomics with Semantic Phenotypes*, Dr. M. Hiller
- HFSP *Human frontiers science program career development award*, Dr. J. Brugues
- VW *The spark of life: initiation of transcription in embryos, and recapitulating such in synthetic nuclei*, Dr. J. Brugues
- VW *Interplay of Proteins and Nucleic Acid Polymers in Compartment Formation*, Prof. Dr. F. Jülicher

3.5.4 Scholarships

- Alexander Eisfeld; Heisenbergstipendium
- Matthew Eiles; AvH
- Daniel Aguilar Hidalgo; University of Geneve
- Petr Karpov; AvH
- Jinbin Li; CsC
- Nishida Naoki; Scholarship from Japan
- Nishida Naoki; Scholarship from South Korea
- Melissa Rinaldin; HFSP

3.5.5 External Cofunding of Workshops and Seminars

2019

- Workshop *Anyons in Quantum Many-Body Systems*
  (6 % of budget)
- Workshop *Quantum Ferromagnetism and Related Phenomena*
  (32 % of budget)
- Focus Workshop *Granular and Particulate Networks*
  (26 % of budget)
- Workshop *Microscale Motion and Light*
  (25 % of budget)
- Seminar and Workshop *Quantum Criticality and Topology in Correlated Electron Systems*
  (9 % of budget)
- Workshop *Dynamical Methods in Data-based Exploration of Complex Systems*
  (3 % of budget)

3.5.6 Patents and Licenses

- *J. Götte, R. Cameron, S. Barnett*
  International patent **PCT/EP2016/076742**
  Chiral rotational spectrometer, since 11/2015
- *A. Pollakis, L. Wetzel, 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 2018/19

- *Quantum simulators* Dr. M. Heyl, Dr. Andre Eckardt, TU Dresden
- *Nonlinear Dynamics* Prof. Dr. Holger Kantz, TU Dresden
- *Strong-coupling QED in materials* Dr. Francesco Piazza, ColOpt Winter School 2019

Sommersemester 2019

- *Quantum Many-Body Dynamics: Correlations and entanglement* Dr. David Luitz, Dr. Markus Heyl, TU Dresden
- *Statistical Physics* Dr. Anne Nielsen, Aarhus University
- *Multidimensional femtosecond spectroscopy* Dr. Alexander Eisfeld, TU Dresden
- *Course: Data science for physicists* Dr. Fabian Rost, Dr. Steffen Rulands, TU Dresden

- *Biophysik III: Theoretical Physics* Prof. Dr. Frank Jülicher, Prof. Dr. Stephan Grill, TU Dresden

Wintersemester 2019/2020

- *Atmospheric Physics* Prof. Dr. Holger Kantz, TU Dresden
- *Non-equilibrium field theory* Dr. Francesco Piazza, Dr. Steffen Rulands, TU Dresden
- *Biological Hydrodynamics* Prof. Dr. Stephan Grill, Dr. Jan Brugues, Dr. Benjamin Friedrich, TU Dresden

Sommersemester 2020

- *Comparative and function genomics* Dr. Michael Hiller, TU Dresden
- *Statistical Physics* Dr. Anne Nielsen, Aarhus University
- *Biophysik III: Theoretical Physics* Prof. Dr. Frank Juelicher, Prof. Dr. Stephan Grill, TU Dresden

Wintersemester 2020/2021

- *Methods for Quantum Many-Body Dynamics* Dr. David Luitz, Dr. Francesco Piazza, TU Dresden
- *Theory of open quantum systems, applied to molecular assemblies* Dr. Alexander Eisfeld, TU Dresden
- *Collective processes in non-equilibrium systems* Dr. Steffen Rulands, TU Dresden

Sommersemester 2021

- *Atmospheric Physics* Prof. Dr. Holger Kantz, TU Dresden
- *Biophysik III: Theoretical Physics* Prof. Dr. Frank Juelicher, Dr. Christoph Weber, TU Dresden

3.6.2 Professional Skills Training

Talk series on professional skills topics

- *Touching the Invisible*
  Orestis Georgiou, Ultrahaptics (April 2019)
- *Experiences in Data Science*
  David Schönleber, esentri AG (May 2019)
- *From PhD Student to IT Professional*
  Martin Mucha, Freelance IT Business Analyst (May 2019)
- *Working in a Ministry as a Former Scientist*
  Johannes Baumgart (June 2021)

