Dynamics and Statistical Physics Division
Fachverband Dynamik und Statistische Physik (DY)

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Overview of Invited Talks and Sessions

(Lecture halls H3, H6, H19, and H20; Poster B2)

Prize talk and Plenary talks

PLV I	Mon	8:30– 9:15	H1	**Linking the International System of Units to Fundamental Constants** — •Joachim Ullrich
PRV II	Mon	13:15–13:45	H1	**Ultimate Rayleigh-Bénard and Taylor-Couette turbulence** — •Detlef Lohse
PLV II	Mon	14:00–14:45	H1	**Self-propelled topological defects in biological systems** — •Julia M Yeomans
PLV IV	Tue	8:30– 9:15	H1	**Impact of Turbulence on Cloud Microphysics** — •Eberhard Bodenschatz
PLV IX	Wed	14:00–14:45	H2	**Vestigial order in quantum materials** — •Jörg Schmalian
PLV XIII	Thu	14:00–14:45	H2	**The Physics of Inference and Community Detection** — •Cristopher Moore
PLV XIV	Fri	8:30– 9:15	H1	**Soft Matter: Topological constraints do matter** — •Kurt Kremer

Invited Talks

DY 3.1	Mon	9:30–10:00	H20	**Collective behavior and self-organisation of active granular particles** — •Thorsten Pöschel, Michael Engel, Christian Scholz, Harol Torres
DY 5.1	Mon	10:00–10:30	H3	**Direct numerical simulations towards ultimate turbulence** — •Richard Stevens, Roberto Verzicco, Detlef Lohse
DY 12.1	Tue	9:30–10:00	H3	**Active Cell Nematics: Architectures and flows.** — •Pascal Silberzan
DY 14.1	Tue	9:30–10:00	H19	**The Fibonacci family of dynamical universality classes** — •Gunter M. Schütz
DY 18.1	Tue	10:00–10:30	H20	**Bursting, amplitude explosions and mixed mode oscillations at the onset of shear flow turbulence** — •Björn Hof, Chaitanya Paranjape, Yohann Duguet, Vasudevan Mukund, Nazmi B Budanur
DY 25.1	Wed	9:30–10:00	H3	**Why the desert is not flat** — •Klaus Kroy
DY 29.1	Wed	9:30–10:00	H19	**Dynamical localization in Z_2 lattice gauge theories** — •Dmitry Kovrizhin
DY 30.1	Wed	10:00–10:30	H6	**Fluctuations and responses in nonequilibrium fluids** — •Matthias Krüger
DY 32.1	Wed	15:00–15:30	H3	**Phase-separation in an elastic matrix: from living cells to synthetic materials** — •Eric Dufresne
DY 36.1	Wed	15:00–15:30	H20	**Quantum Machine Learning** — •Anatole von Lilienfeld
DY 40.1	Thu	9:30–10:00	H3	**Non-Brownian diffusion: from disorder to physical insights** — •Ralf Metzler
DY 42.1	Thu	9:30–10:00	H20	**Quantum dynamics in strongly correlated one-dimensional Bose gases** — •Hanns-Christoph Nägerl
DY 42.2	Thu	10:00–10:30	H20	**Extreme Decoherence and Quantum Chaos** — Zhenyu Xu, Aurélia Chenu, Luis Pedro García-Pintos, Javier Molina-Vilaplana, •Adolfo Del Campo

DY 42.10	Thu	12:30–13:00	H20	**Semiclassical approach in Bose-Hubbard models: from universal spectral statistics to far-out-of-equilibrium dynamics** — •Remy Dubertrand
DY 57.1	Fri	9:30–10:00	H3	**Toroidal droplets, active nematics and topological defects** — •Alberto Fernandez-Nieves
DY 59.1	Fri	9:30–10:00	H19	**Energy landscape exploration approach for non-ergodic soft matter systems** — •Michael Schmiedeberg

Invited talks of the joint Symposium SKM Dissertation-Prize 2019

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:50	H2	**Synchronization and Waves in Confined Complex Active Media** — •Jan Frederik Totz
SYSD 1.2	Mon	9:50–10:10	H2	**Spin scattering of topologically protected electrons at defects** — •Philipp Rüssmann
SYSD 1.3	Mon	10:10–10:30	H2	**Beyond the molecular movie: Revealing the microscopic processes behind photo-induced phase transitions** — •Chris W. Nicholson
SYSD 1.4	Mon	10:30–10:50	H2	**Thermodynamic bounds on current fluctuations** — •Patrick Pietzonka
SYSD 1.5	Mon	10:50–11:10	H2	**Lightwave-driven quasiparticle acceleration** — •Fabian Langer
SYSD 1.6	Mon	11:10–11:30	H2	**Ultrafast plasmon-driven point-projection electron microscopy** — •Jan Vogelsang
SYSD 1.7	Mon	11:30–11:50	H2	**Helimagnets, sand patterns and fingerprints linked by topology** — •Peggy Schönherr

Invited talks of the joint Symposium Patterns in Nature: Origins, Universality, Functions

See SYPN for the full program of the symposium.

SYPN 1.1	Mon	15:00–15:30	H1	**Engineering spatial-temporal organization of bacterial suspensions** — •Igor Aronson
SYPN 1.2	Mon	15:30–16:00	H1	**Collective behaviour and pattern formation in phoretic active matter** — •Ramin Golestanian
SYPN 1.3	Mon	16:00–16:30	H1	**Control and selection of spatio-temporal patterns in complex systems** — •Svetlana Gurevich
SYPN 1.4	Mon	16:45–17:15	H1	**Self-organization of Active Surfaces** — •Frank Jülicher
SYPN 1.5	Mon	17:15–17:45	H1	**Front instabilities can reverse desertification** — •Ehud Meron

Invited talks of the joint Symposium Geometry, Topology, and Condensed Matter

See SYGT for the full program of the symposium.

SYGT 1.1	Tue	9:30–10:00	H1	**Thermal Properties of Vortices on Curved Surfaces** — •José Lorenzana
SYGT 1.2	Tue	10:00–10:30	H1	**Curvature–induced effects in manomagnets** — •Denis Sheka
SYGT 1.3	Tue	10:30–11:00	H1	**Magnetization configurations and reversal of individual ferromagnetic nanotubes** — •Martino Poggio
SYGT 1.4	Tue	11:15–11:45	H1	**An experimental perspective on topology and nanoelectronics in graphene and related 2D materials.** — •Ivan J. Vera-Marun
SYGT 1.5	Tue	11:45–12:15	H1	**Roles of the curvature in two-dimensional nematic films** — •Gaetano Napoli

Invited talks of the joint Symposium Hydrodynamic Electronics: Transport in ultra-pure Quantum Systems

See SYHE for the full program of the symposium.

SYHE 1.1	Wed	9:30–10:00	H1	**Hydrodynamic theory of dissipative magnetophonons** — •Sean Hartnoll
SYHE 1.2	Wed	10:00–10:30	H1	**Unconventional transport in mesostructures of ultra-pure delafossite metals** — •Andrew Mackenzie
SYHE 1.3	Wed	10:30–11:00	H1	**Topological Materials with liquid electrons** — •Claudia Felser
SYHE 1.4	Wed	11:15–11:45	H1	**Hydrodynamic approach to electronic transport** — •Boris Narozhny

SYHE 1.5	Wed	11:45–12:15	H1	**Electron hydrodynamics in graphene: introduction and status** — •Denis Bandurin

Invited talks of the joint Symposium Czech Republic as Guest of Honor

See SYCZ for the full program of the symposium.

SYCZ 1.1	Thu	9:30–10:00	H4	**Crystal symmetries and transport phenomena in antiferromagnets** — •Tomas Jungwirth
SYCZ 1.2	Thu	10:00–10:30	H4	**Terahertz subcycle charge and spin control** — •Rupert Huber
SYCZ 1.3	Thu	10:30–11:00	H4	**1D molecular system on surfaces** — •Pavel Jelinek
SYCZ 1.4	Thu	11:15–11:45	H4	**Tunneling microscopy on insulators provides access to out-of-equilibrium charge states** — •Jascha Repp
SYCZ 1.5	Thu	11:45–12:15	H4	**Occam's razor and complex networks from brain to climate** — •Jaroslav Hlinka
SYCZ 1.6	Thu	12:15–12:45	H4	**Long range temporal correlations in complex systems** — •Holger Kantz

Invited talks of the joint Symposium Physics of Self-Organization in DNA Nanostructures

See SYDN for the full program of the symposium.

SYDN 1.1	Thu	9:30–10:00	H1	**Functional DNA Nanostructures and Their Applications** — •Itamar Willner
SYDN 1.2	Thu	10:00–10:30	H1	**Gaining control of DNA-based nanodevices** — •Francesco Ricci
SYDN 1.3	Thu	10:30–11:00	H1	**Self-assembly and optical properties of single molecule polymers on DNA origami** — •Kurt Gothelf
SYDN 1.4	Thu	11:15–11:45	H1	**DNA origami route to dynamic plasmonics** — •Laura Liu
SYDN 1.5	Thu	11:45–12:15	H1	**DNA templated metal nanostructures** — •Ralf Seidel

Sessions

DY 1.1–1.3	Sun	16:00–18:30	H3	**Tutorial: Statistical Physics Methods for Data Science in Physics (joint SOE/DY/CPP/BP/jDPG) (joint session SOE/DY/TUT)**
DY 2.1–2.10	Mon	9:30–12:15	H8	**Responsive and Adaptive Systems (joint session CPP/DY)**
DY 3.1–3.11	Mon	9:30–12:45	H20	**Active Matter A (joint session DY/CPP)**
DY 4.1–4.12	Mon	9:30–12:45	H22	**Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/DY)**
DY 5.1–5.9	Mon	10:00–12:45	H3	**Convection**
DY 6.1–6.11	Mon	10:00–13:00	H19	**Dynamics in many-body systems: Equilibration and localization I (joint session DY/TT)**
DY 7.1–7.8	Mon	15:00–17:15	H14	**Interfaces and Thin Films (joint session CPP/DY)**
DY 8.1–8.10	Mon	15:00–17:45	H20	**Networks: From Topology to Dynamics (joint session DY/SOE)**
DY 9.1–9.9	Mon	15:30–18:00	H19	**Dynamics in many-body systems: Equilibration and localization II (joint session DY/TT)**
DY 10.1–10.5	Mon	16:15–17:30	H8	**Glasses and Glass Transition (joint session CPP/DY)**
DY 11.1–11.8	Tue	9:30–13:00	H2	**Focus Session: Quantum Dynamics of Kinetically Constrained Many-Body Systems (joint session TT/DY)**
DY 12.1–12.1	Tue	9:30–10:00	H3	**Talk Pascal Silberzan**
DY 13.1–13.12	Tue	9:30–13:00	H13	**Wetting, Fluidics and Liquids at Interfaces and Surfaces (joint session CPP/DY)**
DY 14.1–14.1	Tue	9:30–10:00	H19	**Talk Gunter M. Schütz**
DY 15.1–15.12	Tue	10:00–13:15	H3	**Pattern Formation**
DY 16.1–16.6	Tue	10:00–11:30	H6	**Quantum Dynamics, Decoherence and Quantum Information**
DY 17.1–17.10	Tue	10:00–12:45	H19	**Statistical Physics (General) I**
DY 18.1–18.10	Tue	10:00–13:00	H20	**Fluid physics and turbulence**
DY 19.1–19.5	Tue	11:45–13:00	H6	**Complex Systems**
DY 20.1–20.7	Tue	14:00–15:45	H3	**Active Matter B (joint session DY/CPP)**
DY 21.1–21.6	Tue	14:00–15:30	H6	**Statistical Physics (General) II**

DY 22.1–22.6	Tue	14:00–15:30	H19	**Critical Phenomena and Phase Transitions**
DY 23.1–23.6	Tue	14:00–15:30	H20	**Stochastic Thermodynamics**
DY 24.1–24.8	Tue	14:00–16:00	H23	**Spintronics (joint session TT/MA/DY)**
DY 25.1–25.10	Wed	9:30–12:30	H3	**Granular Matter / Contact Dynamics**
DY 26.1–26.12	Wed	9:30–13:00	H4	**Active matter I (joint session BP/CPP/DY)**
DY 27.1–27.11	Wed	9:30–12:45	H14	**Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)**
DY 28.1–28.5	Wed	9:30–12:00	H17	**Dynamics of Multilayer Networks I (Focus Session SOE/DY/BP) (joint session SOE/DY/BP)**
DY 29.1–29.12	Wed	9:30–13:00	H19	**Many-body Quantum Dynamics**
DY 30.1–30.9	Wed	10:00–12:45	H6	**Statistical Physics far from Thermal Equilibrium**
DY 31.1–31.12	Wed	10:00–13:15	H20	**Nonlinear Dynamics, Synchronization and Chaos**
DY 32.1–32.15	Wed	15:00–19:15	H3	**Complex Fluids and Soft Matter (joint session DY/CPP)**
DY 33.1–33.9	Wed	15:00–17:30	H4	**Statistical physics of biological systems I (joint session BP/DY)**
DY 34.1–34.5	Wed	15:00–16:45	H17	**Dynamics of Multilayer Networks II (Focus Session SOE/DY/BP) (joint session SOE/DY/BP)**
DY 35.1–35.8	Wed	15:00–17:00	H18	**Modeling and Simulation of Soft Matter I (joint session CPP/DY)**
DY 36.1–36.13	Wed	15:00–18:45	H20	**Condensed-matter simulations augmented by advanced statistical methodologies (joint session DY/CPP)**
DY 37.1–37.6	Wed	15:30–17:00	H6	**Quantum Chaos**
DY 38.1–38.9	Wed	15:30–18:00	H19	**Microswimmers (joint session DY/CPP)**
DY 39.1–39.5	Wed	17:15–18:30	H6	**Quantum matter: Chaos, correlation**
DY 40.1–40.1	Thu	9:30–10:00	H3	**Talk R. Metzler**
DY 41.1–41.8	Thu	9:30–12:00	H13	**Modeling and Simulation of Soft Matter II (joint session CPP/DY)**
DY 42.1–42.10	Thu	9:30–13:00	H20	**Focus: Many-Body Quantum Chaos**
DY 43.1–43.12	Thu	10:00–13:15	H3	**Anomalous diffusion / Brownian motion**
DY 44.1–44.10	Thu	10:00–12:45	H19	**Active Matter C (joint session DY/CPP)**
DY 45.1–45.3	Thu	10:30–11:15	H6	**The Physics of Power grids (joint session DY/SOE)**
DY 46.1–46.4	Thu	11:30–12:30	H17	**Energy Networks (joint SOE/DY) (joint session SOE/DY)**
DY 47.1–47.9	Thu	15:00–17:30	H11	**Statistical physics of biological systems II (joint session BP/DY)**
DY 48.1–48.8	Thu	15:00–18:45	H17	**Theory of Stochastic Processes with Applications in Biology (joint session SOE/BP/DY/AKjDPG)**
DY 49.1–49.11	Thu	15:00–18:00	H23	**Quantum-Critical Phenomena (joint session TT/DY)**
DY 50.1–50.24	Thu	15:00–18:00	Poster B2	**Poster: Nonlinear Systems, Patterns, Flows ..**
DY 51.1–51.11	Thu	15:00–18:00	Poster B2	**Poster: Stat. Phys., Comp. Meth**
DY 52.1–52.13	Thu	15:00–18:00	Poster B2	**Poster: Active Matter, Microswimmer, Microfluidics**
DY 53.1–53.11	Thu	15:00–18:00	Poster B2	**Poster Quantum Systems**
DY 54.1–54.11	Thu	15:00–18:00	Poster B2	**Poster: Complex, Fluids, Glasses, Granular**
DY 55.1–55.14	Thu	15:00–18:00	Poster B2	**Poster: Noneq. Stat. Phys., Stat. Bio. Phys., Brownian**
DY 56	Thu	18:30–19:30	H3	**Annual General Meeting of the Dynamics and Statistical Physics Division**
DY 57.1–57.1	Fri	9:30–10:00	H3	**Talk Alberto Fernandes-Nieves**
DY 58.1–58.10	Fri	9:30–12:00	H11	**Active matter II (joint session BP/CPP/DY)**
DY 59.1–59.1	Fri	9:30–10:00	H19	**Talk Michael Schmiedeberg**
DY 60.1–60.7	Fri	10:00–11:45	H3	**Statistical Physics in Biological Systems III**
DY 61.1–61.8	Fri	10:00–12:15	H6	**Microfluidics (joint session DY/CPP)**
DY 62.1–62.7	Fri	10:00–11:45	H19	**Glasses and Glass transition (joint session DY/CPP)**
DY 63.1–63.6	Fri	10:00–11:30	H20	**Modeling and Data Analysis**
DY 64.1–64.1	Fri	12:30–13:15	H1	**Closing talk (joint session BP/CPP/DY)**

Annual General Meeting of the Dynamics and Statistical Physics Division

Do 4. April 18:30–19:30 H3

- Bericht
- Verschiedenes

DY 1: Tutorial: Statistical Physics Methods for Data Science in Physics (joint SOE/DY/CPP/BP/jDPG) (joint session SOE/DY/TUT)

Big Data is an ubiquitious buzzword, but beyond storing and processing large datasets, challenges in applications often lie in high-dimensional and nontrivial structures (= the content!) within the datasets. Artificial intelligence approaches, paired with statistical physics methods, can provide powerful tools which can go far beyond standard statistical methods. The tutorial gives an overview both on methods from stochastic blockmodeling, network analysis, inference and machine learning and on applications ranging from socioeconomic networks to biomolecular simulations. (Session organized by Jens Christian Claussen and Andreas Fery with the divisions of SOE, DY, BP and CPP.)

Time: Sunday 16:00–18:30 Location: H3

Tutorial DY 1.1 Sun 16:00 H3

Statistical network inference and community detection — •Tiago Peixoto — University of Bath, UK

Network structures are shaped by evolutionary mechanisms and determine the central aspects of how a system functions. However, differently from systems that are naturally embedded in space, we cannot simply "look" at network in order to extract its most important structural patterns. Instead, we must rely on well-founded algorithmic methods to extract this information from data in an interpretable way. In this tutorial, we review a principled approach to this problem based on the elaboration of probabilistic models of network structure, and their statistical inference from empirical data. We focus in particular on the detection of modules (or "communities") in networks.