3.6.3 Degrees

Dissertations

- Krueger, S.: *Positioning of Droplets in Inhomogeneous Fluids.* Dresden, 2019
- Kruining, K.v.: *Spin and helicity in structured waves for light and electrons.* Dresden, 2019
- Lezama Mergold Love, T.: *Some dynamical aspects of generic disordered systems.* Dresden, 2019
- Luensmann, B.: *Detection of Coherent Structures in Two-Dimensional Oceanic Flows: On Improvements of the Transfer Operator Approach and Convexity as a Condition of Coherence.* Dresden, 2019
- Mueller, P.: *Extreme value analysis of non-stationary time series: Quantifying climate change using observational data throughout Germany.* Dresden, 2019
- Ortmann, L.: *Trajectory-based analyses of ultrafast strong field phenomena.* Dresden, 2019
- Schaumann, F.: *Investigation of nonhyperbolic systems.* Dresden, 2019
- Schreiber, L.: *Extreme Value Analysis of Precipitation Time Series - Quantifying Precipitation Changes Globally.* Dresden, 2019

- Seyboldt, R.: *The dynamics of chemically active droplets.* Dresden, 2019
- Verresen, R.: *Topology and Excitations in Low-Dimensional Quantum Matter.* Dresden, 2019
- Adame-Arana, O.: *Chemical control of liquid phase separation in the cell.* Dresden, 2020
- Dickmann, J.: *Formation of long-ranged morphogen gradients by cell-to-cell relay.* Dresden, 2020
- Giri, S. K.: *Statistical learning for ultrafast light-matter interactions.* Dresden, 2020
- Manna, S.: *Quasiparticles in Quantum Many-Body Systems.* Dresden, 2020
- Meyer, P. G.: *Anomalous statistical properties and fluctuations on multiple timescales.* Dresden, 2020
- Witkowski, P.: *Hydrodynamics in solid state transport, from microscopic to mesoscopic scales.* Dresden, 2020
- Dantas, R. M. A.: *Quantum anomalies, transport and optical properties of topological semimetals.* Dresden, 2021
- Dutta, S.: *Attoclock Induced Electron Dynamics.* Dresden, 2021
- Matsyshyn, O.: *Berry's phase driven nonlinear optical and transport effects in solids.* Dresden, 2021
- Mukherjee, A.: *Physics of Oocyte Growth and Selection: a mesoscopic perspective.* Dresden, 2021
- Polotzek, K.: *Modeling and analysis of non-Gaussian long-range correlated data - Extreme value theory and effective sample sizes with applications to precipitation data.* Dresden, 2021
- Srivatsa, N. S.: *Special states in quantum many-body spectra of low dimensional systems.* Dresden, 2021
- Trapin, D.: *Dynamical quantum phase transitions.* Dresden, 2021
- Verdel Aranda, R.: *Nonequlibrium dynamics in lattice gauge theories: disorder-free localization and string breaking.* Dresden, 2021

Master Thesis

- Roost, M.: *Thermodynamic and Dynamic Modelling of the Vertical Temperature Profile of the Atmosphere.* Dresden, 2020
- Schulz, A.: *Parameter-dependent deterministic diffusion in intermittent Pomeau-Manneville maps.* Dresden, 2020

Bachelor Thesis

- Vanelli, C.: *Scenario Development and Analysis of an Agent-based Model for Environmentally-induced Human Migration in Ethiopia.* Dresden, 2020

3.6.4 Appointments and Awards

Appointments

- Prof. M. Carney accepted the offer for a professorship at the *University of Queensland, Brisbane, Australia*.
- Prof. M. Das accepted the offer for an assistant professorship at the *IIT Mandi, India*.
- Prof. A. Eckardt accepted the offer for a professorship at the *TU Berlin, Germany*.
- Prof. E. Filippidi accepted the offer for an assistant professorship at the *University of Crete, Greece*.
- Prof. M. Heyl accepted the offer for a professorship at the *University of Augsburg, Germany*.
- Prof. M. Hiller accepted the offer for a professorship at the *Senckenberg Society for Nature Research and Goethe University, Frankfurt/Main, Germany*.
- Prof. L. Jawerth accepted the offer for a professorship at the *University of Leiden, Netherlands*.
- Prof. A. Landsman accepted the offer for an associate professorship at the *Ohio State University, USA*.
- Prof. X. Li accepted the offer for an assistant professorship at the *Anhui University, China*.
- Prof. D. Luitz accepted the offer for a professorship at the *University of Bonn, Germany*.
- Prof. A. E. B. Nielsen accepted the offer for an associate professorship at *Aarhus University, Denmark*.

- Prof. T. Oka accepted the offer for a professorship at the *University of Tokyo, Japan*.
- Prof. F. Pientka accepted the offer for a tenure-track junior professorship at the *Goethe University, Frankfurt/Main, Germany*.
- Prof. J. Rau accepted the offer for an assistant professorship at the *University of Windsor, Canada*.
- Prof. B. Roy accepted the offer for an assistant professorship at the *Lehigh University, USA*.
- Prof. P. Surowka accepted the offer for an associate professorship at *Wrocław University of Science and Technology, Poland*.
- Prof. A. Tejedor accepted the offer for an assistant professorship at *Sorbonne University, Abu Dhabi*.
- Prof. C. Weber accepted the offer for a professorship at the *University of Augsburg, Germany*.

Awards

- Bauermann, J.: *Physik-Studienpreis 2019 der DPG Berlin*
- Hänggi, P.: *Marian-Smoluchowski-Emil-Warburg-Preis 2019*
- Heyl, M.: *ERC starting grant*
- Moessner, R.: *Honorary Fellowship, Hertford College, Oxford University*
- Nielsen, A. E. B.: *Ørsted Reserach Talent Prize 2020*
- Nielsen, A. E. B.: *Carlsberg Foundation Young Researcher Fellowship*
- Rulands, S.: *ERC starting grant 2020*
- Ünal, N.: *Newton International Fellowship of the Royal Society*
- Verresen, R.: *Otto-Hahn-Medal 2021*
- Verresen, R.: *2. Dresdner Promotionspreis Physik*
- Weber, C.: *ERC starting grant*
- Wüster, S.: *Dresden Excellence Award 2019 in the category habilitation*

3.7 Public Relations

3.7.1 Long Night of the Sciences

Over the last 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. In 2020, the *Long Night of the Sciences* unfortunately had to be cancelled due to the pandemic. In 2021, there was a virtual *Long Night of the Sciences* with 1600 interested visitors.

DRESDNER
LANGE NACHT DER
WISSENSCHAFTEN

3.7.2 Science in the Theater

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.

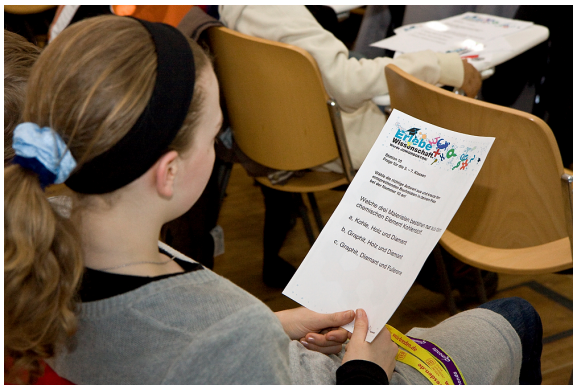
Science in the Theatre

2019 - 2021

- *Gefangen auf Ewigkeit: Das kosmische Antimaterie-Rätsel*
  Prof. Klaus Blaum, (about 280 participants)

3.7.3 mpipks School Contact Program

JUNIOR DOKTOR



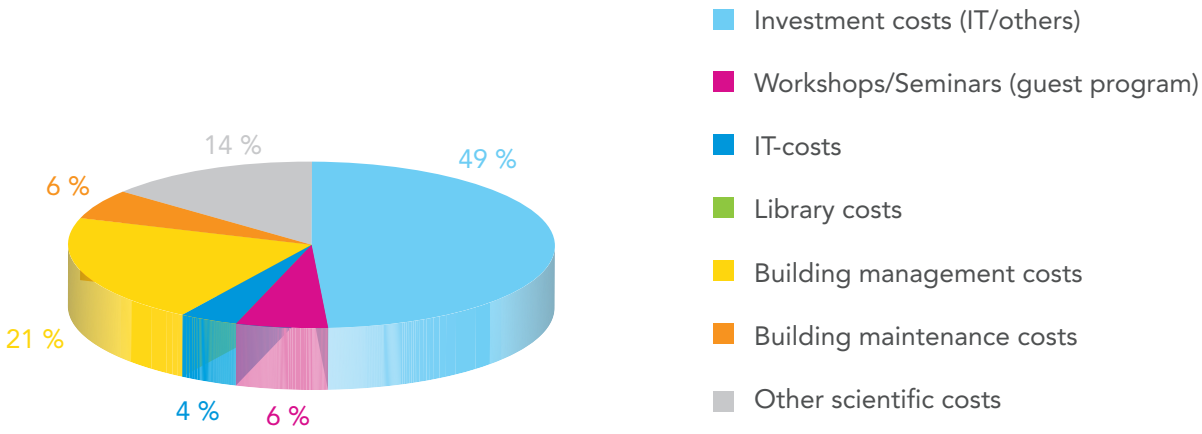
Public lecture for Junior Doctors

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.