We aim to cover the following topics: 1. The stochastic block model (SBM) and its variants (degree correction, overlapping groups, etc.); 2. Bayesian inference and model selection: Distinguishing structure from noise; 3. Generalizing from data: Prediction of missing and spurious links; 4. Model extensions: Layered, dynamic SBMs, and generalized models on continuous latent spaces; 5 Fundamental limits of inference, and the undetectability phase transition; 6. Efficient inference algorithms; 7. Network reconstruction from noisy or indirect data.

Tutorial DY 1.2 Sun 16:50 H3

Network filtering for big data — •Tiziana Di Matteo — Department of Mathematics - King's College London

In this lecture I will present network-theoretic tools to filter information in large-scale datasets and I will show that these are powerful tools to study complex datasets. In particular I will introduce correlation-based information filtering networks and the planar filtered graphs (PMFG) and I will show that applications to financial data-sets can meaningfully identify industrial activities and structural market changes. It has been shown that by making use of the 3-clique structure of the PMFG a clustering can be extracted allowing dimensionality reduction that keeps both local information and global hierarchy in a deterministic manner without the use of any prior information. To advance the PMFG (currently O(N3)), I will introduce a new algorithm, the TMFG (Triangulated Maximally Filtered Graph), that efficiently extracts a planar subgraph which optimizes an objective function. The method is scalable to very large datasets and it can take advantage of parallel and GPUs computing. The method is adaptable allowing online updating and learning with continuous insertion and deletion of new data as well changes in the strength of the similarity measure. Finally I will also show that filtered graphs are valuable tools for risk management and portfolio optimization too and they allow to construct probabilistic sparse modeling for financial systems that can be used for forecasting, stress testing and risk allocation.

Tutorial DY 1.3 Sun 17:40 H3

Multiscale simulations of soft matter augmented by data-driven methods — •Tristan Bereau — Max Planck Institute for Polymer Research

Multiscale simulations, all the way from quantum chemistry to continuum mechanics, probe a variety of length and time scales relevant to soft-matter systems. In this tutorial, I will describe different strategies to help improve physics-based simulations with recently-developed data-driven methods and concepts. Applications discussed will include Bayesian inference for molecular kinetics, machine learning to vastly improve force-field transferability, and high-throughput screening to explore chemical compound space.

DY 2: Responsive and Adaptive Systems (joint session CPP/DY)

Time: Monday 9:30–12:15 Location: H8

DY 2.1 Mon 9:30 H8

H2O / D2O swelling and exchange kinetics of a multi-stimuli responsive PNIPAM-based block copolymer thin film — •Lucas Kreuzer[1], Tobias Widmann[1], Nuri Hohn[1], Kun Wang[1], Jean-Francois Moulin[2], Viet Hildebrand[3], André Laschewsky[3], Christine M. Papadakis[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Helmholtz-Zentrum Geesthacht at Heinz Maier-Leibnitz Zentrum, Lichtenbergstr. 1, 85747 Garching — [3]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Straße 24-25, 14476 Potsdam Golm

Stimuli-responsive polymers can react with a drastic change in properties towards even slight changes in their surrounding environment. Especially in thin film morphology, such films are well-suited for a manifold of applications such as nano-switches, artificial muscles in soft-robotics or sensors. In order to implement stimuli-responsive polymers in the aforementioned application fields, a fundamental understanding of the underlying kinetics is necessary. In our recent work, we followed the H2O and D2O swelling and the corresponding exchange kinetics in a multi-stimuli responsive block copolymer thin film with in-situ time of flight (TOF) neutron reflectometry (NR). TOF-NR enables high time resolution with which the mechanisms of water uptake and exchange can be followed. A theoretical model is applied to describe the swelling and exchange kinetics in order to obtain detailed insights about the underlying mechanisms of these dynamic processes.

DY 2.2 Mon 9:45 H8

Morphology of Thermoresponsive Molecular Brushes with Copolymer Side Arms in Aqueous Solution — •Jia-Jhen Kang[1], Junpeng Zhao[2], Henrich Frielinghaus[3], Lester Barnsley[3], Fabian Kohler[1], Hendrik Dietz[1], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, Athens, Greece — [3]FZ Jülich, JCNS at MLZ, Garching, Germany

Poly (ethylene oxide) (PEO) and poly (propylene oxide) (PPO) are known to be thermoresponsive polymers both exhibiting lower critical solution temperature (LCST) behavior, with the cloud points >100 °C and 8 °C, respectively. In the present work, we aim to investigate the LCST behavior of their densely-grafted analogues, namely molecular brushes, which are polymers composed of a polymeric backbone and side arms attached to virtually every monomer of the backbone. Molecular brushes with PEO-ran-PPO and PEO-block-PPO copolymer side arms were studied in aqueous solution using dynamic light scattering (DLS) and small angle neutron scattering (SANS). They display mixed LCST behavior based on the two components, indicating new properties induced by the densely-grafted architecture.

DY 2.3 Mon 10:00 H8

Formation and growth of mesoglobules in aqueous poly(N-isopropylacrylamide) solutions at low and high pressures revealed with fast pressure jumps — •Bart-Jan Niebuur[1], Leonardo Chiappisi[2], Florian Jung[1], Xiaohan Zhang[1], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]TU München, Physik Department, Physik weicher Materie, Garching, Germany — [2]Institut Laue-Langevin, Large Scale Structures Group, Grenoble, France — [3]University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando, U.S.A.

Understanding the kinetics of phase separation is of importance for numerous systems. The thermoresponsive polymer poly(N-isopropylacrylamide) (PNIPAM) presents a model system to investigate the kinetics of phase separation. In aqueous solutions at temperatures above the cloud point, PNIPAM forms stable mesoglobules with their size and hydration state depending strongly on pressure [1]. To elucidate the formation and early stage growth of the mesoglobules, we applied time-resolved small-angle neutron scattering after rapid pressure jumps inducing phase separation at low and high pressures. We find that mesoglobule formation includes the formation of small clusters, growth by diffusion-limited coalescence, and the formation of a dense shell, slowing down further coalescence [2]. The strong dehydration at low pressures results in much slower kinetics than at high pressures, where the chains stay more hydrated. [1] B.-J. Niebuur, C. M. Papadakis et al., *ACS Macro Lett.* 2017, **6**, 1180. [2] B.-J. Niebuur, C. M. Papadakis et al., *ACS Macro Lett.* 2018, **7**, 1155

DY 2.4 Mon 10:15 H8

The structural and dynamic behavior of the thermoresponsive polymer Poly(N-isopropylmethacrylamide) — •Chia-Hsin Ko[1], Kora-Lee Claude[1], Dirk Schanzenbach[2], Bart-Jan Niebuur[1], Henrich Frielinghaus[3], Lester Barnsley[3], Vitaliy Pipich[3], Alfons Schulte[4], Peter Müller-Buschbaum[1], André Laschewsky[2,5], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Universität Potsdam, Institut für Chemie, Germany — [3]FZ Jülich, JCNS at MLZ, Garching, Germany — [4]University of Central Florida, Department of Physics, Orlando, U.S.A — [5]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany

Poly(N-isopropylmethacrylamide) (PNIPMAM) is a thermoresponsive polymer, exhibiting lower critical solution temperature (LCST) behavior in aqueous solution. Compared to the well-investigated poly(N-isopropylacrylamide) (PNIPAM), which has similar chemical structure, PNIPMAM has a higher transition temperature (43 °C instead of 32 °C). This may be due to the presence of the additional methyl groups on the vinyl backbone, which cause steric hindrance and weaken the intramolecular interactions. We investigate the temperature- and concentration-dependent phase behavior of PNIPMAM in D_2O using turbidimetry, dynamic light scattering (DLS), small-angle neutron scattering (SANS) and Raman spectroscopy. The main difference from PNIPAM are inhomogeneities in the one-phase state due to physical crosslinks caused by the methyl groups.

DY 2.5 Mon 10:30 H8

All-in-One 'Schizophrenic' Self-assembly of Orthogonally Tuned Thermo-responsive Diblock Copolymers — Natalya S. Vishnevetskaya[1], Viet Hildebrand[2], Peter Müller-Buschbaum[1], André Laschewsky[2,3], and •Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Universität Potsdam, Institut für Chemie, Germany — [3]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany

Smart, fully orthogonal switching was realized in a diblock copolymer system with variable trigger-induced aqueous self-assembly [1]. The polymers are composed of non-ionic and zwitterionic blocks featuring lower and upper critical solution temperatures (LCST, UCST). Due to the salt-sensitivity of the zwitterionic block, the UCST can be varied by addition of salt. Superimposed orthogonal switching by electrolytes results in 'schizophrenic' micellization, in which the roles of the core and the shell block are interchanged. The following switching scenarios are observed by turbidimetry and SANS: i) via a molecularly dissolved state at low NaBr concentrations, or (ii) via an insoluble state at high NaBr concentrations. The versatile and tunable self-assembly of such diblock copolymers offers manifold opportunities, e.g. for smart emulsifiers.

1. N. S. Vishnevetskaya et al., Macromolecules 51, 2604 (2018)

DY 2.6 Mon 10:45 H8

PNIPAM microgel-stabilized aqueous foams and foam films — •Matthias Kühnhammer and Regine von Klitzing — Technical University of Darmstadt, Soft Matter at Interfaces, Darmstadt, Germany

Cross-linked, short-chained poly-N-isopropylacrylamide (NIPAM) polymers have been in the focus of numerous studies in the past years and are still being discussed very actively in the context of multiple possible applications, because of their ability to respond to external stimuli like temperature. A prominent example are thermo-responsive emulsions stabilized by microgel particles adsorbed at the water-oil interface. In these systems the emulsion stability can be controlled by changing the temperature.

In this contribution the interfacial activity of PNIPAM microgels is exploited to stabilize aqueous foams. These foams are very stable at temperatures below the volume phase transition temperature (VPTT) of NIPAM and can be destabilized by increasing the temperature above the VPTT. In addition, the relation between the properties of individual microgels (e.g. size, elasticity, particle concentration) and the properties of foams prepared with them is studied. The properties of foam films are studied with a thin film pressure balance and are related to features of macroscopic foams investigated in drainage experiments and with neutron scattering.

DY 2.7 Mon 11:00 H8

Reversible surface structuring of photosensitive polymer films: In-situ atomic force microscopy and diffraction efficiency measurements — •Joachim Jelken, Burkhard Stiller, Carsten Henkel, and Svetlana Santer — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Here we report on light induced reversible structuring of azobenzene containing polymer films under dynamic changing of local distribution of electrical field vector in interference pattern used for the polymer irradiation. This is achieved utilizing a homemade setup which consists of three parts: a two beam interference setup for topography structuring, an atomic force microscope (AFM) for in-situ recording (during irradiation) of surface morphology[1,2], and a diffraction efficiency (DE) setup which enables to obtain information about the birefringence grating at the same time. Introducing a phase delay between the two interfering beams results in a shift of the whole interference pattern along the sample plane. Depending on the shifting speed the topography grating follows the redistribution of electrical field vector. In this way one can reversible structure and flatten surface topography in controlled manner. Using the measured kinetics of topography and birefringence gratings we aim to further understand the process of surface relief grating formation in azobenzene containing polymer films [3]. [1]S. N. Yadavalli, M. Saphiannikova and S. Santer, Appl. Phys. Lett., 2014, 105, 051601 [2]S. N. Yadavalli and S. Santer, J. of Appl. Phys., 2013, 113, 224304-12 [3]V. Toshchevikov, J. Ilnytskyi and M. Saphiannikova, J. Phys. Chem. Lett. 2017, 8, 1094

15 min. break

DY 2.8 Mon 11:30 H8

Modelling of light-induced deformations in side-chain azopolymers — •Bharti Yadav, Jan Domurath, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Str. 6, 01069 Dresden

Photopolymers deform in the presence of light, even below the glass transition temperature, because the stress produced by the light is greater than the yield stress [1]. The deformations in the photopolymers are directional i.e. they depend on the polarization of light [2]. For linearly polarized light the deformation is in the direction of the polarization and for circularly polarized light in the plane perpendicular to the propagation vector. These directional deformations are caused by the light-induced orientation potential, which acts on each chromophore attached to the main chain. From the orientation potential one can calculate the light-induced stress in the sample. We model these photopolymers as visco-plastic materials by implementing the light-induced stress using ANSY, a finite element modelling software. We calculate the strain and elongation as a function of time for both linearly and circularly polarized light.

[1] Toshchevikov, V. et al. J. Phys. Chem. Lett. 8 (2017) p.1094-1098

[2] Kang., H. S. et al. Adv. Funct. Mater. 24 (2014) p.7273-7283

DY 2.9 Mon 11:45 H8

Columnar clusters of three-arm azobenzene stars - MD simulations of a light-induced phase transition — •Markus Koch[1], Marina Saphiannikova[1], Svetlana Santer[2], and Olga Guskova[1] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, Germany

In this study we investigate star-shaped molecules consisting of a central benzenetricarboxamide (BTA) core and three symmetrically attached azobenzene groups. In aqueous solution these molecules exhibit a distinctive photoresponsive self-assembly behavior. In the absence of light or exposed to blue visible light they form long fibrous structures. When irradiated with UV light the columns disassemble but can be restored after resuming exposure to the initial conditions [1]. This phase transition is a result of the trans-cis photoisomerization of the centrally anchored azobenzene arms. We demonstrate, using DFT and MD simulations, that the solvophilicity of azo stars increases with the number of azo groups present in the cis state [2]. Further on using MD simulations, the stability of the columnar clusters in water is tested, while again varying the amount of trans and cis arms per molecule. Our results indicate that clusters with a large fraction of cis-arms display higher disorder or may even break apart. Lastly, also the kinetics of cluster self-assembly from random initial distributions is studied.

We gratefully acknowledge support from the German Research Foundation (DFG), projects GU 1510/3-1 and SA 1657/13-1.

[1] Lee, S. et al. Langmuir 29 (19), 5869 (2013)
[2] Koch, M. et al. J. Phys. Chem. B 121, 8854 (2017)

DY 2.10 Mon 12:00 H8

Dissipative systems with nonlocal delayed feedback — •Josua Grawitter, Reinier van Buel, Christian Schaaf, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

We present a linear model, which mimics the response of a spatially extended dissipative medium to a distant perturbation and investigate its dynamics under delayed feedback control [Grawitter *et al.*, New J. Phys. **20**, 113010 (2018)]. In our model the time it takes a perturbation to travel to the location of measurement is described by an inherent delay time. We investigate the resulting double-delay differential equation using linear stability analysis and numerical integration.

For nonzero delay, linear stability analysis reveals that sufficiently strong feedback destabilizes the system's trivial fixed point. When feedback is bounded by a smooth sigmoid function, the stability-instability transition follows a supercritical Hopf bifurcation and a stable limit cycle occurs. Its frequency and amplitude respond to parameter changes like the dominant eigenvalue of the linearized problem. In particular, they show similar discontinuities along specific lines. These results are largely independent of the chosen sigmoid function and match previous findings on the feedback-induced instability of vortex diffusion in a rotationally driven Newtonian fluid. Because our model captures the essential features of nonlocal delayed feedback in dissipative systems, we consider it a valuable reference case for studies of more complex and spatially extended systems such as photoresponsive fluid interfaces.

DY 3: Active Matter A (joint session DY/CPP)

Time: Monday 9:30–12:45 Location: H20

Invited Talk DY 3.1 Mon 9:30 H20

Collective behavior and self-organisation of active granular particles — •Thorsten Pöschel, Michael Engel, Christian Scholz, and Harol Torres — Friedrich-Alexander-Universität Erlangen-Nürnberg

Biological organisms and artificial active particles self-organize into swarms and patterns. Open questions concern the design of emergent phenomena by choosing appropriate forms of activity and particle interactions. A particularly simple and versatile system are 3D-printed robots on a vibrating table that can perform self-propelled and self-spinning motion. Here we study a mixture of minimalistic clockwise and counter-clockwise rotating robots, called rotors. Our experiments show that rotors move collectively and exhibit super-diffusive interfacial motion and phase separate via spinodal decomposition. On long time scales, confinement favors symmetric demixing patterns. By mapping rotor motion on a Langevin equation with a constant driving torque and by comparison with computer simulations, we demonstrate that our macroscopic system is a form of active soft matter.

C. Scholz, T. Pöschel, Phys. Rev. Lett. 118, 198003 (2017)
C. Scholz, M. Engel, T. Pöschel, Nature Comm. 9, 931 (2018)
C. Scholz, S. D'Silva, T. Pöschel, New J. Phys. 18, 123001 (2016)
C. Scholz, T. Pöschel, Revista Cubana de Física 34, 69 (2017)

DY 3.2 Mon 10:00 H20

Approximating microswimmer dynamics by active Brownian motion: Energetics and efficiency — •Jannik Ehrich and Marcel Kahlen — Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany

We consider the dynamics of a microswimmer and show that they can be approximated by active Brownian motion. The swimmer is modeled by coupled overdamped Langevin equations with periodic driving. We compare the energy dissipation of the real swimmer to that of the active Brownian motion model finding that the latter can massively underestimate the complete dissipation. This discrepancy is related to the inability to infer the full dissipation from partial observation of the complete system. We introduce an efficiency that measures how much of the dissipated energy is spent on forward propulsion.

[1] J. Ehrich and M. Kahlen, arXiv:1809.07235 (2018)

DY 3.3 Mon 10:15 H20

Magnetocapillary Microswimmers — •Maxime Hubert[1,2], Galien Grosjean[2], and Nicolas Vandewalle[2] — [1]PULS group, Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]GRASP Lab, CESAM UR, University of Liège, Liège, Belgium

The study of artificial microswimmers is of major interest in many area of physics, from the understanding of microorganisms swimming strategies to applications in microfluidic and micromanipulation. While there exists numerous theoretical studies on microswimmers, experimental realizations are technologically challenging. We focus in this presentation on a simple system made of three soft ferromagnetic particles trapped at air-water interfaces and self-assembling in triangles. Complex behaviors can arise under a time-dependent magnetic field. In particular, those assemblies can undergo deformations in non-time-reversible sequences, a necessary condition for low Reynolds number locomotion. Because of their controllability, such structures can be used for capture, transport and release of a microcargo, or the mixing of fluids at low Reynolds number. During this talk, the key mechanism for the collective motion of the beads is described from a numerical point of view and a model for their dynamics is discussed, opening the way for optimal control and efficiency of experimental magnetocapillary microswimmers.

DY 3.4 Mon 10:30 H20

Self-assembly of dipolar active Brownian particles in two dimensions — •Guo-Jun Liao and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

We computationally study the self-assembly behavior of self-propelled Brownian particles with additional dipole-dipole interactions, stemming from a point dipole in the particle center. The propulsion direction of each particle is parallel to its dipole moment. At low densities and small dipolar coupling, the system undergoes a transition from a homogeneous state to a state with finite-sized (and orientationally disordered) clusters, when the particle motility is increased. Such cluster formation could be regarded as the asymptotic behavior of conventional active Brownian particles [1]. For strongly coupled dipolar colloids and zero motility, the model exhibits gel-like structures. On increasing particle motility, we observe a transition into a state with orientationally-ordered, finite-sized clusters. We analyze this state via the cluster size distribution and the net orientation. We also propose a mechanism to describe the emergence of such clusters.

Reference:
[1] G.-J. Liao and S. H. L. Klapp, Soft Matter 14, 7873 (2018)

DY 3.5 Mon 10:45 H20

Experimental optimization of escape strategies in active systems. — •Hugo Wendehenne, François Lavergne, and Clemens Bechinger — Department of Physics, University of Konstanz, 78464 Konstanz, Germany

Groups formed by living organisms frequently react to external perturbations which can be repulsive (incoming predator) or attractive (presence of food). These responses are a combination of individuals reacting directly to the perturbation and collective mechanisms within the group. However, it is unclear whether collective interactions are a real benefit for an individual to escape from a repulsive perturbation. Here, we show that a change of the individuals' motilities and polarities in response to their visual perception of a perturbation leads to an effective escaping motion. Experimentally, this is demonstrated using active particles whose propulsion velocities and orientations are individually light-controlled by an external feedback-loop. We show that for a single active particle reacting to the perturbation within a restricted field of view, there is an increase of its rotational diffusion. The escape dynamics is characterized by ballistic transport, which is maximized for an optimal width of the particle's field of view. Interestingly, for a multi-particle system where individuals interact with their peers using a cohesion-based mechanism, we show that the escaping motion becomes more efficient. We expect this escaping mechanism to be relevant for cases where the perturbation is mobile, such as prey-predator interactions.

DY 3.6 Mon 11:00 H20

Dynamics and configurations of active polymers — •Paolo Malgaretti — Max Planck Institute for Intelligent Systems, Stuttgart, Germany

We study the dynamics and conformation of polymers composed by active monomers. By means of Brownian dynamics simulations we show that, when the direction of the self-propulsion of each monomer is aligned with the backbone, the polymer undergoes a coil-to-globulelike transition, highlighted by a marked change of the scaling exponent of the gyration radius. Concurrently, the diffusion coefficient of the center of mass of the polymer becomes essentially independent of the polymer size for sufficiently long polymers or large magnitudes of the self-propulsion. These effects are reduced when the self-propulsion of the monomers is not bound to be tangent to the backbone of the polymer. Our results, rationalized by a minimal stochastic model, open new routes for activity-controlled polymers and, possibly, for a new generation of polymer-based drug carriers[1].

[1] V. Bianco, E.Locatelli, P. Malgaretti PRL 121, 217802 (2018)

15 min. break

DY 3.7 Mon 11:30 H20

Collapse Dynamics of Polymers with Vicsek-like Activity — •Subhajit Paul[1], Suman Majumder[1], Subir K Das[2], and Wolfhard Janke[1] — [1]Institute for Theoretical Physics, University of Leipzig, Leipzig, Germany. — [2]Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore, India

Many biologically active systems can effectively be understood within the framework of active matter models in statistical physics. In this regard, even modeling a single component Lennard-Jones-type fluid with Vicsek-like activity shows both rich phase and dynamical behavior. Motivated by this we construct a flexible bead-spring polymer model with Vicsek-like activity of the monomer beads. We pay particular emphasis on exploring the pathways of its collapse, following a quench from a high-temperature random coil state into a low-temperature phase where the equilibrium phase is a compact globule in the passive limit of the model. In the active case, however, our results from molecular dynamics simulations reveal that depending upon the strength of activity there is a rich phase behavior of the model that ranges from compact globule to dumbbells. On the nonequilibrium dynamics front, we compare our results with the passive polymer case, from the perspective of various scaling laws related to the collapse time, cluster coarsening, etc.

DY 3.8 Mon 11:45 H20

Collective guiding of self-acoustophoretic particles in complex environments* — Tobias Nitschke and •Raphael Wittkowski — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

Using self-propelled microparticles for medical applications like targeted drug delivery has been a dream for many decades. With the recent discovery of self-acoustophoretic particles, which move when they are exposed to ultrasound, a new type of particles with a biocompatible propulsion mechanism has become available. It turned out that these particles can be made from biocompatible materials and be equipped with mechanisms for the encapsulation and release of drugs. However, the hitherto insufficient capabilities for controlling the collective motion of the particles remained as a big obstacle preventing far-reaching medical applications.

In this talk, we present a method that allows to guide a large number of self-acoustophoretic particles collectively to a prescribed target region. The method is based on combining a moving focused ultrasound beam with a synchronized time-dependent magnetic field. Our method is harmless to patients and works even in complex environments like a patient's vasculature, when the particles are distributed throughout the body, and without information about the positions or orientations of the particles. Furthermore, we present a particle design that is particularly advantageous for applications.

**Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

DY 3.9 Mon 12:00 H20

Emergent biomechanics in growing bacterial colonies — •Anupam Sengupta — Physics of Living Matter Group, Physics and Materials Science Research Unit, University of Luxembourg

Bacterial colonies, known to mediate key ecological and industrial processes, constitute a class of active matter within which geometry, order, and topology emerge spontaneously over the lifespan of a colony. Although numerous studies have been carried out on growing colonies, so far we have lacked a comprehensive biomechanical framework that could capture the cell-to-colony dynamics and the consequences thereof. In this talk I will present recent results [1] obtained by combining micro-scale experiments, molecular dynamics simulations, and continuous modeling, that capture the continuous evolution of the geometry, order and topology in a growing colony of non-motile strain of E.coli bacteria. We reveal how steric forces between neighboring cells (favoring cell alignment), compete with the extensile stresses due to the cell growth (reducing the local order), leading to emergent biomechanics within the growing colony: spontaneous hydrodynamic flows, anisotropy of internal stresses, and emergent motility due to non-motile cells. The results indicate at activity-driven cell-cell communications preceding biofilm formation, and can be extended beyond bacterial communities, for instance, to study mammalian cells, many of which exist as non-motile elongated phenotypes.

[1] Geometry and Mechanics of Microdomains in Growing Bacterial Colonies: Z. You, D. Pearce, A. Sengupta*, and L. Giomi*, Phys. Rev. X 8, 031065, 2018.

DY 3.10 Mon 12:15 H20

Phase transitions in huddling emperor penguins — •Alexander Winterl[1], Sebastian Richter[1,2], Richard Gerum[1], Ben Fabry[1], and Daniel Paranhos Zitterbart[1,2] — [1]Biophysics Group, Friedrich-Alexander University, Erlangen, Germany — [2]Applied Ocean Physics and Engineering, Woods Hole Oceanographic Institution, Woods Hole, MA 02543, United States of America

Emperor penguins (*Aptenodytes forsteri*) breed under the harsh conditions of the Antarctic winter. To save energy and survive for 120 days of fasting, they from tight huddles. Using time-lapse images of an emperor penguin colony in Terre Adelie, we study huddle formation in response to environmental conditions (temperature, humidity, solar radiation, and wind speed). Huddle formation can be described as a phase transition from a freely moving state to a solid-like state where individual movements stall. We find a larger huddling probability with decreasing temperature and solar radiation and with increasing wind speed and humidity. These environmental factors can be lumped to an apparent temperature that would result in the same huddling probability in the absence of wind, humidity, and solar radiation, with weights of 1°C/°C for temperature, 2.9°C/(m/s) for wind, 0.5°C/% for rel. humidity, and 0.3°C/(W/m^2) for solar radiation. For the month of May, we find a critical temperature of −48.2°C for a 50% huddling probability. We expect this critical temperature to rise during fasting as the animals consume their insulating fat layer, and propose that the critical temperature can serve as an indicator for energy reserves and thus colony health.

DY 3.11 Mon 12:30 H20

Delayed feedback control of active particles: a controlled journey towards the destination — Seyed Mohsen Jebreiil Khadem and •Sabine H. L. Klapp — Institut für Theoretische Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin.

We explore theoretically the navigation of an active particle based on delayed feedback control. The delayed feedback enters in our expression for the particle orientation which, for an active particle, determines (up to noise) the direction of motion in the next time step. Here we estimate the orientation by comparing the delayed position of the particle with the actual one. This method does not require any real-time monitoring of the particle orientation and may thus be relevant also for controlling sub-micron sized particles, where the imaging process is not easily feasible. We apply the delayed feedback strategy to two experimentally relevant situations, namely, optical trapping and photon nudging. To investigate the performance of our strategy, we calculate the mean arrival time analytically (exploiting a small-delay approximation) and by simulations.

References:
[1] S. M. J. Khadem and Sabine H. L. Klapp arXiv:1811.06849v2 (2018).

DY 4: Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/DY)

Time: Monday 9:30–12:45 Location: H22

DY 4.1 Mon 9:30 H22

Quantum Loschmidt echo in quenched Hubbard model — •Nikodem Szpak[1] and Ralf Schützhold[2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Institut für Theoretische Physik, Technische Universität Dresden

A quantum Loschmidt echo (also referred to as quantum time mirror) corresponds to an effective time inversion after which the quantum wave function reverses its previous time evolution and eventually reaches its initial distribution again. We consider a Hubbard model describing free dispersion in a lattice and impose a sudden pulse-like perturbation (pi-pulse) which reverses the sign of all quasi-momenta simultaneously. After equal period of time, we observe the rebuild of the initial state. We generalize previous results obtained in this field and propose a comparably simple protocol for ultra-cold atoms in optical lattices which should be easier to realize experimentally than previous proposals.

DY 4.2 Mon 9:45 H22

Ion Impact induced Doublon Creation in Strongly Correlated Finite Hubbard Systems — •Maximilian Rodriguez Rasmussen, Karsten Balzer, Niclas Schlünzen, Jan-Philip Joost, and Michael Bonitz — CAU Kiel, Germany

Under certain conditions strongly correlated fermions in lattice systems are known to form doublons - quasi-particles consisting of two electrons on the same site. Due to the interesting resulting electronic properties doublon formation processes have been the subject of various studies. Here a new mechanism of doublon production due the impact of energetic ions is presented. The processes leading to doublon creation are described and verified by numerical results [1, 2] obtained by exact diagonalization for small systems and non-equilibrium Green functions approach [3] for larger systems.

[1] K. Balzer, M.R. Rasmussen, N. Schlünzen, J.-P. Joost, M. Bonitz, submitted to Phys. Rev. Lett., arXiv:1801.05267
[2] M. Bonitz, K. Balzer, N. Schlünzen, M.R. Rasmussen, J.-P. Joost, Phys. Stat. Sol. (b) (2018), arXiv:1808.07868
[3] K. Balzer and M. Bonitz, "Nonequilibrium Green's Functions Approach to Inhomogeneous Systems", Springer 2013

DY 4.3 Mon 10:00 H22

Hidden phases in the photodoped two-band Hubbard model — •Jiajun Li and Martin Eckstein — University of Erlangen-Nuremberg, Erlangen, Germany

Recent years have witnessed intense interest in controlling materials through non-equilibrium protocols. In particular, a strong electric pulse can drastically disturb a Mott insulator, giving rise to a transient photo-doped state featuring charge excitations across the insulating gap. This protocol of photo-doping can yield non-trivial physical consequences, such as non-thermal melting of symmetry-breaking phases and the formation of hidden states with entangled spin-orbital ordering which are inaccessible in equilibrium. We demonstrate the scenarios in a two-band Hubbard model using non-equilibirum Dynamical Mean-Field Theory. Furthermore, controlled studies of the photo-doped state are often prone to the limited time range that is numerically accessible. Thus, we adopt a non-equilibrium steady-state formulation of Dynamical Mean-Field Theory to describe a longlived photo-doped system, which is constantly perturbed to maintain a stationary state containing charge excitations across the gap. The perturbation can be adjusted to control the excitation density continuously. Using this method, we study a photo-doped two-band Hubbard model. We find the photo-doping drives the system to a hidden phase, which exhibits non-thermal ordering essentially distinct from an equilibrium or Floquet engineered system.

DY 4.4 Mon 10:15 H22

Non-equilibrium optical conductivity for the antiferromagnetic single-band Hubbard model: Time-dependent Gutzwiller analysis — •Christian Martens[1], Jörg Bünemann[2], and Götz Seibold[1] — [1]Institut für Physik, BTU Cottbus-Senftenberg, Postfach 101344, 03013 Cottbus, Germany — [2]Fakultät Physik, TU Dortmund, 44227 Dortmund, Germany

Based on the time-dependent Gutzwiller approximation (TDGA) for the Hubbard model we analyze the optical conductivity $\sigma(\omega)$ in an out-of equilibrium situation for underlying antiferromagnetic ground states. The equilibrium state is perturbed by an instant quench of the local Coulomb interaction parameter U or by an electric field $E(t)$. We analyze various shapes for the applied electric field and discuss our results with regard to the optical conductivity determination from pump-probe experiments. In the linear response regime, RPA corrections to the TDGA vanish, so that the optical response is determined by the bare current-current correlation function. In contrast, far from the linear response regime the out-of equilibrium case shows a more interesting behavior and in particular mixes double occupancy fluctuations to the current response.

DY 4.5 Mon 10:30 H22

Time-dependent wave functions with multiple correlators for the Hubbard model in nonequilibrium — •Patricia Mayer[1], Masud Haque[2], and Marcus Kollar[1] — [1]Theoretische Physik III, Universität Augsburg — [2]Department of Theoretical Physics, Maynooth University, Ireland

For the solvable $1/r$-Hubbard chain [1], the double occupation relaxes to nonthermal values after an interaction quench [2]. We apply time-dependent variational wave functions to this problem to assess their descriptive capabilities. We find that the Gutzwiller wave function, which acts on the Fermi sea with the exponentiated double occupation as correlator, can describe the time evolution accurately only for short times and then keeps oscillating with a single frequency, similar to the infinite-dimensional case [3]. On the other hand, in the Gutzwiller-Baeriswyl wave function the exponentiated kinetic energy is applied in turn to the Gutzwiller wave function [4], which leads to accurate expectation values up to longer times followed by a more complicated oscillating pattern. We conclude that multiple variational correlators substantially improve the description of Hubbard models in nonequilibrium.

[1] F. Gebhard and A.E. Ruckenstein, Phys. Rev. Lett. **68**, 244 (1992)
[2] M. Kollar and M. Eckstein, Phys. Rev. A **78**, 013626 (2008)
[3] M. Schiró and M. Fabrizio, Phys. Rev. Lett. **105**, 076401 (2010)
[4] M. Dzierzawa et al., Phys. Rev. B **51**, 1993 (1995)

DY 4.6 Mon 10:45 H22

Dynamics of densities and currents in spin ladders — •Jonas Richter[1], Fengping Jin[2], Lars Knipschild[1], Jacek Herbrych[3], Hans De Raedt[4], Kristel Michielsen[2], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]University of Osnabrück, Germany — [2]Forschungszentrum Jülich, Germany — [3]The University of Tennessee, USA — [4]University of Groningen, The Netherlands

The impact of integrability or nonintegrability on the dynamics of isolated quantum systems is a longstanding issue. For integrable models, a macroscopic set of (quasi)local conservation laws can lead to partially conserved currents and ballistic transport. In generic situations, however, integrability is lifted due to various perturbations and currents are expected to decay. Still, since the dynamics of interacting quantum many-body systems poses a formidable challenge to theory and numerics, it remains open whether nonintegrability as such already implies the emergence of diffusion. In this context, we study the dynamics of spin and energy in the two-leg spin-1/2 ladder with up to 40 lattice sites, using an efficient pure-state approach based on the concept of typicality. We discuss correlation functions in real and momentum space, and in the time and frequency domain, providing a comprehensive picture of high-temperature dynamics in this archetypal nonintegrable quantum model. Particularly, we unveil the occurence of diffusion for both spin and energy.

[1] J. Richter *et al.*, Phys. Rev. B **97**, 174430 (2018)
[2] J. Richter *et al.*, arXiv:1811.02806

15 min. break.

DY 4.7 Mon 11:15 H22

Inhomogeneous quench on the Bethe lattice — •Marc Alexander and Marcus Kollar — Theoretische Physik III, Universität Augsburg

An abrupt change of the on-site energy for a single site in a one-dimensional non-interacting tight-binding model generates dynamical Friedel oscillations of the disturbed Fermi sea [1]. In order to study this phenomenon in higher dimensions we obtain exact time evolution for such an inhomogeneous quench for a Bethe lattice with arbitrary coordination number. We use the exact eigenstates of finite Cayley trees without [2,3] or with an impurity at the central site. For the Bethe lattice with infinite coordination number we observe dynamical Friedel oscillations with two qualitative different long-time limits depending on the strength of the impurity potential.

[1] J. M. Zhang and Y. Liu, Phys. Rev. B. **97**, 075151 (2018)
[2] M. van den Berg et al., J. Stat. Phys. **69**, 307 (1992)
[3] G. D. Mahan, Phys. Rev. B **63**, 155110 (2001)

DY 4.8 Mon 11:30 H22

Steady-state charge transport through Falicov-Kimball system connected to metallic leads — Martin Žonda and •Michael Thoss — Institute of Physics, Albert-Ludwig University of Freiburg, Hermann-Herder-Strasse 3, 791 04 Freiburg, Germany

We study steady-state nonequilibrium charge transport in a model heterostructure, where a two-dimensional spin-less Falicov-Kimball system is coupled to two noninteracting leads, using a combination of a sign-problem-free Monte Carlo approach and nonequilibrium Green's function techniques. We show that the transport characteristic depends sensitively on the electrostatic potential in the system and exhibits different properties for different phases of the Falicov-Kimball model. In particular, pronounced step-like changes of the current and transmission are observed at the phase boundaries, evident even on a logarithmic scale. Analyzing finite size effects, we find that with the method used a relatively small system can be utilized to address specific thermodynamic limits.