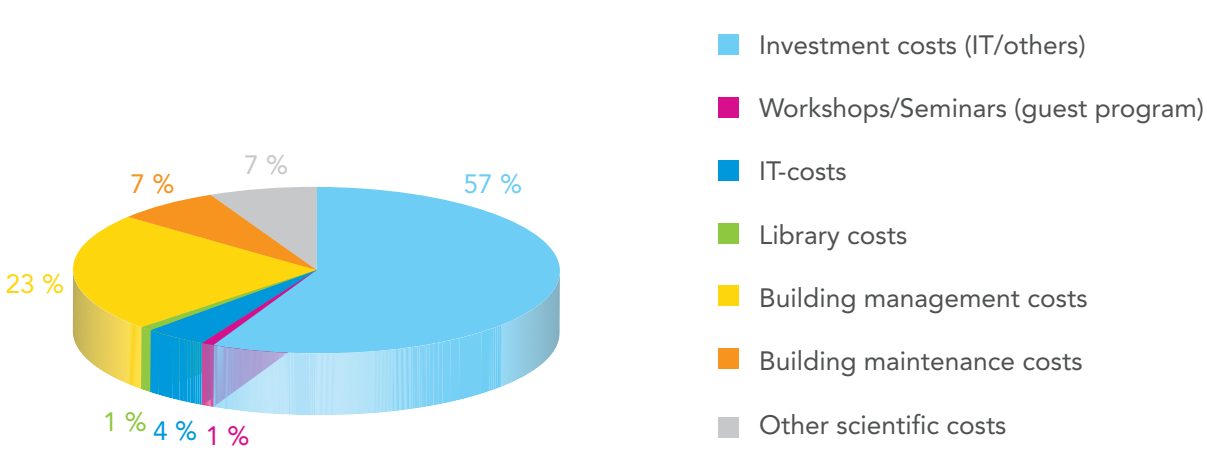
In addition, the institute participates in the program *Junior Doctor* organized by the network *Dresden - Stadt der Wissenschaft*. The participating research institutes offer a variety of lectures for children, who are awarded a "Junior Doctor degree" when attending a stated number of talks. Each school year, the **mpipks** contributes to the curriculum with four lectures for students from the 3rd grade onwards.