DY 4.9 Mon 11:45 H22

Heating Dynamics in a Periodically Driven SYK-Model — •Clemens Kuhlenkamp, Simon Weidinger, and Michael Knap — Technische Universität München

Periodically driven quantum matter can realize exotic dynamical phases that do not even exist in equilibrium. In order to understand how ubiquitous and robust these phases are, it is important to understand the heating dynamics of generic interacting quantum systems. We study the thermalization and heating dynamics in a generalized SYK-model subjected to a periodic drive, which realize a Fermi-Liquid (FL) to Non-FL crossover at a certain energy scale. Using an exact field theoretic approach we determine two regimes in the heating dynamics. Only at energies above this crossover scale the system is efficiently thermalizing and heats up exponentially. The crossover in the heating dynamics may be experimentally studied by measuring the absorption of THz laser light that impinges on an irregularly shaped graphene flake in a strong magnetic field, which has been proposed to realize exotic SYK physics.

DY 4.10 Mon 12:00 H22

Periodically Driven Manybody System: a Density Matrix Renormalization Group Study — Shaon Sahoo, •Imke Schneider, and Sebastian Eggert — Department of Physics and Research Center OPTIMAS, Technical University of Kaiserslautern

Driving a quantum system periodically in time can profoundly alter its long-time dynamics and trigger exotic quantum states of matter. We propose a new DMRG method which directly deals with the Fourier components of the eigenstates of a periodically driven system using Floquet theory. With this new method we can go beyond effective Hamiltonians and take into account higher Floquet modes. Numerical results are presented for the isotropic Heisenberg antiferromagnetic spin-1/2 chain under both local (edge) and global driving for energies, spin-spin correlation and temporal fluctuations. As the frequency is lowered, the spin system enters into a Floquet regime with coherent excitations of a large number of Floquet modes, which shows characteristic quantum correlations that cannot be described by any effective static model.

DY 4.11 Mon 12:15 H22

Matrix Product Operator Algorithm for Quantum Hydrodynamics — •Tibor Rakovszky[1], Curt von Keyserlingk[2], Ehud Altman[3], and Frank Pollmann[1] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]University of Birmingham, School of Physics & Astronomy, B15 2TT, UK — [3]Department of Physics, University of California, Berkeley, California 94720, USA

Motivated by recent understanding of the Heisenberg picture evolution of operators in many-body systems, and the growth of quantum entanglement in systems subject to weak measurements, we propose a novel numerical algorithm for extracting the long-time hydrodynamic transport properties of strongly interacting spin chains. Our algorithm is based on time evolving local operators corresponding to conserved densities, making use of the so-called matrix product operator representation, and adding an artificial dissipative term that reduces the weight of large, un-physical operators that do not contribute to the physically relevant few-point correlations. The dissipation leads to a significant reduction in the number of parameters needed to represent the operator and allows us to compute the aforementioned correlation functions up to much longer times then would otherwise be possible. Using this we extract the diffusion constants of several model Hamiltonians and benchmark them against existing results in the literature.

DY 4.12 Mon 12:30 H22

Diffusion and operator spreading in matrix product operators — •Johannes Hauschild and Frank Pollmann — Department of Physics, Technische Universität München, Garching, Germany

Matrix product states (MPS) became one of the standard tools for the simulation of real time dynamics in quantum many-body systems in one dimensional systems. The fast growth of entanglement during a real time evolution usually restricts the evolution of pure MPS to short to intermediate times. In certain cases, the operator entanglement entropy of a single-site operator evolved in the Heisenberg picture grows much slower. We discuss advantages and disadvantages of the different methods in the context of extracting diffusion constants and the study of operator spreading in disordered systems. Starting from a model which displays diffusion already after short times, we study the transition to a many-body localized phase and perform a careful convergence analysis in the bond dimension.

DY 5: Convection

Time: Monday 10:00–12:45 Location: H3

Invited Talk DY 5.1 Mon 10:00 H3

Direct numerical simulations towards ultimate turbulence — •Richard Stevens[1], Roberto Verzicco[2], and Detlef Lohse[1,3] — [1]Physics of Fluids, University of Twente, Enshede, The Netherlands — [2]University of Rome Tor Vergata, Roma, Italy — [3]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Both in experiments and simulations of Rayleigh-Bénard (RB) convection it is a major challenge to reach the ultimate regime in which the boundary layers transition from laminar to turbulent. In the ultimate regime the scaling exponent γ in the relation $Nu \sim Ra^{\gamma}$, where Nusselt Nu is the dimensionless heat transport and Rayleigh Ra is the dimensionless temperature difference between the plates, increases. The critical Rayleigh number (Ra^*) for the transition to the ultimate regime has been observed in the Göttingen experiments around $Ra^* \approx 2\times10^{14}$. So far, the highest Ra obtained in direct numerical simulations (DNS) is $Ra = 2 \times 10^{12}$ for aspect ratio $\Gamma = 0.5$ (Stevens, Lohse, Verzicco, JFM 688, 31 (2011)). Here we present a comparison between the Göttingen experiments and DNS up to $Ra = 10^{13}$. We find perfect agreement between experiments and simulations, both for the heat transfer and for the mean and temperature variance profiles close to the sidewall. In addition, we discuss simulations for $\Gamma = 0.23$ up to $Ra = 10^{14}$, which agree well with measurements by Roche et al., NJP 12, 085014 (2010). In addition, we discuss the influence of the aspect ratio on the heat transfer and flow structures in high Rayleigh number convection.

DY 5.2 Mon 10:30 H3

Boundary layers and scaling relations in natural thermal convection — •Olga Shishkina — Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany

Classical setups to study natural thermal convection are vertical convection (VC), where the fluid is confined between two differently heated vertical walls, horizontal convection (HC), where the fluid is heated at one part of the bottom plate and cooled at some other part, and Rayleigh-Benard convection (RBC). Here we consider the boundary-layer (BL) equations in natural thermal convection and derive for some flow configurations the mean flow characteristics and the scaling relations of the Nusselt and Reynolds numbers (Nu, Re) with the Rayleigh and Prandtl numbers (Ra, Pr). For VC the scaling relations are obtained directly from the BL equations (Shishkina, Phys. Rev. E 93 (2016)), while for HC they are derived by extending the Grossmann-Lohse theory for RBC (J. Fluid Mech. 407 (2000)) to the case of VC (Shishkina, Grossmann, Lohse, Geophys. Res. Lett. 43 (2016)).

The work is supported by the Deutsche Forschungsgemeinschaft (DFG) under the grant Sh 405/4 - Heisenberg fellowship.

DY 5.3 Mon 10:45 H3

Experimental analysis of superstructures in large-aspect-ratio Rayleigh Bénard convection — Christian Kästner, •Christian Resagk, and Jörg Schumacher — Institute of Thermodynamics and Fluid Mechanics, TU Ilmenau, Ilmenau

We report about measurement and analysis of horizontal velocity fields in a square Rayleigh-Bénard convection cell at an aspect ratio Gamma = 10 with compressed air and sulfur hexafluoride as working fluid. 2D3C horizontal cuts through the convective flow were obtained from stereoscopic particle image velocimetry (SPIV) measurements. Optical access for laser light sheet and PIV cameras was provided by transparent side-walls and a transparent heating plate. The application of a transparent heating plate, a glass plate coated with a transparent and electrically conductive metal oxide (TCO), allowed first time experimental observation of horizontal velocity fields in turbulent thermal convection at large aspect ratio. The horizontal cuts were taken in midplane of the convection cell and below the cooling plate at a Rayleigh number ranging from Ra = 10^4 - 10^7. Spatial and transient analysis of the velocity fields revealed superstructures, steadily increasing in size with increasing Rayleigh number. Hence the present experimental approach and results provide further insights into large-scale coherent flow pattern formation in turbulent thermal convection.

DY 5.4 Mon 11:00 H3

Resolved energy budget of superstructures in Rayleigh-Bénard convection — •Gerrit Green[1,2], Dimitar Vlaykov[1,3], Juan-Pedro Mellado[4], and Michael Wilczek[1] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Faculty of Physics, University of Göttingen, Germany — [3]University of Exeter, Exeter, England — [4]Max-Planck-Institute for Meteorology, Hamburg, Germany

The dynamics of turbulent Rayleigh-Bénard convection exhibits a complex interaction between coherent large-scale flow patterns, so-called superstructures, and small-scale fluctuations. In this contribution we employ direct numerical simulations to investigate the interaction between scales and clarify the impact of turbulence on large-scale patterns. A filtering approach is used to separate the superstructures and turbulent fluctuations. It complements spectral analysis techniques by retaining physical space information. This allows us to study the energy budget at the scale of superstructures and to characterize the different contributions, such as the power input due to buoyancy, the direct dissipation and the energy transfer between scales. We find that the energy transfer in the bulk differs significantly from the one close to the walls. In the bulk, most of the energy input in the superstructures is balanced by the energy transfer between scales, which acts primarily as a dissipation for the large scales. Close to the wall, there is a layer in which the energy transfer is up-scale, driving the superstructures. Our investigations therefore provide insights which will help to derive an effective description of turbulent superstructures.

DY 5.5 Mon 11:15 H3

The evolution of the large-scale flow in magnetoconvection — •Till Zürner[1], Felix Schindler[2], Tobias Vogt[2], Sven Eckert[2], and Jörg Schumacher[1] — [1]Institute of Thermodynamics and Fluid Mechanics, Technische Universität Ilmenau, Postfach 100565, 98684 Ilmenau — [2]Department Magnetohydrodynamics, Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

We investigate the effect of a vertical magnetic field on the flow properties of turbulent Rayleigh-Bénard convection. The large-scale flow of a low-Prandtl number liquid metal alloy in a cylindrical convection cell of aspect ratio 1 is reconstructed by a combination of temperature and direct velocity measurements, using ultrasound Doppler velocimetry (UDV). In accordance to theory and simulations the flow strength is reduced by the induced Lorentz forces. With increasing magnetic field strength a transition from the turbulent one-roll large-scale circulation to a weakly non-linear cell-like structure is observed. Increasing the field strength even further finally supresses the flow in the centre of the cell almost completely. However, even at such high fields significant flows can still be observed near the side walls of the cell, far above the critical Hartmann number of the Chandrasekhar limit for the onset of magnetoconvection for a fluid layer without lateral boundaries. This destabilising effect of non-conducting side walls was predicted by theory and simulations, and is here confirmed by experiments for the first time.

292,314,312,321

DY 5.6 Mon 11:45 H3

Rotating turbulent Rayleigh-Bénard convection at very large Rayleigh numbers — •Marcel Wedi[1], Dennis van Gils[2], Stephan Weiss[1], and Eberhard Bodenschatz[1] — [1]Max-Planck-Institut for Dynamics and Self-Organization, Göttingen, Germany — [2]Twente University, The Netherlands

Thermal convection in astro- and geophysical systems is both, highly turbulent and strongly influenced by Coriolis forces caused by the rotation of their celestial body. We aim to study the influence of rotation on the heat transport and the temperature field at very large thermal driving in the High Pressure Convection Facility (HPCF) in Göttingen. The facility consists of a cylindrical cell with a diameter of 1.10 m and a height of 2.20 m that can be filled with pressurized sulfur hexafluoride (SF_6) or Helium at up to 19 bar. The height of the cell and the large density of SF_6 enables us to reach large thermal drivings with Rayleigh numbers up to 2×10^{15}. The cell is mounted on a rotating table and connected to the non-rotating world via water feed-throughs and slip rings. We reach Ekman numbers down to 10^{-8}, possibly entering the geostrophic regime. At very high rotation rates the Froude number increases and centrifugal forces may not be negligable. The effects of rotation and applied temperature settings are looked at in

the temperature field. In our talk, we discuss these effects and the behavior of the flow field as well as the heat transport.

DY 5.7 Mon 12:00 H3

Non-Oberbeck-Boussinesq effects and flow structures in Rotating Rayleigh–Bénard convection in pressurized SF_6 — •Xuan Zhang and Olga Shishkina — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen

Rotating Rayleigh–Bénard convection (RBC) in pressurized sulfur hexafluoride (SF_6) in a cylindrical cell of the diameter-to-height aspect ratio 1/2 is studied using our finite-volume code Goldfish. The results based on direct numerical simulations (DNS) at Prandtl number 0.8, Rayleigh number 10^8 to 10^{10} and Rossby number 0.02 to 50 are presented. Non-Oberbeck-Boussinesq effects are studied by considering temperature dependence of the fluid properties, and the results are compared to those under Oberbeck-Boussinesq approximation. Effects of rotation on the flow structures are investigated in terms of the global heat transfer, dynamics of large-scale circulation, long-term bulk temperature statistics and local historical temperature signals.

Funding Acknowledgment: The work is supported by the German Research Foundation under the grant SH405/8 and Heisenberg fellowship SH405/4. We acknowledge the Leibniz Supercomputing Centre (LRZ) for providing computing resources on SuperMUC.

DY 5.8 Mon 12:15 H3

Inclined thermal convection in liquid metals — •Lukas Zwirner and Olga Shishkina — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen

Any tilt of a Rayleigh-Benard convection (RBC) cell against gravity changes the global flow structure inside the cell. Recent experiments by Vasil'ev et al. (2015, Tech. Phys. 60) and Frick et al. (2015, Europhys. Lett. 109) with liquid sodium (Prandtl number $Pr<<1$) demonstrated that the heat transport in low-Prandtl number fluids is especially sensitive to the inclination angle. Our study is based on direct numerical simulations of inclined convection in a cylindrical cell of diameter-to-height aspect ratios 1 and 1/5 and we consider Prandtl numbers down to Pr=0.0083. We demonstrate that the global flow structure like the large scale circulation is influenced by both the inclination angle and the lateral confinement of the cell. For inclined convection we observe the formation of two system-sized plume columns, a hot and a cold one, that impinge on the opposite boundary layers (Zwirner and Shishkina, 2018, J. Fluid Mech. 850). In RBC the confined cell supports the formation of multiple rolls on top of each other.

The work is supported by the German Research Foundation under the grant SH405/7 and Heisenberg fellowship SH405/4. We acknowledge the Leibniz Supercomputing Centre (LRZ) for providing computing resources on SuperMUC.

DY 5.9 Mon 12:30 H3

Heat and momentum transport in symmetric horizontal convection — •Philipp Reiter, Mohammad Emran, and Olga Shishkina — Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany

Horizontal convection (HC) is a paradigm system to study natural turbulent convection, in which heating and cooling is applied solely to one horizontal surface of a fluid layer. This type of convection is relevant in different geophysical and astrophysical systems, e.g., in the meridional-overturning circulation of the oceans. Recent progress in understanding of the scaling relations of the mean heat and momentum transport has been done theoretically (Shishkina et al., Geophys. Res. Lett 43(2016)) and numerically, but further investigations are required.

Here, using an advanced version of the computational code goldfish, we investigate a modified symmetric elongated HC setup, where heat is applied to the central part of the bottom plate and cooling to both ends of the HC cell. Such meridional symmetry bypasses some difficulties that arise in the measurements in the classical configuration and it leads to a more natural setup with less artificial constraints. For the modified and classical HC, we compare global flow structures and their time evolution, as well as the scaling relations, over a wide range of Rayleigh numbers.

This work is supported by the DFG grants Sh405/10 and Sh405/4.

DY 6: Dynamics in many-body systems: Equilibration and localization I (joint session DY/TT)

Time: Monday 10:00–13:00 Location: H19

DY 6.1 Mon 10:00 H19

Modern Principles of Equilibration in Closed Quantum Systems do Not Rule Out Strange Relaxation Dynamics — Lars Knipschild and •Jochen Gemmer — Universität Osnabrück, Germany

The quest for equilibration and thermalization in closed quantum systems has stimulated vast scientific effort, especially in the last decades. Various principles and approaches have been put forth, such as the eigenstate thermalization hypothesis, quantum chaos, typicality, the non-resonance principle, the unfeasibility of fine-tuned initial states, etc. While these approaches are well suited to explain that observables will assume specific "equilibrium" values for most points in time in between some initial time and a very distant future, they do not address the concrete dynamics towards these values. Furthermore they do not rule out substantial observable revivals on relevant timescales . We demonstrate that indeed very unexpected dynamics may result for systems and observables complying with all the above principles. This occurs for a very large set of non-fine tuned initial states.

DY 6.2 Mon 10:15 H19

Entanglement-ergodic quantum systems equilibrate exponentially well — Henrik Wilming[1], •Marcel Goihl[2], Ingo Roth[2], and Jens Eisert[2] — [1]Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

One of the outstanding problems in non-equilibrium physics is to precisely understand when and how physically relevant observables in many-body systems equilibrate under unitary time evolution. General equilibration results have been proven that show that equilibration is generic provided that the initial state has overlap with sufficiently many energy levels and the energy spectrum is sufficiently generic. At the same time results showing that natural initial states fulfill this condition are lacking. We present stringent results for equilibration of lattice systems in which the amount of entanglement in energy eigenstates with finite energy density is extensive for some subset of the lattice. Concretely, we carefully formalize a notion of "entanglement-ergodicity" in terms of Rényi entropies and derive that systems fulfilling this condition equilibrate exponentially well. Our proof uses insights about Rényi entropies and combines them with recent results about the probability distribution of energy in local lattice systems with initial states that are weakly correlated.

DY 6.3 Mon 10:30 H19

Out-Of-Time-Ordered Correlators in critical systems - Instability and the onset of chaos — •Dominik Hahn, Benjamin Geiger, Quirin Hummel, and Klaus Richter — Universität Regensburg

It is known from mean field theory that a system of bosons with attractive contact interaction in one dimension exhibits a quantum phase transition at a certain critical coupling. This transition has its manifestation in the formation of a local instability in the integrable mean-field dynamics. By adding an external potential, we investigate the transition from integrability to chaos in this system. A characteristic feature of chaotic motion, the exponential sensitivity to initial conditions, can be also detected in the corresponding quantum mechanical system using Out-Of-Time-Ordered Correlators (OTOCs). It can be shown, that a local instability is sufficient to generate an exponential growth of certain OTOCs. After breaking the integrability, we find evidence, that the OTOC growth is affected by an additional exponent, which can be related to the largest Lyapunov exponent of the system.

DY 6.4 Mon 10:45 H19

Thermalization and eigenstate thermalization hypothesis in the Holstein polaron model — David Jansen[1], •Jan Stolpp[2], Lev Vidmar[3], and Fabian Heidrich-Meisner[2] — [1]Arnold-Sommerfeld-Center for Theoretical Physics, LMU Munich — [2]Institute for Theoretical Physics, University of Göttingen — [3]Jozef

Stefan Institute, Ljubljana

The 1d Holstein model is a paradigmatic system to study polaron physics and the nonequilibrium dynamics of charge carriers coupled to phonons. While the electronic relaxation dynamics of a single charge carrier is a much studied topic (see, e.g. [1]), here, we systematically investigate whether the 1d Holstein model in the single-polaron limit is ergodic by checking the criteria of the eigenstate thermalization hypothesis and by testing for established quantum chaos indicators. Using exact diagonalization techniques we find that the level spacing distribution is Wigner-Dyson, which is characteristic for a quantum chaotic system. Remarkably, both the diagonal and offdiagonal matrix elements of typical observables obey properties predicted by the eigenstate thermalization hypothesis. Thus, we found an example in which the coupling term between the electronic and phononic subspaces leads to ergodic behavior, even though the phonon system itself consists of uncoupled, local harmonic oscillators.

[1] Phys. Rev. B 91, 104302 (2015)

DY 6.5 Mon 11:00 H19

Bounds on equilibration time scales — •Robin Heveling, Lars Knipschild, and Jochen Gemmer — University of Osnabrueck, Osnabrueck, Germany

We consider closed quantum systems consisting of a single system-spin and a spin-bath. Starting from a product state of a microcanonical bath at some energy and a fully aligned system-spin, equilibration time scales of the magnetization are calculated for various coupling strengths. The paper PRX 7, 031027 (2017) conjectures a relation between short time behaviour and long equilibration time scales. We probe this conjecture. For small couplings, we find exponential relaxation to an equilibrium value. The exponential nature of the decay may break down at some point when decreasing the coupling strength.

DY 6.6 Mon 11:15 H19

Decoherence Entails Exponential Forgetting in Systems Complying with the Eigenstate Thermalization Hypothesis — •Lars Knipschild and Jochen Gemmer — University of Osnabrück, D-49069 Osnabrück, Germany

According to the eigenstate thermalization ansatz, matrices representing generic few-body observables exhibit a specific form when displayed regarding the eigenbasis of the Hamiltonian. We examine the effect of environmental induced decoherence on the expectation value dynamics of observables confirming with said eigenstate thermalization ansatz. We find that this influence is equivalent to an exponential damping of the memory-kernel appearing in an equation of motion for the expectation value. The statement is formulated as a rigorous theorem.

15 min. break

DY 6.7 Mon 11:45 H19

Many body localized system weakly coupled to thermal environment — •Ling-Na Wu, Alexander Schnell, Giuseppe De Tomasi, Markus Heyl, and André Eckardt — Max Planck Institute for the Physics of Complex Systems

Many body localization (MBL), which describes the failing of an interacting system under disorder to reach thermalization, has attracted widespread attentions. In recent years, the imperfect experimental environment has excited an intense interest in the effect of dissipations on MBL. We formulate an efficient method for the description of MBL systems in weak contact with thermal environments at temperature T. As an example, we study the transport property of a fermion Hubbard chain coupled to a thermal bath and recover a conductivity following Mott's law for variable range hopping. Weak attractive (repulsive) interactions are found to enhance (decrease) the transport, which is attributed to an interaction-induced modification of the density of states due to spatio-energetic correlations. We also study the effect of dissipations on disorder-free localized system and compare it with the conventional disorder-induced localized system.

DY 6.8 Mon 12:00 H19

Many-body localization and delocalization in large quantum chains — •Elmer V. H. Doggen[1], Frank Schindler[2], Konstantin S. Tikhonov[1,3], Alexander D. Mirlin[1,3,4,5], Titus Neupert[2], Dmitry G. Polyakov[1], and Igor V. Gornyi[1,3,4,6] — [1]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Department of Physics, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland — [3]L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia — [4]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [5]Petersburg Nuclear Physics Institute, 188300 St. Petersburg, Russia — [6]A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia

We theoretically study the quench dynamics for an isolated Heisenberg spin chain with a random on-site magnetic field, which is one of the paradigmatic models of a many-body localization transition. We use the time-dependent variational principle as applied to matrix product states, which allows us to controllably study chains of a length up to L=100 spins. We find that the consideration of the larger system sizes substantially increases the estimate for the critical disorder that separates the ergodic and many-body localized regimes, compared to the values in the literature. From a technical perspective, we develop an adaptation of the "learning by confusion" machine-learning approach that can determine the critical disorder.

DY 6.9 Mon 12:15 H19

Detection and characterization of many-body localization in central spin models — •Daniel Hetterich[1,4], Norman Yao[2], Maksym Serbyn[3], Frank Pollmann[4], and Björn Trauzettel[1] — [1]Institute for theoretical Physics, University of Würzburg — [2]Department of Physics, University of California, Berkeley — [3]Insitute of Science and Technology, Wien — [4]Department of Physics, Technical University Munich

We analyze a disordered central spin model, where a central spin interacts equally with each spin in a periodic one-dimensional (1D) random-field Heisenberg chain. If the Heisenberg chain is initially in the many-body localized (MBL) phase, we find that the coupling to the central spin suffices to delocalize the chain for a substantial range of coupling strengths. We calculate the phase diagram of the model and identify the phase boundary between the MBL and ergodic phase. Within the localized phase, the central spin significantly enhances the rate of the logarithmic entanglement growth and its saturation value. We attribute the increase in entanglement entropy to a nonextensive enhancement of magnetization fluctuations induced by the central spin. Finally, we demonstrate that correlation functions of the central spin can be utilized to distinguish between MBL and ergodic phases of the 1D chain. Hence, we propose the use of a central spin as a possible experimental probe to identify the MBL phase.

DY 6.10 Mon 12:30 H19

Magnetization and Entanglement after a geometric quench in the XXZ chain — •Matthias Gruber and Viktor Eisler — TU Graz, Graz, Österreich

We consider the XXZ spin chain in the gapless regime and study magnetization and entropy profiles after a geometric quench. This quench is realized by preparing the ground states with zero and maximum magnetizations on the two halves of a chain and letting it evolve subsequently. The magnetization profiles during time evolution are studied numerically by tDMRG and compared to the predictions obtained from generalized hydrodynamics (GHD). We find that the GHD description of the dynamics provides a very good agreement with the numerical data. Furthermore, entanglement entropy profiles are also studied, finding a closed form expression in the non-interacting XX case. For the general interacting case, the propagation velocities of the entropy fronts are studied both before and after the reflection from the boundaries. Finally, we also study the relationship between magnetization fluctuations and entanglement entropy.

DY 6.11 Mon 12:45 H19

Equilibration of expectation values for statically and dynamically generated initial conditions — •Christian Bartsch — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, D-49069 Osnabrück

We investigate dynamical equilibration of expectation values in closed quantum systems for realistic non-equilibrium initial states. For statically generated initial states we find that the long time expectation values depend on the initial expectation values if eigenstate thermalization is violated. An analytical expression for the deviation from the expected ensemble value is derived for small displacements from equilibrium based on linear response theory. Analogous derivations show that this deviation vanishes for dynamically generated initial states, at least within the linear response regime. Additional numerics for magnetization and energy equilibration in an asymmetric anisotropic spin-1/2-ladder illustrate the behavior beyond linear response for both cases.

DY 7: Interfaces and Thin Films (joint session CPP/DY)

Time: Monday 15:00–17:15 Location: H14

DY 7.1 Mon 15:00 H14

In situ GISAXS Investigations of Multi-responsive Block Copolymer Thin Films during Solvent Vapor Annealing — •Florian Jung[1], Panayiota A. Panteli[2], Detlef-M. Smilgies[3], Dorthe Posselt[4], Constantinos Tsitsilianis[5], Costas S. Patrickios[2], and Christine M. Papadakis[1] — [1]Physics Department, Soft Matter Group, Technical University of Munich, Garching, Germany — [2]Department of Chemistry, University of Cyprus, Nicosia, Cyprus — [3]Wilson Laboratory, Cornell University, Ithaca, USA — [4]Department of Science and Environment, Roskilde University, Roskilde, Denmark — [5]Department of Chemical Engineering, University of Patras, Patras, Greece

In the present work, we investigate the structure of a pH and temperature responsive, CBABC type pentablock terpolymer in thin films during solvent vapor annealing (SVA) using grazing-incidence small-angle X-ray scattering. The C end blocks are statistical copolymers of the hydrophobic n-BuMA and the thermoresponsive TEGMA, the B blocks are the weak cationic polyelectrolyte PDMAEMA and the A block is the hydrophilic PEG. Films were prepared by spin coating from aqueous solutions of different pH values. SVA experiments were carried out using both water and toluene as solvents. Films prepared at low pH feature a spherical morphology, and swell strongly in water, but only weakly in toluene vapor. At high pH, no structural features are observed, indicating the importance of ionization for microphase separation. During swelling in toluene, a morphology of small spheres is observed in the swollen state, while water has no noticeable effect.

DY 7.2 Mon 15:15 H14

Competition of structural and electrostatic forces in colloidal dispersions confined between of two charged surfaces — •Michael Ludwig and Regine von Klitzing — Soft Matter at Interfaces, Department of Physics, Technische Universität Darmstadt

Structural forces can be observed when pure solvents and ionic liquids, as well as dispersions containing nanoparticles, micelles, polymers or polyelectrolytes are confined between two smooth surfaces into a thin liquid film. Upon surface-approach, liquid matter has to be depleted from the vicinity of the surfaces, altering the interactions between the surfaces.

The present study addresses structural forces across thin films of suspensions of nanoparticles (NP) confined between two charged surfaces measured with a colloidal-probe atomic force microscope (CP-AFM). Special attention is drawn to the transition from diluted to concentrated NP-packing and to the effect of the outer surface charge. An extended fitting procedure was introduced to accurately fit experimental data. The need of an additional repulsive contribution to the fitting formula will be discussed in terms of the DLVO-framework.

DY 7.3 Mon 15:30 H14

Growth Kinetics and Molecular Mobility of Irreversibly Adsorbed Layers in Thin Films of P2VP and PVME — •Marcel Gawek, Sherif Madkour, Andreas Hertwig, and Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin

In well-annealed thin polymer films, with non-repulsive polymer/substrate interactions, an irreversibly adsorbed layer is formed. These adsorbed layers have shown enormous potential for technological applications. Due to the hard accessibility of these layers, their growth kinetics and molecular dynamics are still not fully understood. Here, the irreversibly adsorbed layers of Poly(2-vinylpyridine) (P2VP) and Poly(vinyl methyl ether) (PVME) thin films are revealed by solvent-leaching experiments. The growth kinetics of these layers is investigated as a function of original film thickness and annealing times. The thickness, topography and quality of the adsorbed layer is determined with Atomic Force Microscopy (AFM) and spectroscopic ellipsometry. Additionally, the molecular mobility of the adsorbed layer is investigated with Broadband Dielectric Spectroscopy (BDS). A recently developed nanostructured capacitor (NSC) is employed to measure the adsorbed layers with a free surface layer depending on annealing and solvent-leaching time. The results are quantitatively compared and discussed with respect to recently published work.

DY 7.4 Mon 15:45 H14

Enhanced protein adsorption near a phase transition — •Madeleine R. Fries[1], Daniel Stopper[1], Fajun Zhang[1], Robert M. J. Jacobs[2], Maximilian W. A. Skoda[3], Roland Roth[1], and Frank Schreiber[1] — [1]University of Tübingen, Germany — [2]University of Oxford, UK — [3]ISIS Facility, Didcot, UK

Protein adsorption at the solid-liquid interface is an important phenomenon that often can be observed as a first step in biomedicine. In particular, globular proteins tuned by multivalent ions give rise to a rich phase behavior including reentrant condensation and liquid-liquid phase separation (LLPS) through ion-bridges connecting individual proteins [1, 2]. Multivalent ions can be used not only to modify the bulk behaviour, but also the adsorption behaviour of proteins at the solid-liquid interface [3]. Here, we demonstrate experimentally that protein adsorption at attractive substrates can be enhanced significantly by approaching the LLPS regime through an increase in temperature or protein concentration, pointing towards the ability to control protein adsorption by means of suitably tailoring thermodynamic conditions. This is supported by theoretical calculations treating proteins as limited-valence (patchy) particles. These results could enable better biocompatibility in implants through guided protein-substrate interactions. [1] Zhang et al, PRL (2008); [2] Roosen-Runge et al, Sci. Rep. (2014); [3] Fries et al, PRL (2017)

15 min. break

DY 7.5 Mon 16:15 H14

Templated electrodeposition of nanoscale semiconductors — •Li Shao[1], Andrew Hector[1], Philip Bartlett[1], Francis Sweeney[2], Samantha Soule[1], Richard Beanland[2], and Gilles Moehl[1] — [1]Chemistry, Southampton University, University Rd, SO17 1BJ, United Kingdom — [2]Department of Physics, University of Warwick, Coventry CV4 7AL

The Advanced Devices by ElectroPlaTing (ADEPT) project, an interdisciplinary research project funded by the EPSRC (EP/N035437/1), aims to develop new techniques and materials for thermoelectric devices, infrared detection, and phase change memory, by using electrodeposition methods. In previous work, Sn nanowires were deposited into mesoporous silica templates with pores of 1.5nm diameter.1 In this work, well-ordered mesoporous silica films with 3D pore structures were prepared by the evaporation-induced self-assembly (EISA) method. Using these silica films as templates, tellurium was deposited into the 3D pores. Grazing incidence small-angle X-ray scattering (GISAXS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were used to characterize film nanostructures before and after electrodeposition. Programmes based on the distorted wave Born approximation (DWBA) were used for analysis and simulation of the 2D diffraction patterns from GISAXS. The patterns show that silica films with different structures including cubic, hexagonal and orthorhombic were synthesized. 1.*Philip N. Bartlett et al, Nano Lett. 2018, 18, 941*947. Type: Talk Topic: Thin films division Email: L.Shao@soton.ac.uk

DY 7.6 Mon 16:30 H14

In-situ GISAXS during sputter deposition of metal nanolayers on functional polymer thin films for lithium-ion batteries — •Simon J. Schaper[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Pallavi Pandit[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, 22607 Hamburg — [3]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel — [4]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden

Understanding the interface between metals, commonly used as current collectors, and ion-conducting polymers used in polymer lithium-ion batteries (LIBs) is crucial to develop highly reproducible, low-cost and reliable devices. To address these issues, sputter deposition is the technique of choice to fabricate scalable, reproducible and controllable nanometer and sub-nanometer metal layers on polymer thin films. The sputter deposition process, being well understood and controlled, offers advantages over chemical methods to tailor metal thin-flim morphologies on the nanoscale and offers a superior adhesion of the deposited

material. We use in-situ grazing incidence small angle X-ray scattering (GISAXS) to investigate the formation, growth and, self-assembled structuring on polymer thin films and composites used in LIBs. Different polymer films are compared with respect to the metal layer growth.

DY 7.7 Mon 16:45 H14

Using GISAXS to reveal spatial correlations in the electrochemical nucleation of gold particles — •Gilles Moehl, Philip Bartlett, and Andrew Hector — Chemistry, Southampton University, University Rd, SO17 1BJ, United Kingdom

Gilles E. Moehl, Philip N. Bartlett and Andrew L. Hector Chemistry, University of Southampton, Southampton, SO17 1BJ, UK. Developing the next generation of electronic devices requires the deposition of high-quality functional materials in a controlled fashion in complex structures in order to unleash the true potential of devices such as thermoelectrics, phase change memory (PCM) and infra-red detectors. Within EPSRC programme grant ADEPT *Advanced Devices by ElectroPlaTing* (EP/N035437/1), new techniques and materials are to be developed for that matter. Electrochemical nucleation was generally described theoretically many years ago as a random process, which mainly depends on the deposition rate applied through the set current or potential, resulting in either instantaneous or progressive nucleation. Further development of theory and experiments has shown that the underlying process is just random, but that every newborn nucleus has the potential to influence the evolution of further nucleation steps. In this work, we show how grazing incidence small angle scattering can reveal spatial correlations in seemingly randomly arranged gold particles from electrolytic metal deposition.

DY 7.8 Mon 17:00 H14

An Extended Transfer Matrix Approach to Calculate the Scattering of Light in an Interface Profile — •Reinhard Sigel — 83301 Traunreut

The transfer matrix method is a reliable work horse for the calculation of the reflection at an interface profile. In this contribution, the approach is extended by additional fluctuations $\Delta\varepsilon$ of the relative permittivity ε within the profile, which cause light scattering. For small amplitudes, such fluctuations can be treated within the first Born approximation. The incident light as well as the exit of the scattered light through the layered profile are handled by the transfer matrix method. Based on a model which yields the interface profile and the fluctuation amplitudes, the intensity and the polarization properties of the light scattered in any solid angle are predicted. Applications to grazing incidence small angle X-ray scattering (GISAXS), evanescent wave dynamic light scattering (EWDLS) and scattering ellipsometry are discussed.

DY 8: Networks: From Topology to Dynamics (joint session DY/SOE)

Time: Monday 15:00–17:45 Location: H20

DY 8.1 Mon 15:00 H20

Inhibition induced explosive synchronization in multiplex networks — •Sarika Jalan — IIT Indore

To date, explosive synchronization (ES) is shown to be originated from either degree-frequency correlation or inertia of phase oscillators. Of late, it has been shown that ES can be induced in a network by adaptively controlled phase oscillators. We show that ES can occur in any network by appropriately multiplexing it with another layer. We devise an approach which leads to the occurrence of ES with hysteresis loop in a network upon its multiplexing with a negatively coupled (or inhibitory) layer. We discuss the impact of various structural properties of positively coupled (or excitatory) and inhibitory layer along with the strength of multiplexing in gaining control over the induced ES transition. This investigation is a step forward in highlighting the importance of multiplex framework not only in bringing novel phenomena which are not possible in an isolated network but also in providing more structural control over the induced phenomena.