3.8 Budget of the Institute

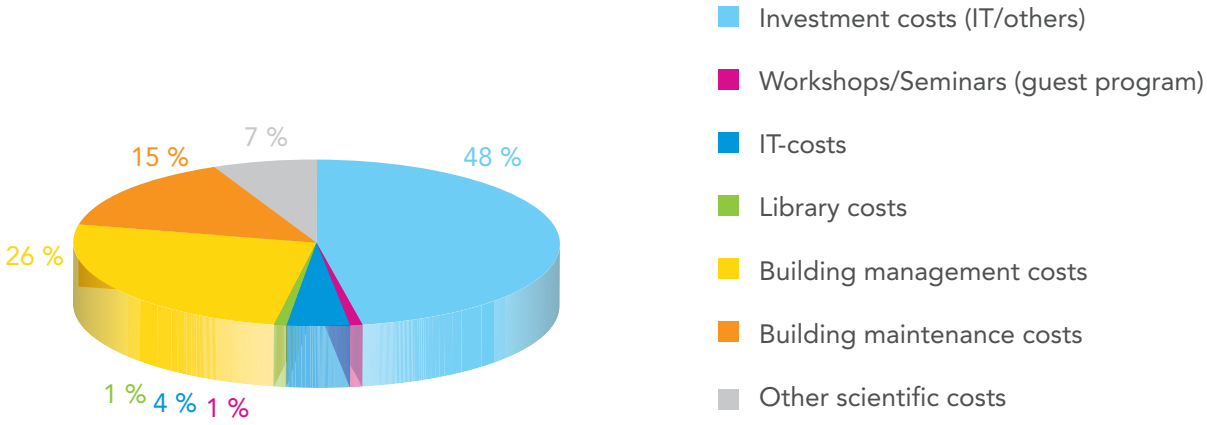
Research Budget 2019



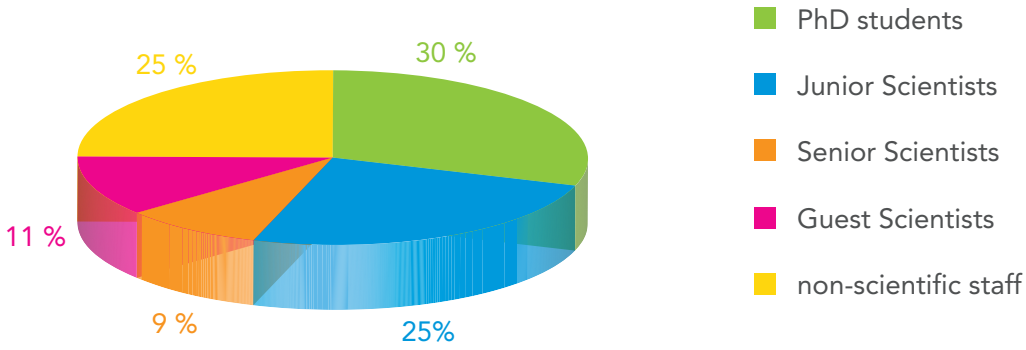
Research Budget 2020



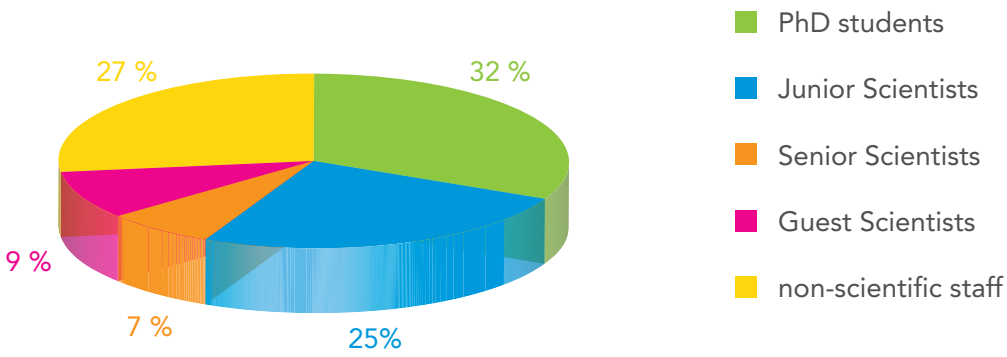
Research Budget 2021



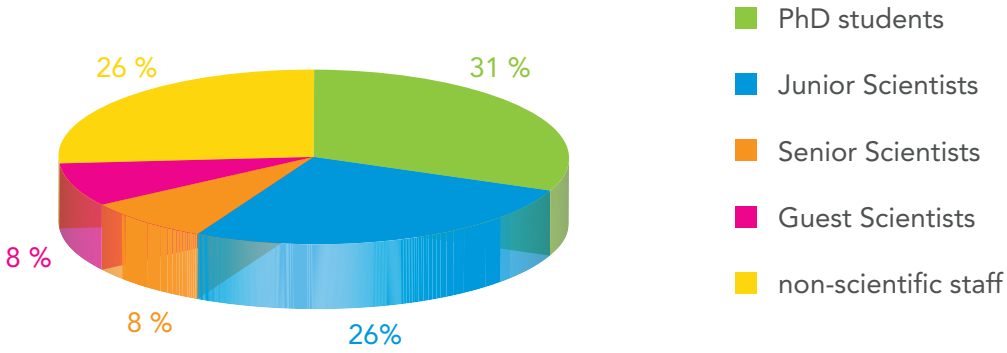
Personnel Budget 2019



Personnel Budget 2020



Personnel Budget 2021



3.9 Equipment and Premises

3.9.1 Computing Facilities

While video conferences were rarely used for scientific lectures before 2020, they suddenly became common early 2020 due to the pandemic situation. Since many scientists were already used to communicate via videotelephony, though usually in face to face situations or sometimes in small groups, they got acquainted with using video conferencing systems very quickly. New video conferencing platforms came into play which were easier to use than the ones that were available before. Quite early there was the wish to be able to realize hybrid talks and seminars as soon as there would be some relief with respect to the very strict social distancing rules that we faced in the beginning. Thus one of the main projects in 2020 was to equip one of our seminar rooms such that it can easily be used for hybrid formats of scientific seminars and workshops. The key features are ceiling microphones which allow people to be heard from everywhere within the seminar room, several cameras, a large display in the front and a software setup which permits to realize a very wide variety of configurations, including the conversion between several video conferencing softwares.

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. At the same time the possibility to develop programs which make heavy use of GPUs was requested by our scientists. This is why we completed our local cluster by several nodes with powerful GPUs during the last three years.

Since early 2019 we are hosting part of our cluster 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 are able to integrate 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.

As there is an ever growing requirement for more computing power by our scientists, our main server room had to be upgraded both with respect to power supply and cooling capacity. At the same time the usual server racks were to be replaced with racks with an heat exchanger in the read door, providing more efficient cooling. This construction work originally planned for 2020 had to be shifted to 2021 and was successfully finished late 2021. This will now give us enough capacity to run new air-cooled servers for the coming years.

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 800 servers with a total of approximately 55,000 CPU cores on site. The cluster located at the MPCDF in Garching, shared by the Fritz Haber Institute, the MPI for the Structure and Dynamics of Matter (Hamburg) and our institute was dismantled in June 2021 and will be followed by a new cluster with fast GPU cards which is going to be put in operation early 2022. This cluster was approved and subsidized by the BAR in 2021.

Our compute nodes have up to 128 CPU cores and a maximum of 6 Terabytes of main memory and a maximum of fifty Terabytes of local disk space. Several nodes with powerful GPUs are available for our scientists. We run 100, 10 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. 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 120 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 Workstations 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 1 GBit/s. Redundancy is achieved by automatic failover to a second line to our neighboring institute (and vice versa for their connection) in case of problems with our primary Internet connection.

The computer department is run by five employees with their respective main tasks being Unix/Linux, Mac OS and cloud services, hardware and web, network and Windows, video conferencing. In addition to those five 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

Since we expect that online formats of workshops and seminars will continue to play an important role even after the current pandemic is gone, we will equip our largest seminar room with technical devices suitable for hybrid events. This is planned to be realized early 2022.

Linux will continue to be the main operating system for our number crunchers in the near future, presently running on Intel Xeon and AMD EPYC based hardware. Other operating systems like AIX might only come into play if particularly fast hardware is required by our scientists that is not supported by Linux. The highly specialized GPUs are used by a growing number of scientists, partly due to the fact that there is now software available which hides the complexity of GPU programming from the user. As the overall speedup in some cases is significant, more scientists are expected to make use of those GPUs in the near future. This is why we decided to join the MPI for the Structure and Dynamics of Matter and apply for the GPU based cluster mentioned above. As the servers in the HPC area tend to show an ever growing power consumption with every new generation, it might become necessary to purchase such servers which require direct cooling. In this case we will most likely try to host such systems either at the Lehmannzentrum of the TU Dresden or the MPCDF in Garching as our facilities are not suitable for the requirements of such systems.

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 was installed at the RZG in Garching and was 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 shared 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. Since early 2019 some of our computers are located at the Lehmann Zentrum of the TU Dresden which is nearby and connected to our institute via fibre optic cable, allowing us to integrate those servers seamlessly into our cluster.

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
2021	800	1000	4500

3.9.2 Library

The library of the mpi**pks** is a service unit with a wide range of duties. It is accommodated in guest house 4 on three floors ablaze 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 mpi**pks** 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 5,700 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, mpi**pks** 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. All these services also work when connecting to the mpi**pks** compute environment through VPN from home, which was of high relevance during the times of lock-down and home office obligations because of the CoViD pandemic.

As an additional service, the librarian has access to online document delivery systems. Books or references which are not avail-

able 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 had failed in 2018, we do 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 are, as long as there is no positive outcome of new negotiations, ordered through the document delivery service on demand.

Finally, the library is also responsible for reporting the publication activities of the mpi**pks**, e.g., for the yearbook of the Max Planck Society or the 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 mpi**pks** 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 mpi**pks** makes sure that the needs of scientists are optimally served by the library. In quarterly meetings decisions such as new journal subscriptions are made.

Our library, 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 mpi**pks** 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 eight large two-bedroom apartments which are well-suited for families with children. On the ground floor, two apartments have been converted into offices in the past, which were used by short term guest scientists or scientists with children. Since additional office space has been created in guest house 4 in summer/autumn 2021, the offices in guest house 3 will be re-converted to regular apartments, further increasing the capacities of mpi**pks** to host visitors with families.

The guest houses 1-3 were built in the course of the institute foundation and after 25 years of extensive use they are now showing signs of wear. Since their operational readiness is essential for the scientific mission of mpi**pks**, the institute is now embarking on their renovation. The refurbishment of guest house 1 began in May 2021 and is currently expected to be completed by March 2022, with the refurbishment of guest house 2 and 3 envisaged for 2022/2023.

Guest house 4 was built in 2012 and offers nine single and two double rooms (with two separate bedrooms). All rooms are equipped with TV connection ports and telephones. Furthermore, the building has a multi-purpose room, which for example is used for German classes, a large terrace and a light garden for the common use and enjoyment. In autumn 2021, it has been further improved by the installation of a fully equipped kitchen with a meeting/dining room. Guest house 4 also accommodates six offices for up to 11 short term guests, a parent-child office, in case family circumstances require a colleague to bring children to work, 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 mpi**pks** has a Scientific Advisory Board. The members of the Board advise the board of directors concerning the research at the institute. The Board assesses the research direction of the institute, the scientific relevance and likelihood of success of the research projects, as well as the collaborations among members of the institute, with universities, other research institutions and with industry. The Scientific Advisory Board evaluates the results of the research work presented by the board of directors in the triennial research report and prepares, usually every three 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:

Blume, D.
Professor Dr.