DY 8.2 Mon 15:15 H20

Coarsening dynamics of transient ferrogranular networks under influence of a horizontal magnetic field - network alignment and magnetization in experiments and simulations — Justus Miller[1], Pedro Sanchez[2], Sofia Kantorovich[2,3], and •Reinhard Richter[1] — [1]Experimentalphysik 5, Universität Bayreuth, Bayreuth, Germany — [2]University of Vienna, Vienna, Austria — [3]Ural Federal University, Ekaterinburg, Russia

We investigate the phase separation of a shaken mixture of glass and magnetised steel spheres after a sudden quench of the shaker amplitude. Then transient networks of steel spheres emerge in the experiment, as well as in simulations. Analyzing the network evolution by network specific parameters like the mean number of neighbours or network efficiency we have uncovered three regimes (Kögel et al. Soft Matter **14** 2018), previously established by H. Tanaka (2000) for the viscoelastic phase separation of dynamically asymmetric mixtures.

Here we present new results for the network evolution under influence of a horizontally applied magnetic field. With increasing field strength the branched networks are more and more replaced by linear chains. We quantitatively characterize the average orientation of the network edges with respect to the direction of the applied field in experiment and simulations and explore the consequences for the magnetization curves.

DY 8.3 Mon 15:30 H20

Asymptotically Exact Solution of the Fredrickson-Andersen Model — Koray Önder[1,2], •Till Kranz[1,2], and Matthias Sperl[2,1] — [1]Institut für Theoretische Physik, Uni Köln — [2]Institut für Materialphysik im Weltraum, DLR Köln

Kinetically constrained models describe many phenomena from opinion dynamics to amorphous solids [1]. The Fredrickson-Andersen model—a kinetically constrained lattice model—displays an ergodic to non-ergodic transition. Simulations indicate a slow two-step relaxation of dynamical correlation functions close to the transition point. We derive an asymptotically exact solution for the dynamical occupation correlation function of the Fredrickson-Andersen model on the Bethe lattice by identifying an exact expression for its memory kernel. The exact solution proves an empirical scaling relation [2] between critical exponents and allows to calculate the exponents explicitly. In addition, we propose an approximate dynamics that describes numerical data away from the critical point over many decades in time.

[1] F. Ritort and P. Sollich, Adv. Phys. **52**, 219 (2003)
[2] M. Sellitto, Phys. Rev. Lett. **115**, 225701 (2015)

DY 8.4 Mon 15:45 H20

Assessing and improving the replication of chaotic attractors by means of reservoir computing — •Alexander Haluszczynski[1,3], Christoph Raeth[2], Ingo Laut[2], and Mierk Schwabe[2] — [1]Ludwig-Maximilians-Universität, München, Deutschland — [2]Deutsches Zentrum für Luft- und Raumfahrt, Weßling, Deutschland — [3]Allianz Global Investors, München, Deutschland

The prediction of complex nonlinear dynamical systems with the help of machine learning techniques has become increasingly popular. In particular, the so-called "reservoir computing" method turned out to be a very promising approach especially for the reproduction of the long-term properties of the system [1]. Yet, a thorough statistical analysis of the forecast results is missing. So far the standard approach is to use purely random Erdös-Renyi networks for the reservoir in the model. It is obvious that there is a variety of conceivable network topologies that may have an influence on the results. Using the Lorenz System we statistically analyze the quality of predicition for different parametrizations - both the exact short term prediction as well as the reproduction of the long-term properties of the system as estimated by the correlation dimension and largest Lyapunov exponent. We find that both short and longterm predictions vary significantly. Thus special care must be taken in selecting the good predictions. We investigate the benefit of using different network topologies such as Small World or Scale Free networks and show which effect they have on the prediction quality. Our results suggest that the overall performance is best for small world networks. [1] J. Pathak et al., Chaos, 27, 121102 (2017)

DY 8.5 Mon 16:00 H20

Principal Eigenvector Localization in Multilayer Networks

— •Priodyuti Pradhan[1] and Sarika Jalan[1,2] — [1]Complex Systems Lab, Discipline of Physics, Indian Institute of Technology Indore, Khandwa Road, Simrol, Indore-453552, India — [2]Centre for Biosciences and Biomedical Engineering, Indian Institute of Technology Indore, Khandwa Road, Simrol, Indore-453552, India

Starting with a multilayer network (MN) corresponding to a delocalized PEV, we rewire the network edges using an optimization technique such that the PEV of the rewired MN becomes more localized. The localization of an eigenvector refers to a state where few components of the vector take very high values, and rest of the components take very small values. For a two layers MN, the optimization process can be implemented in two different edge rewiring protocols; (1) by rewiring edges in both-layers or (2) by rewiring edges in only one layer. We reveal that for both the rewiring protocols, though there is an emergence of various specific structural features, the different rewiring protocols lead to a noticeable difference in the spectral properties of the optimized MN. For the both-layers rewiring protocol, PEV is sensitive to a single edge rewiring in the optimized MN, and however, interestingly, we get rid of this sensitivity of PEV for the single-layer rewiring protocol. This sensitivity in the localization behavior of PEV is accompanied by the second largest eigenvalue lying very close to the largest one. Furthermore, analysis of MNs constructed using real-world social and biological data show a good agreement with the simulation results for model MN.

15 min. break

DY 8.6 Mon 16:30 H20

Topology vs. Node Dynamics in Collective Adaptation to Risk — Matthew Grobis[1], Colin Twomey[2], Joseph Bak-Coleman[1], •Winnie Poel[3,4], Bryan Daniels[5], Pawel Romanczuk[3,4], and Iain Couzin[6,7] — [1]Princeton University, USA — [2]University of Pennsylvania, USA — [3]Humboldt Universität zu Berlin — [4]Bernstein Center for Computational Neuroscience Berlin, Germany — [5]Arizona State University, USA — [6]Max Planck Institute for Ornithology, Germany — [7]University of Konstanz, Germany

Our research focuses on the mechanism used by large animal groups to reliably collectively process information on external threats like predation. Specifically, we are interested in the role of an individual's internal state vs. the structure of the group in collective reaction to perceived risk. Using a generic contagion model [1], we study behavioral response cascades in fish schools based on empirically inferred visual interaction networks [2]. We aim to uncover if and how the spatial configuration of the group (i.e. structure of its visual interaction network) and the individual response parameters affect the collective responsiveness.

[1] Dodds PS, Watts DJ (2005) Journal of Theoretical Biology 232(4):587-604

[2] Rosenthal et Al. (2015) PNAS 112(15):4690-4695

DY 8.7 Mon 16:45 H20

Structure and dynamics of non-normal networks — •Malbor Asllani — University of Limerick, Limerick, Ireland

Network theory has been a groundbreaking research field in science for the last 20 years, conceivably the only one that could glue together disparate and even contrasting disciplines such as physics, economy, biology or sociology. A network materializes the complex interactions between the composing entities of large systems, it thus defines the natural and structural backbone for describing complex systems, which dynamics is unavoidably bound to the network properties. Based on a detailed study involving a large set of empirical networks arising from a wide spectrum of research fields, we claim that strong non-normality is indeed a universal property in network science [1]. Dynamical processes evolving on non-normal networks exhibit a peculiar behavior, initial small disturbances can undergo a transient phase and be strongly amplified although the system is linearly stable [2]. We hence propose several models to generate complex non-normal networks to explain the origin of such property. Because of the non-normality of the networked support, the comprehension of the dynamical properties goes beyond the classical linear spectral methods, while we show that the pseudo-spectrum is able to capture such behavior. This response is very general and it challenges our understanding of natural processes grounded in real networks, as we illustrate in the Generalised Lotka-Volterra model.

[1] M. Asllani and T. Carletti, Sci. Adv. 4, eaau9403 (2018). [2] M. Asllani and T. Carletti, Phys. Rev. E 97, 042302 (2018).

DY 8.8 Mon 17:00 H20

Chimera States in Networks of Type-I Morris-Lecar Neurons — •Philipp Hövel[1], Ali Calim[2], Mahmut Ozer[3], and Muhammet Uzuntarla[2] — [1]School of Mathematical Science, University College Cork, Ireland — [2]Department of Biomedical Engineering, Bulent Ecevit University, Turkey — [3]Department of Electrical and Electronics Engineering, Bulent Ecevit University, Turkey

Chimeras are complex spatio-temporal patterns that emerge as coexistence of both coherent and incoherent groups of coupled dynamical systems. Here, we investigate the emergence of chimera states in nonlocal networks of type-I Morris-Lecar neurons coupled via chemical synapses. This constitutes a more realistic neuronal modeling framework than previous studies of chimera states, since the Morris-Lecar model provides biophysically more relevant control parameters to describe the activity in actual neural systems. We explore systematically the transitions of dynamic behavior and find that different types of synchrony appear depending on the excitability level and nonlocal network features. Furthermore, we map the transitions between incoherent states, traveling waves, chimeras, synchronized states and global amplitude death in the parameter space of interest. This work contributes to a better understanding of biological conditions giving rise to the emergence of chimera states in neural medium.

Reference: A. Calim, M. Ozer, P. Hövel, M. Uzuntarla, Phys. Rev. E (2018) in print.

DY 8.9 Mon 17:15 H20

Terminal Transient Phase of Chimera States — •Thomas Lilienkamp[1] and Ulrich Parlitz[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Germany

In spatially homogeneous systems regions with regular and coherent motion may coexist with regions where irregular and incoherent dynamics occurs. In many cases, chimera states are actually chaotic transients which self-terminate abruptly e.g. towards the completely coherent state. Recent studies of chaotic transients in various systems show, that although the process of self-termination seems to be abrupt [1], a particular final transition phase in state space could be verified, called the "Terminal Transient Phase" [2, 3]. Using small but finite perturbations it was shown, that the state space structure is significantly different in this transition zone. We detected this behavior also in different spatially extended systems which exhibit chimera states. Furthermore, the spatial distribution of perturbations which have a significant impact on trajectories just before the collapse turns out to be correlated with the state of the system. Thus, before its self-termination the chimera state is mostly "vulnerable" only at specific regions of the spatial domain.

[1] T. Lilienkamp, J. Christoph, and U. Parlitz. Phys. Rev. Lett. 119, 054101 (2017)

[2] T. Lilienkamp and U. Parlitz. Phys. Rev. Lett. 120, 094101 (2018)

[3] T. Lilienkamp and U. Parlitz, Phys. Rev. E 98, 022215 (2018)

DY 8.10 Mon 17:30 H20

Synchronization of time-varying networks with coupling delays — •Otti D'Huys[1], Javier Rodríguez-Laguna[2], Manuel Jiménez-Martín[2], and Elka Korutcheva[2] — [1]Department of Mathematics, Aston University, B4 7ET Birmingham, United Kingdom — [2]Departamento de Física Fundamental, UNED, Spain

We study the effect of a fluctuating topology in delay-coupled networks. Such network fluctuations are common, for instance, between interacting neurons, or networks modeling social interactions.

We concentrate on the synchronization properties of chaotic maps. The topology fluctuates between an ensemble of small-world networks. The dynamics is characterized by three timescales: the internal time scale of the node dynamics, the connection delay along the links, and the timescale of the network fluctuations. When the network fluctuations are faster than the coupling delay and the internal time scale, the synchronized state can be stabilized by the fluctuations. As the network time scale increases, the synchronized state becomes unstable when both time scales collide.

We complement these results with an analytical theory in the linearized limit. Two limit cases allow an interpretation in terms of an 'effective network': When the network fluctuations are much faster than the internal time scale and the coupling delay, the effective network topology is the average over the different topologies. When coupling

delay and network fluctuation time scales collide, the effective topology is the geometric mean over the different topologies.

DY 9: Dynamics in many-body systems: Equilibration and localization II (joint session DY/TT)

Time: Monday 15:30–18:00 Location: H19

DY 9.1 Mon 15:30 H19

Environment induced pre-thermalization in the Hubbard dimer — •Nikodem Szpak[1], Eric Kleinherbers[1], Friedemann Queisser[2], Jürgen König[1], and Ralf Schützhold[2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Institut für Theoretische Physik, Technische Universität Dresden

We study a strongly interacting two-site Fermi-Hubbard model representing two coupled quantum dots and couple them to Markovian baths. We compare the real-time diagrammatic technique derived within the Keldysh formalism with a simplified model in the form of a Lindblad master equation for the reduced density matrix based on the Born-Markov approximation. Solving it exactly, we observe equilibration at different time-scales corresponding to thermalization and pre-thermalization processes.

DY 9.2 Mon 15:45 H19

Prethermalization and typical response of weakly perturbed quantum many-body systems — •Lennart Dabelow and Peter Reimann — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld

We explore the temporal relaxation of quantum many-body systems under the influence of weak-to-moderate perturbations. Situations we have in mind include, for instance, a sudden quench from one Hamiltonian to a related but different second Hamiltonian. Another example are integrable systems subject to a small integrability-breaking perturbation, commonly leading to prethermalization. Using a typicality approach, we show that the perturbed dynamics resembles the unperturbed time evolution modulated by an exponential decay towards the (possibly modified) long-time limit. We support our theory by comparison with both experimental and numerical data.

DY 9.3 Mon 16:00 H19

How to teach equilibration to the Boltzmann equation: a noisy relaxation time approximation — •Philipp Weiss and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

Equilibration of closed systems is controlled by diffusive transport of conserved quantities. After a quench these systems approach thermal equilibrium only slowly, hydrodynamic long-time tails emerge. As an analog in space one expects long-distance tails to appear when the system is perturbed only locally. A natural example for this situation is a current-carrying wire coupled to leads. We expect the connections to induce long-distance tails which show up as correction in the voltage drop.

The Boltzmann equation is widely used for tackling transport problems. However, it predicts exponential relaxation as it does not capture fluctuations of the hydrodynamic modes. Close to equilibrium a fluctuation-dissipation relation restores the missing piece of information, giving rise to a stochastic Boltzmann-Langevin equation.

Here, we present a simplified version, a "noisy relaxation time approximation", which we derive from a conserving relaxation time approximation supplemented with a suitably correlated noise term. We use our new tool to track the equilibration of a one-dimensional wire after a quench. Our prime goal is to detect long-time tails and long-distance tails indicating the diffusive built-up of the equilibrium correlations.

DY 9.4 Mon 16:15 H19

Boltzmann relaxation dynamics in strongly interacting quantum lattice systems — •Friedemann Queisser[2,3] and Ralf Schützhold[1,2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

To the best of our knowledge, we present the first derivation of the Boltzmann equations for strongly interacting spinless fermions on a lattice in higher dimensions. Our derivation is based on a hierarchy of correlations [1]. For a large repulsive nearest neighbor interaction, the ground state at half filling is given by a charge density wave state. In this limit, we find that the collisions between particles and holes dominate over particle-particle and hole-hole scattering. Furthermore we shall discuss the validity of the η-theorem and the dependence of the thermalization dynamics on the type of excitation (particles or holes).

[1] P. Navez and R. Schützhold, Phys. Rev. A **82**, 063603 (2010)

DY 9.5 Mon 16:30 H19

Effect of anisotropic diffusion on spinodal decomposition — •Abhinav Sharma[1], Hidde Vuijk[1], and Joseph Brader[2] — [1]Leibniz Institute for polymer research, Dresden, Germany — [2]University of Fribourg, Fribourg, Switzerland

We study the phase transition dynamics of a fluid system in which the particles diffuse anisotropically in space. The motivation to study such a situation is provided by systems of interacting magnetic colloidal particles subject to the Lorentz force. The Smoluchowski equation for the many-particle probability distribution then acquires an anisotropic diffusion tensor. Using the method of dynamical density functional theory we predict that the intermediate-stage decomposition dynamics can be slowed down significantly by anisotropy; the coupling between different Fourier-modes is strongly reduced. Numerical calculations are performed for a model (Yukawa) fluid that exhibits gas-liquid phase separation.

15 min break

DY 9.6 Mon 17:00 H19

Cooperative efficiency boost for quantum heat engines — David Gelbwaser-Klimovsky[1], Wassilij Kopylov[2], and •Gernot Schaller[2] — [1]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, USA — [2]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

The power and efficiency of many-body single-stroke heat engines can be boosted by performing cooperative non-adiabatic operations in contrast to the commonly used adiabatic implementations. The key property relies on the fact that non-adiabaticity allows for cooperative effects, that can use the thermodynamic resources only present in the collective non-passive state of a many-body system. In particular, we discuss an analytic formula for the efficiency of a quantum Otto cycle, which increases with the number of copies used and reaches a many-body bound, which we discuss analytically.

[1] D. Gelbwaser-Klimovsky, W.Kopylov, and G. Schaller, *Cooperative efficiency boost for quantum heat engines*, arXiv:1809.02564.

DY 9.7 Mon 17:15 H19

Light-induced Hall current in Graphene: beyond the high-frequency limit — •Marlon Nuske[1] and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging, 22761 Hamburg, Germany

In the high-frequency limit driving graphene with circularly-polarized light leads to a quantized Hall effect. In experiment, however, this idealized theoretical limit is often not achievable. We therefore investigate the effects of a finite-frequency circularly-polarized pulse on the Hall conductivity of graphene. For such a setup it is crucial to include decay processes in the theoretical model. We analyze the additional resonant contributions to the Hall current that arise from finite frequency driving. We explore different regimes, where either the resonant or the effective high-frequency contributions dominate the Hall current.

DY 9.8 Mon 17:30 H19

Environment induced pre-thermalization in the Mott-Hubbard model — •Friedemann Queisser[2,3], Ralf Schützhold[1,2,3], Nikodem Szpak[1], and Patrick Navez[2] —

[1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

Using a hierarchy of correlations, we discuss the strongly interacting Fermi-Hubbard model in the Mott insulating regime coupled to a Markovian environment [1,2]. The environment is chosen such that the particle number is constantly monitored at each lattice site. As expected, the environment induces a decay rate of γ the quasi-particles frequencies and tends to diminish the correlations between lattice sites. Surprisingly, the environment does also steer the state of the system on intermediate time scales $\mathcal{O}(1/\gamma)$ to a pre-thermalized state very similar to a quantum quench. The full thermalization and the approach to an infinite temperature state occurs via local on-site heating and takes much longer.

[1] P. Navez and R. Schützhold, Phys. Rev. A **82**, 063603
[2] F. Queisser and R. Schützhold, arXiv:1808.09906

DY 9.9 Mon 17:45 H19

Laser driven ultrafast crystallization of phase-change material Ge1Sb2Te4 — •Jingyi Zhu[1], Shuai Wei[2], Julian Merten[2], Christoph Persch[2], Lin Yang[1], Matthias Wuttig[2], and Paul H. M. van Loosdrecht[1] — [1]Physics institute 2, University of Cologne, 50937, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Aachen, 52074, Germany

Rapid and reversible switching between amorphous and crystalline phases of the phase-change materials are either used or very promising in a wide range of applications in the electronic, optoelectronic, and photonic memory devices. Here we use time-resolved spontaneous Raman spectra to monitor the ultrafast process of melting, bond softening and crystallization in the phase changing material Ge1Sb2Te4 upon laser excitation. We demonstrate ultrafast crystallization on a ps timescale by monitoring the transient formation of a well-defined phonon mode signaling the crystalline state emerging from a broad vibrational continuum typical for the amorphous state.

DY 10: Glasses and Glass Transition (joint session CPP/DY)

Time: Monday 16:15–17:30 Location: H8

DY 10.1 Mon 16:15 H8

A coarse-grained model for studying polymer melts toward the glass transition point under cooling — •Hsiao-Ping Hsu and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

For studying polymer melts of weakly semiflexible chains under cooling at zero pressure by molecular dynamics simulations, a coarse-grained model based on the standard bead-spring model is developed. We introduce a short range attractive potential between non-bonded monomers such that the pressure of polymer melts is tuned to zero. Additionally, the common used bond-bending potential [Everaers et al., Science 303, 823 (2004)] controlling the chain stiffness is replaced by another new bond-bending potential. With our newly developed model, we show that the Kuhn length and the internal distance of chains in a melt are independent of temperatures under cooling. The glass transition is probed by the volume change of polymer melts and the slowing down of the mobility of chains. Thus, our coarse-grained model can be served as an optimal model for studying glass-forming polymer melts and understanding the effect of free surface on the glass transition of thin polymer films.

DY 10.2 Mon 16:30 H8

Molecular Dynamics of Dipole Functionalized Triphenylene-based Discotics — •Arda Yildirim[1], Andrea Bühlmeyer[2], Shunsuke Hayashi[3], Johannes Christian Haenle[2], Kathrin Sentker[4], Patrick Huber[4], Sabine Laschat[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und *prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Institut für Organische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany — [3]Department of Applied Chemistry, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan — [4]Materials Physics and Technology, Hamburg University of Technology (TUHH), 21073 Hamburg, Germany

In this study, the molecular dynamics of a series of dipole functionalized triphenylene-based discotics, forming a columnar mesophase, were investigated by broadband dielectric spectroscopy (BDS). In addition to conductivity and localized dynamics, glassy dynamics were also observed. At higher temperatures an α1-processes and at low temperatures an α2 processes were detected having a completely different temperature dependence of its relaxation times. Different molecular assignments of α1- and α2-processes are suggested. The phase behavior of the material was explored under helium purge down to 100 K by differential scanning calorimetry (DSC). Besides the phase transition temperatures and enthalpies, one or two thermal glass transitions were found for all the materials. Moreover, the glassy dynamics were further investigated by Flash DSC, which is a chip-based calorimetry technique allowing for fast heating and cooling rates as high as 10000K

DY 10.3 Mon 16:45 H8

System size-dependent non-affine displacements in a model glass: the impact of yield strain — •Moumita Maiti and Andreas Heuer — University of Muenster, Institute for physical chemistry, Corrensstr. 28/30, 48149, Muenster

The probability distribution of non-affine displacements has an exponential tail, which is scaled with the system size. The scaling exponent is zero for all strains below a critical value which turns out surprisingly to be the overshoot strain. Above, the scaling exponent is finite. This picture holds for the system size larger than approx. 4000 particles. For small system size we find that the scaling exponent is finite and constant irrespective of any strain value. In order to understand these two pictures we calculate the mobility correlation of nearest neighbours. Around the mobility range where percolation of mobile particles takes place, the correlation increases again up to sizes of approx. 4000 particles and saturates above that size. This yields additional insight into the physical mechanisms of yielding.

DY 10.4 Mon 17:00 H8

Tuning the Temperature-Dependent Thermal Conductivity via Complex Colloidal Superstructures — Fabian Nutz and •Markus Retsch — Physical Chemistry I, University of Bayreuth, 95447 Bayreuth, Germany

The ability to specifically tune the temperature dependence of the thermal conductivity possess a vital challenge to develop and conceive future heat management devices. In this contribution, we demonstrate the vast potential of polymer colloidal crystals to address and master these challenges. We achieve this goal based on the constriction controlled thermal transport through well-defined colloidal crystal superstructures.[1,2,3,4] These colloidal superstructures are specifically built by tailor-made latex particles with distinct glass transition temperatures. We exploit their multiresponsive film formation at various temperatures to demonstrate unprecedented control over thermal conductivity at temperatures between 25 °C and 200 °C. Based on the film formation process, we can irreversibly increase the thermal conductivity by a factor of about three. We show how to control: i) the temperature, where the increase in thermal conductivity happens ii) the sharpness of the thermal conductivity increase iii) the height of the increase in thermal conductivity iv) the incorporation of a multistep increase in thermal conductivity

[1] Nutz et al. J. Colloid Interface Sci. 2015, 457, 96. [2] Ruckdeschel et al, Nanoscale 2015, 7, 10059. [3] Nutz et al, Phys. Chem. Chem. Phys. 2017, 19, 16124

DY 10.5 Mon 17:15 H8

Direct Determination of the Thermodynamic Properties of Melting for Amino Acids — •Y.Z. Chua[1], H.T. Do[3], D. Zaitsau[2], S.P. Verevkin[2], C. Held[3], and C. Schick[1] — [1]Uni. Rostock, Inst. Physics and CALOR, Rostock, Germany — [2]Uni. Rostock, Inst. Chemistry, Rostock, Germany — [3]TU Dortmund Uni., Depart. Biochem. Chem. Eng., Dortmund, Germany

The properties of melting are used for the prediction of solubility of

solid compounds. Unfortunately, by using the conventional DSC or adiabatic calorimetry direct determination of the melting enthalpy and melting temperature is often not possible for biological compounds due to the decomposition during the measurement. The apparent activation energy of decomposition is at least one order of magnitude smaller than that of melting. This allows shifting of the decomposition process to higher temperature without seriously disturbing the melting by applying very high heating rates. High scanning rates up to $2 \cdot 10^4\ K \cdot s^{-1}$ are utilized with fast-scanning calorimeter Mettler Toledo Flash DSC1, which employs thin film chip sensors with sub $\mu J \cdot K^{-1}$ addenda heat capacities. With the help of this technique the melting parameters for a series of amino acids and dipeptides were successfully determined. The ultra-fast cooling of the melted samples allows the studied compounds to retain in the liquid state and to determine for the first time its glass transition temperatures. The determined glass transition temperatures agree with the Beaman-Kauzmann rule. The correlation between the melting properties of the amino acids and dipeptides with their molecular structures were investigated.

DY 11: Focus Session: Quantum Dynamics of Kinetically Constrained Many-Body Systems (joint session TT/DY)

Over the past few years it has been shown that quantum many-body systems far from equilibrium can exhibit very rich and exciting physics, including the emergence of thermodynamics in closed quantum systems, dynamical quantum phase transitions, and many-body localization. This topic became of particular relevance as closed quantum many body states can now be prepared experimentally and coherent quantum dynamics can be observed over long time scales. Strongly correlated systems that are subject to a kinematic constraints receive currently a lot of attention. Such constrained quantum matter is characterized by a Hilbert space structure that is different from a conventional tensor product structure. Well known examples are frustrated quantum magnets described by effective dimer models, fractional quantum Hall liquids, and so called fracton models with excitations that are only mobile in certain directions. In a recent experiment, constrained models have also been realized in synthetic quantum matter in which Rydberg excitations of one-dimensional ultracold atoms are energetically forbidden to occupy neighbouring sites*a constrained model that can be mapped onto a 1D quantum dimer model. While the equilibrium properties of constrained systems have been studied in depth over the past decades in the context of frustrated magnetism and gauge theories, we just begin to understand the rich non-equilibrium physics of these systems. The proposed session aims to give an overview ofrecent developments and point towards the open questions.

Organized by: Michael Knap (Technical University of Munich), Frank Pollmann (Technical University of Munich), Roderich Moessner (Max-Planck-Institute for the Physics of Complex Systems)

Time: Tuesday 9:30–13:00 Location: H2

Invited Talk DY 11.1 Tue 9:30 H2

Quantum dynamics, scars, and integrability in constrained Rydberg systems — •Vedika Khemani[1], Christopher Laumann[2], and Anushya Chandran[2] — [1]Harvard University, Cambridge, Massachusetts, USA — [2]Boston University, Boston, Massachusetts, USA

A recent experiment on a 51-atom chain of Rydberg atoms observed anomalously long-lived temporal oscillations of local observables after quenching from an antiferromagnetic initial state. This coherence is surprising as the initial state should have thermalized rapidly to infinite temperature. I will describe the novel dynamics of this system using various diagnostics, and provide some insights into the underlying causes for the unusual dynamical properties of this system.

Invited Talk DY 11.2 Tue 10:00 H2

DMRG investigation of constrained models: from quantum dimer and quantum loop ladders to hard-boson and Fibonacci anyon chains — •Natalia Chepiga[1] and Frederic Mila[2] — [1]University of California, Irvine, USA — [2]EPFL, Lausanne, Switzerland

Motivated by the presence of Ising transitions that take place entirely in the singlet sector of frustrated spin-1/2 ladders and spin-1 chains, we study two types of effective dimer models on ladders, a quantum dimer model and a quantum loop model. We further show that both models can be mapped rigorously onto a hard-boson model first studied by Fendley, Sengupta and Sachdev [Phys. Rev. B 69, 075106 (2004)]. Building on a density-matrix renormalization group algorithm that takes full advantage of the dimers constraints, we study systems with up to 9'000 sites and calculate the correlation length and the wave-vector of the incommensurate short-range correlations with unprecedented accuracy. We discuss the full phase diagram of these models, with special emphasis on the phase transitions. In particular, we provide strong numerical evidence that there is an intermediate floating phase far enough from the integrable Potts point, while in its vicinity, our numerical data are consistent with a unique transition in the Huse-Fisher chiral universality class. Moreover, using conformal field theory, we fully characterize the tricritical Ising point, with a complete analysis of the boundary-field correspondence including partially polarized edges.

Invited Talk DY 11.3 Tue 10:30 H2

Localization in Fractonic Random Circuits — Shriya Pai, •Michael Pretko, and Rahul Nandkishore — University of Colorado Boulder

In this talk, I will describe a new mechanism for many-body localization, making use of ideas drawn from the field of fractons. Specifically, I will present results on the spreading of initially local operators under random unitary evolution in spin chains subject to fracton conservation laws, such as conservation of dipole moment. We find that fractons remain permanently localized at their initial positions, providing a crisp example of a non-ergodic dynamical phase of random unitary evolution. These results can be interpreted as a consequence of the properties of low-dimensional random walks. This mechanism for localization remains robust in one and two dimensions, but breaks down in three-dimensional fracton systems. We argue that these results extend to Floquet and Hamiltonian time evolution, even in the absence of disorder, thereby providing a mechanism for many-body localization in a translationally invariant system.

15 min. break.

Invited Talk DY 11.4 Tue 11:15 H2

Many-body localization dynamics from gauge invariance — •Markus Heyl — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

In this talk I will show how lattice gauge theories can display many-body localization dynamics in the absence of disorder as a consequence of local constraints induced by gauge invariance. The starting point is the observation that, for some generic homogeneous initial conditions, the time-evolved state can be decomposed into different superselection

sectors as a consequence of Gauss law in such a way that it realizes an effective disorder average. By carrying out extensive exact simulations on the real-time dynamics of a lattice Schwinger model, describing the coupling between U(1) gauge fields and staggered fermions, it is shown that the dynamics can become nonergodic leading to a slow, double-logarithmic entanglement growth. These findings are immediately relevant to cold atoms and trapped ion experiments realizing dynamical gauge fields and suggest a new and universal link between confinement and entanglement dynamics in the many-body localized phase of lattice models.

Invited Talk DY 11.5 Tue 11:45 H2

Slow dynamics due to kinetic constraints, from classical to quantum — •Juan Garrahan — School of Physics and Astronomy, University of Nottingham

Classical many-body systems that display slow collective relaxation - the canonical example being those that form glass - often do so due to effective constraints in the their dynamics. The simplest manifestation of this principle is in so-called kinetically constrained models (KCMs) where dynamical constraints are explicit. After reviewing the basic properties of constrained dynamics in classical systems, I will dis- cuss how similar ideas can be made relevant for quantum many-body systems. I will describe quantum KCMs which display slow thermalization and even in certain cases (apparent) non-ergodicity in the absence of disorder. Like in the classical case, I will show how slow relaxation goes together with spatially fluctuating dynamics, giving rise to heterogeneous growth of entanglement. I will also discuss connections with other quantum systems with complex dynamics such as fracton models. My main aim will be to highlight links between concepts and methods of classical and quantum non-equilibrium.

DY 11.6 Tue 12:15 H2

Dynamical Phase Transitions in a 2D Quantum Dimer Model — •Johannes Feldmeier, Michael Knap, and Frank Pollmann — Technische Universität München

The study of dynamical properties in systems with local constraints has attracted a lot of interest, spurred by experiments with Rydberg blockaded atoms, that naturally implement constrained many-body models. We study the quench dynamics in a 2D quantum dimer model to identify dynamical phase transitions in constrained models by means of exact diagonalization on systems of sizes up to 8x8 sites. We find that the quenched quantum system thermalizes efficiently by determining the relaxation dynamics of both the order parameter (OP) and local correlation functions. The observed fast relaxation to thermal expectation values allows us to study the underlying thermal BKT-transition between a columnar ordered valence bond solid (VBS) and a symmetric liquid (VBL) phase in the form of a dynamical phase transition. The existence of this finite-temperature transition in the dynamics is confirmed by the long-time averaged values of the OP. Moreover, upon quenching across the VBS-VBL phase boundary, the dynamical transition can be shown to be manifest in the Loschmidt-echo, whose rate-function displays kinks at the zero-crossings of the columnar OP.

DY 11.7 Tue 12:30 H2

Hamiltonian systems with charge and dipole conservation far from equilibrium — •Pablo Sala, Tibor Rakovszky, Ruben Verresen, Michael Knap, and Frank Pollmann — Technische Universität München, Physics Department T42, 85747 Garching, Germany

Recently so-called fracton phases, which are characterized by excitations with restricted mobility, have been discovered. The mobility constraints are related to the conservation of a U(1) charge and its associated dipole moment. Motivated by results on random unitary circuits [1], we study one dimensional spin-1/2 and spin-1 Hamiltonian systems conserving these two intertwined quantities and consider the implications of a U(1) local gauge invariance. We investigate the effects of these conservation laws on the dynamics, and the implications for higher dimensional systems following the same construction. [1] S. Pai, M. Pretko and R. M. Nandkishore. arXiv:1807.09776 [cond-mat.stat-mech]

DY 11.8 Tue 12:45 H2

Apparent slow dynamics in the ergodic phase of a driven many-body localized system without extensive conserved quantities — •Talía Lezama Mergold Love[1], Soumya Bera[2], and Jens H. Bardarson[1,3] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India — [3]Department of Physics, KTH Royal Institute of Technology, Stockholm, 106 91 Sweden

One of the distinguishing features of the ergodic phase in systems exhibiting many-body localization (MBL) is a slowing down of the dynamics as they approach the MBL transition. Using a fast Walsh-Hadamard transform, we numerically study the former scenario in a Floquet model with no global conservation laws. In this model, the ergodic-MBL transition can be tuned by the disorder strength within a region of the frequency-amplitude space. Similarly to models with conserved quantities, our data is consistent with a subballistic spread of entanglement and a stretched-exponential decay of an autocorrelation function, with their associated exponents reflecting slow dynamics near the transition for a fixed system size. However, with access to larger system sizes, we find a clear flow of the exponents towards faster dynamics. We further observe examples of non-monotonic dependence of the exponents with time, consistent with the slow dynamics being a crossover phenomena with a localized critical point.

DY 12: Talk Pascal Silberzan

Time: Tuesday 9:30–10:00 Location: H3

Invited Talk DY 12.1 Tue 9:30 H3

Active Cell Nematics: Architectures and flows. — •Pascal Silberzan — Institut Curie, Paris, France

When cultured in monolayers, spindle-shaped cells such as NIH-3t3 fibroblasts form domains of common orientation. These domains don't fuse because of the presence of intrinsic topological defects characteristic of these 2D nematic phases. The characteristic size of these domains is very large compared to a cell size (up to 0.5 mm). Confining these fibroblasts in stripes whose width is smaller than this length ensures a defect-free nematic ordering whose director aligns with the stripe's direction. However, in the same confinement condition, other cell types adopt a more complex nematic architecture and develop spontaneous shear flows. This particular situation is reminiscent of in vivo observations where cancer cells escaping collectively from a tumor can locally migrate in antiparallel directions within the same strand. Confining the cells in circular domains imposes a topological charge that results in a pair of defects whose position indicates that cell activity is eventually overcome by friction with the underlying substrate.

DY 13: Wetting, Fluidics and Liquids at Interfaces and Surfaces (joint session CPP/DY)

Time: Tuesday 9:30–13:00 Location: H13

DY 13.1 Tue 9:30 H13

Non-monotonous wetting of graphene-mica and MoS_2-mica interfaces with a molecular layer of water — •Abdul Rauf, Andre Schilo, Nikolai Severin, Igor M. Sokolov, and Jürgen P. Rabe — Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Hydration of interfaces with a layer of water is a ubiquitous phenomenon. Nevertheless, the understanding of the wetting process is still limited, since it is experimentally difficult to follow. Here, graphene and monolayers of MoS_2 deposited on dry mica are used to investigate wetting of the 2D material-mica interfaces with a molecularly thin layer of water employing scanning force microscopy in different modes. Wetting starts at relative humidities (RH) of 10-17% for graphenes and 8-9% for MoS_2, and it concludes with a homogeneous layer at 25-30% and 15-20%, respectively. Wetting occurs non-monotonously in time and space for both types of interfaces. Initially a highly compliant and unstable layer of water spreads, which subsequently stabilizes by developing labyrinthine nanostructures. These nanostructures exhibit distinct mechanical deformability and dissipation, which is ascribed to different densities of the confined water layer. The laterally structured morphology is explained by the interplay of counteracting long-range dipole-dipole repulsion and short-range line tension, associated with the mechanical deformation of the 2D material. The proposed origins of the interactions are common for thin layers of polar molecules at interfaces, implying that the lateral structuring of thin wetting layers may also be a quite general phenomenon.