University of Oklahoma
Homer L. Dodge Department of Physics and Astronomy
440 W. Brooks St.
NORMAN, OK 73019
USA

Brabec, T.
Professor Dr.

University of Ottawa
Department of Physics
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CANADA

Chen, X.
Professor Dr.

California Institute of Technology
Division of Physics, Mathematics and Astronomy
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USA

Furusaki, A.
Professor Dr.

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Condensed Matter Theory Laboratory
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WAKO, SAITAMA 351-0198
JAPAN

Hlinka, J.
Professor Dr.

Czech Academy of Sciences
Institute of Computer Science
Pod Vodarenskou vezi 271/2
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CZECH REPUBLIC

Howard, M.
Professor Dr.

John Innes Centre
Norwich Research Park
Norwich NR4 7UH
UNITED KINGDOM

Mahadevan, L.
Professor Dr.

The Applied Math Lab
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Martinez, T. J.
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UNITED KINGDOM

Singh, R.
Professor Dr.

University of California, Davis
Department of Physics and Astronomy
One Shields Avenue
DAVIS, CA95616
USA

3.10.2 Board of Trustees

In accord with the rules of the Max Planck Society the mpi**pks** has formed a Board of Trustees. The board members discuss and consult the proposed budget, the annual report, and the budget of the last year of mpi**pks** together with the directors. The Board of Trustees advises the institute on important issues and promotes the connection of the institute to research oriented circles in the society. The Board of Trustees had the following members during the period of this report (current membership is until December 31, 2024):

Birgel, D.	Chefredakteur Dresdner Neueste Nachrichten Dr. Külz-Ring 12 01067 Dresden
Gemkow, S.	Sächsische Staatsminister für Wissenschaft Wigardstraße 17 01097 Dresden
Harms, C. Dr.	Kretschmerstraße 21 01309 Dresden
Hilbert, D.	Oberbürgermeister Landeshauptstadt Dresden Dr.-Külz-Ring 19 01067 Dresden
Hollenders, Ch. Dr.	Honorarkonsul Republik Korea Notariat Dr. Hollenders Königstraße 1 01097 Dresden
Kretschmer, M.	Ministerpräsident des Freistaates Sachsen Staatskanzlei Archivstraße 1 01097 Dresden
Leonhardt, K. Dr.	Vorstandsvorsitzende Sächsische Aufbaubank Pirnaische Straße 9 01069 Dresden
Milbradt, G. Prof. Dr.	Ministerpräsident des Freistaates Sachsen a.D. Stiller Winkel 4 01328 Dresden
Olbertz, J.-H. Prof. Dr.	Humboldt-Universität zu Berlin Institut für Erziehungswissenschaften Unter den Linden 6 10099 Berlin

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Dipl.-Phys.

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01626 Dresden

Schmidt, F.
Dr.-Ing.

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01328 Dresden

Timm, C.
Prof. Dr.

Dekan der Fachrichtung Physik
Technische Universität Dresden
01062 Dresden

3.11 Members of the mpipks

(as of September 2021)

1. mpi**pks positions** — **56**

   - Scientific personnel 16
     Scientific members *3*
     Research staff (including research group leaders) *13*
   - Technical staff 9
   - Administration and infrastructure staff 31

2. **Externally funded research staff** — **8**

3. **PhD students** — **80**

   - PhD students with internal supervision 69
     German PhD students *16*
     Foreign PhD students *64*
   - PhD students with external supervision 11
     PhD students with external funding *7*
     IMPRS PhD students with external supervision *25*

4. **Guest scientists** — **78**

   - German guest scientists 8
   - Foreign guest scientists 70

Chapter 4

Publications

4.1 Atomic and Molecular Structure

2019

Eiles, M. T.: Trilobites, butterflies, and other exotic specimens of long-range Rydberg molecules. Journal of Physics B **52**, 113001 (2019)

Herzog-Arbeitman, J., S. Mantilla, I. Sodemann: Solving the quantum dimer and six-vertex models one electric field line at a time. Physical Review B **99**, 245108 (2019)

Kumar, P., B. Poirier: Isotope shifts and band progressions in SO_2 rovibrational energy levels: using quantum theory to extract rotational constants. Molecular Physics **117**, 2456-2469 (2019)

Scharf, B., F. Pientka, H. Ren, A. Yacoby, E. M. Hankiewicz: Tuning topological superconductivity in phase-controlled Josephson junctions with Rashba and Dresselhaus spin-orbit coupling. Physical Review B **99**, 214503 (2019)

Takayoshi, S., Y. Murakami, P. Werner: High-harmonic generation in quantum spin systems. Physical Review B **99**, 184303 (2019)

2020

Dubois, J., C. Chandre, T. Uzer: Nonadiabatic effects in the double ionization of atoms driven by a circularly polarized laser pulse. Physical Review E **102**, 032218 (2020)

Eiles, M. T., C. Fey, F. Hummel, P. Schmelcher: Triatomic butterfly molecules. Journal of Physics B **53**, 084001 (2020)

Giannakeas, P., M. T. Eiles, F. Robicheaux, J. M. Rost: Dressed Ion-Pair States of an Ultralong-Range Rydberg Molecule. Physical Review Letters **125**, 123401 (2020)

Giannakeas, P., M. T. Eiles, F. Robicheaux, J. M. Rost: Generalized local frame-transformation theory for ultralong-range Rydberg molecules. Physical Review A **102**, 033315 (2020)

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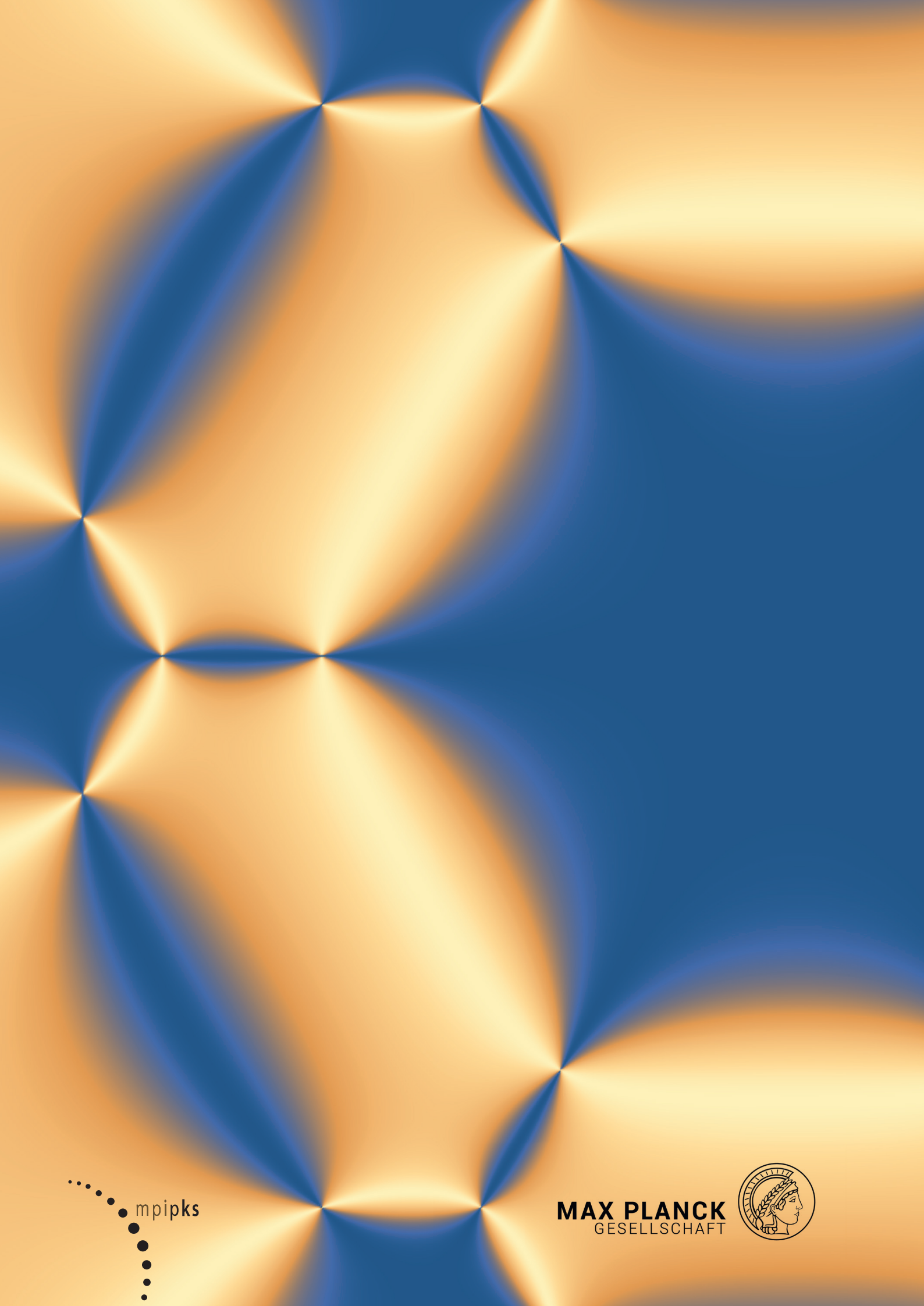

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