DY 13.2 Tue 9:45 H13

Molecular Hydrophobicity at a Macroscopic Hydrophilic Surface — •Jenee D. Cyran[1], Michael Donovan[1], Doris Vollmer[1], Flavio Siro Brigiano[2], Simone Pezzotti[2], Daria R. Galimberti[2], Marie-Pierre Gaigeot[2], Mischa Bonn[1], and Ellen H.G. Backus[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]LAMBRE, Univ Every, Universite Paris-Saclay, Evry, France

Chemical and physical interactions between water and silicates are ubiquitous and relevant for geochemistry and industrial processes, including chromatography, oil extraction and coatings. Characterizing the silica/water interface is important to not only understand the fundamental properties for natural occurring processes but also to improve existing technologies, such as silica coatings, which rely on wettability and thermal-resistant properties to remain effective. At the silica/water interface, we compare the microscopic water organization, from both surface sensitive vibrational sum frequency generation experiments and molecular dynamics simulations, to macroscopic information about the hydrophobicity obtained from contact angle measurements. At the microscopic level, weakly hydrogen-bonded OH groups, typical for hydrophobic interfaces, are observed that originate from water molecules interacting with hydrophobic sites of the silica surface. Surprisingly, we observe the presence of hydrophobic water at a macroscopically hydrophilic water surface.

DY 13.3 Tue 10:00 H13

Interfacial premelting of ice in nano composite materials — •Markus Mezger[1,2], Hailong Li[1], Julian Mars[1,2], and Markus Bier[3,4] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Institute of Physics, Johannes Gutenberg University Mainz — [3]Max Planck Institute for Intelligent Systems, Stuttgart — [4]University of Applied Sciences Würzburg-Schweinfurt

The interfacial premelting in ice/clay nano composites was studied by high energy X-ray diffraction. Below the melting point of bulk water, the formation of liquid water was observed for the ice/vermiculite and ice/kaolin system. For the quantitative description of the molten water fraction in wet clay minerals we developed a continuum model for short range interactions and arbitrary pore size distributions. This model quantitatively describes the experimental data over the entire temperature range. Model parameters were obtained by fitting using a maximum entropy approach. Pronounced differences in the deviation from Antonow's rule relating interfacial free energy between ice, water, and clay are observed for the charged vermiculite and uncharged kaolin minerals. The resultant parameters are discussed in terms of their ice nucleation efficiency. Using well defined and characterized ice/clay nano composite samples, this work bridges the gap between studies on single crystalline ice/solid model interfaces and naturally occurring soils and permafrost.

[1] H. Li et al., Phys. Chem. Chem. Phys. DOI: 10.1039/c8cp05604h (2018)

DY 13.4 Tue 10:15 H13

A Direct Inversion Approach to Local Permittivity at Liquid-Liquid Interfaces — •David Egger, Christoph Scheurer, and Karsten Reuter — Theoretische Chemie, TU München

Realistic models for catalytic reactions at liquid-liquid interfaces (LLIs) require a profound knowledge of the electrostatic properties in the vicinity of the solvated catalytic complex. For polar fluids like water, these properties as described by the static dielectric constant, ε, can be related to thermal equilibrium fluctuations of the polarization at zero field.

The Kirkwood-Fröhlich (KF) approach usually applied in the derivation of such formulas faces two major difficulties: First, correlated polarization fluctuations are long-range and subject to slow convergence, making KF expensive in simulations. Second, the difficulty of the electrostatic boundary value problem one needs to solve in a KF ansatz increases with the systems' complexity. In this contribution, we present a possible alternative procedure, following the reciprocal space formalism described by Neumann for wave-vectors at finite wavelength [1].

Exploiting the convolutional relation between dipole-dipole interaction tensor and polarization, we present a cavity kernel based approach in reciprocal space in order to arrive at local real space averages to calculate a spatially resolved $\varepsilon(r)$ from spheroidal gaussian cavities of different shape and volume, avoiding difficulties with geometry-induced boundary conditions in the electrostatic description. Results are discussed for water bulk and water-dichloroethane LLI systems.

[1] M. Neumann, Mol. Phys. 57:1, 97-121, 1986

DY 13.5 Tue 10:30 H13

Testing dielectric continuum theory at interfaces by atomistic simulations — •Philip Loche[1], Cihan Ayaz[1], Alexander Schlaich[1,2], Douwe Jan Bonthuis[1], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Laboratoire Interdisciplinaire de Physique, CNRS and Université Grenoble Alpes, UMR CNRS 5588, 38000 Grenoble, France

Based on fully atomistic simulations of ions in water, we discuss the validity of continuum models for the dielectric response at aqueous interfaces. For the electrostatic energy of an ion in the vicinity of a hydrophobic graphene surface we find the electrostatic contribution to be dominated by the non-electrostatic contribution. Linear dielectric theory breaks down, and to quantitatively describe the linear dielectric contribution an anisotropic tensorial dielectric model is needed. This demonstrates the limitation of current continuum models for the dielectric response at interfaces.

Invited Talk DY 13.6 Tue 10:45 H13

Dynamic surface tension of soft solids — Mathijs van Gorcum[1], Bruno Andreotti[2], Jacco Snoeijer[1], and •Stefan Karpitschka[3] — [1]University of Twente, Enschede, Netherlands — [2]Université Paris-Diderot, Paris, France — [3]MPI-DS, Göttingen, Germany

The contact line of a liquid drop on top of a solid surface exerts a nanometrically sharp surface traction, providing an unprecedented tool to study highly localized and dynamic deformations of soft polymer networks. The morphology is determined not only by bulk viscoelasticity, but also by solid surface tension. The latter may depend on strain, known as the Shuttleworth effect. Its impact on soft wetting is controversially discussed in recent literature. One of the outstanding problems in this context is the stick-slip instability of a moving contact line, which is observed above a critical velocity. Timeresolved measurements of the solid deformation are challenging, and the mechanism of dynamical depinning has remained elusive. Here we present direct visualizations of dynamic wetting ridges. Unexpectedly, the opening angle of the wetting ridge increases with speed, which cannot be attributed to bulk rheology. Instead, this effect points to an increase of

solid surface tension not only in response to strain, but also depending on the rate of strain. Under this assumption, a criterion for depinning can be derived which is confirmed experimentally. We conclude that the surface tension of a solid is a truly dynamical quantity, following from a surface rheology that is different from the bulk, similar to what is known from liquid interfaces with surfactants.

15 min. break

DY 13.7 Tue 11:30 H13

Raman spectroscopic evaluation of concentration gradients in small drops in binary mixtures on different substrates and in 3d printed small channels — •Alena Bell and Robert Stark — Physics of Surfaces, Materialwissenschaften, TU Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt, Deutschland

The evaluation of concentration gradients plays a big role in medical technology and chemotaxis. Microchannels are used in lab-on-chip devices for quick tests to test fluids directly, for example. Microchannels are also used for chemotaxis applications to mix fluids. The amount of liquid which is needed for these tests is in the microliter range. Raman spectroscopy is a powerful technique to detect changes in molecular structures within reactions in lab-on-chip devices and in chemotaxis devices. Therefore, different fluids are directed through 3d printed channels and changes are measured via Raman spectroscopy. In a first step, these generated fluid mixtures are measured as drops on different substrates. The concentration gradients that build up in the mixtures is measured in the drops. In the next step the gradients are measured in small channels. The concentration gradients are calculated by comparing relative peak intensities and correlating these results with calibration curves.

DY 13.8 Tue 11:45 H13

Shallow water lattice Boltzmann simulations of thin film flows — •Stefan Zitz[1], Andrea Scagliarini[2], Suryanarayana Maddu Kondaiah[3], Anton Darhuber[4], and Jens Harting[1,4] — [1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Nürnberg, Germany — [2]Institute for Applied Mathematics "M. Picone" (IAC-CNR), Rome, Italy — [3]Center for System Biology (MPI-CBG), Dresden, Germany — [4]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

We propose a novel approach to the numerical simulation of thin film flows, based on the viscocapillary shallow water equations. The integration is performed by the means of a suitably devised lattice Boltzmann method.

The numerical scheme is applied to the viscous Rayleigh-Taylor instability of a thin film under the influence of gravity as well as the spreading of a sessile drop towards its equilibrium contact angle. During the spreading we observe a linear correlation between the spreading speed and the contact angle, as theoretically predicted by the Cox-Voinov law.

Further we address the problem of a droplet sliding on an inclined plane. Due to the choice of the substrate friction we observe a pinning region for low forcing. When increasing the forcing by varying the droplet volume the droplet starts to slide and the Capillary number scales linearly with the Bond number.

DY 13.9 Tue 12:00 H13

Complex Wetting: flow profiles close to three phase contact lines — •Benedikt Straub[1], Franziska Henrich[1], and Günter K. Auernhammer[2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Leibniz Institute for Polymer Research, Dresden, Germany

Wetting and dewetting behavior on solid surfaces is the crucial process underlying many natural phenomena as well as technical applications like printing or coating of surfaces. Our aim is to study the wetting behavior of surfactant solutions on solid surfaces. Especially the flow profile close to the three phase contact line is highly interesting for modelling efforts.

Three-dimensional flow profiles are measured with an astigmatism particle tracking velocity setup.

Measurements of a receding contact line for pure water show that the theoretical prediction can be reproduced, which is used to validate the system. First results show that surfactants cause a deviation of the flow field in comparison to theoretical predictions for pure liquids. In the case of a receding contact line new air-liquid interface is formed at the three phase contact line. The freshly formed interface is, in comparison to the already existing air-liquid interface, not completely occupied by surfactants. This causes a Marangoni tension in the direction of the contact line along the interface. This Marangoni tension opposes the bulk flow close to the air-liquid interface and causes a deviation of the flow field. In special cases this can lead to an opposing interface flow compared to the bulk flow.

DY 13.10 Tue 12:15 H13

Direct observation of gas meniscus formation on a superhydrophobic surface — •Doris Vollmer[1], Mimmi Eriksson[2], Agne Swerin[2], Hannu Teisala[1], Michael Kappl[1], and Hans-Jürgen Butt[1] — [1]MPI for Polymer Research, Mainz, Germany — [2]RISE Research Institutes of Sweden, Stockholm, Sweden

The formation of a bridging gas meniscus via cavitation or nanobubbles is considered the most likely origin of the long-range attractive forces measured between hydrophobic surfaces in aqueous solution. On a superhydrophobic surface a thin air layer is present and influences the interaction. Here, we report time and space resolved imaging of the formation and growth of a gas meniscus during force measurements between a superhydrophobic surface and a hydrophobic microsphere immersed in water. This is achieved by combining laser scanning confocal microscopy and colloidal probe force microscopy. The configuration allows determination of the volume and shape of the meniscus, together with direct calculation of the Young-Laplace capillary pressure. The long-range attractive interactions acting on separation are due to meniscus formation and volume growth as air is pulled from the surface layer.

DY 13.11 Tue 12:30 H13

Wetting of n-Alkane Nano-Patterns: Evidence of Macroscopic Line Tension Effects and Adaptive Wetting — •Diego Diaz[1], Tomas P. Corrales[2], Maria J. Retamal[3], Marcelo Cisternas[1], Nicolas Moraga[1], Rodrigo Catalan[1], Mark Busch[4], Patrick Huber[4], Marco Soto-Arriaza[3], and Ulrich G. Volkmann[1] — [1]Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [2]Department of Physics, UTFSM, Valparaiso, Chile — [3]Faculty of Chemistry and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [4]TUHH, Hamburg, Germany

We present a wetting study of silicon samples coated with a single layer of n-alkane molecules self-assembled perpendicular to the surface by velocity-dependent dip-coating. The contact angle was measured with 2 microliters of ultrapure water for different n-alkane surface coverages. The results of the apparent contact angle versus coverage can be grouped in two regimes that depend linearly on coverage. This can be described by the Cassie wetting model along with the consideration of line tension effects. The two wetting regimes are characterized by two line tensions representing distinct alkane monolayer morphologies, i.e. dentritic and stripe patterns resulting from different dip-coating velocities. During drop evaporation, there is a restructuring of the alkane monolayer structure which could be related to adaptive wetting. Acknowledgements: FONDECYT Nos. 3160803 (MJR), 1180939 (UGV) 1171047 (MSA) and 11160664 (TPC), CONICYT Fellowship (MC) and CONICYT-PIA ACT 1409.

DY 13.12 Tue 12:45 H13

Impact of Nanoparticles' Surface Properties on their Physico-Chemical Behavior in Pickering Emulsions — •Sebastian Stock, Dmitrij Stehl, Sandra Forg, and Regine von Klitzing — TU Darmstadt, Darmstadt, Germany

Pickering Emulsions (PEs) were first studied by S. U. Pickering in the beginning of the last century and describe emulsions stabilized by particles that adsorb at the oil water interface and prevent coalescence of the droplets. In the present study Halloysite Nanotubes, fumed colloidal silica and Latex nanospheres are used to stabilize PEs. They display significant differences regarding their surface properties, size and shape. The surface of these particles is modified in order to investigate the influence of surface charge or hydrophobicity on the whole systems behavior including emulsion stability and reaction performance in homogeneous catalysis at the oil-water-interface. Additionally, the effect of the surface-active Rh-catalyst is investigated. The interaction between catalyst and particle surface plays a significant role for mass transfer and conversion.

DY 14: Talk Gunter M. Schütz

Time: Tuesday 9:30–10:00 Location: H19

Invited Talk DY 14.1 Tue 9:30 H19

The Fibonacci family of dynamical universality classes — •Gunter M. Schütz — Forschungszentrum Jülich, Jülich, Deutschland

Using mode coupling theory for nonlinear fluctuating hydrodynamics we predict that in generic quasi one-dimensional systems the transport of mass, energy and other locally conserved quantities is governed by dynamical universality classes with dynamical exponents z which are Kepler ratios of neighboring Fibonacci numbers, starting with $z = 2$ (corresponding to a diffusive mode) or $z = 3/2$ (Kardar-Parisi-Zhang (KPZ) mode). If neither a diffusive nor a KPZ mode are present, all modes have as dynamical exponent the golden mean $z = (1 + \sqrt{5})/2$. The universal scaling functions of the higher Fibonacci modes are Lévy distributions. These results put the well-known diffusive and KPZ universality classes into a larger perspective. The theoretical predictions are confirmed by Monte-Carlo simulations of n-lane asymmetric simple exclusion processes which are also models of directed polymers in $n+1$ dimensions.

DY 15: Pattern Formation

Time: Tuesday 10:00–13:15 Location: H3

DY 15.1 Tue 10:00 H3

Spontaneous center formation in Dictyostelium discoideum — •Estefania Vidal-Henriquez and Azam Gholami — Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077 Göttingen, Germany

Dictyostelium discoideum (D.d.) is a widely studied amoeba due to its capabilities of development, survival, and self-organization. During aggregation it produces and relays a chemical signal (cAMP) which shows spirals and target centers. Nevertheless, the natural emergence of these structures is still not well understood. We present a mechanism for creation of centers and target waves of cAMP in D.d. by adding cell inhomogeneity to a well known reaction-diffusion model of cAMP waves and we characterize its properties. We show how stable activity centers appear spontaneously in areas of higher cell density with the oscillation frequency of these centers depending on their density. The cAMP waves have the characteristic dispersion relation of trigger waves and a velocity which increases with cell density. Chemotactically competent cells react to these waves and create branching aggregation streams even with very simple movement rules. Finally we argue in favor of the existence of a degradation which scales with local density to maintain the wave properties once small cell clusters appear in the high density streams.

DY 15.2 Tue 10:15 H3

Controlling discrete pattern formation with local signals — •Stephan Kremser, Tiago Ramalho, Hao Wu, and Ulrich Gerland — Technical University of Munich

Programmability is a fruitful concept to explore the extent to which a dynamical system can be steered by external inputs or internal feedback signals. Here, we propose a minimal system for studying the programmability of discrete patterning, based on one-dimensional cellular automata, which process discrete local signals to update their internal state according to logical rules. The organization signals are given by individual cells that are located either within the system or at its boundary. This framework is sufficiently general to encompass a broad class of model systems, yet simple enough to permit exhaustive analysis. We study model systems with different update rules and different topologies, to assess their ability to perform programmable pattern formation and their susceptibility to errors. We find that only a small subset of model systems permits local organizer cells to dictate any target pattern. These systems follow a common principle whereby a temporal pattern is transcribed into a spatial pattern. Our results establish a basis for the design of synthetic systems, and for more detailed models of programmable pattern formation closer to real systems.

DY 15.3 Tue 10:30 H3

Effects of time-periodic forcing in a generalized Cahn-Hilliard model for the Langmuir-Blodgett transfer — •Phong-Minh Timmy Ly[1], Uwe Thiele[1], Lifeng Chi[2], and Svetlana V. Gurevich[1] — [1]Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Soochow University, 215123 Suzhou, P.R. China

The Langmuir-Blodgett transfer is a surfactant based dip-coating technique where pattern formation occurs via self-organization. In particular, a solid substrate is pulled out of a liquid bath, covered by a monolayer of surfactants. In this setup the transfer velocity is the main control parameter and leads to deposition of different kinds of patterns depending on its magnitude. The procedure excels in through-put in comparison to traditional lithographic methods as means for pattern creation but lacks in terms of uniformity and ways to control the patterns. Therefore, we investigate the effect of a time-periodically modulated velocity on the pattern formation by means of a generalized Cahn-Hilliard equation. 1D and 2D direct numerical simulations reveal various synchronization phenomena as well as the deposition of a variety of complex patterns. Interestingly, it is also possible to influence the system in the spatial direction which is transversal to the direction of the forcing which can lead to the formation of synchronized patterns in two-spatial dimensions.

DY 15.4 Tue 10:45 H3

DNS of liquid films under lateral and normal excitations — •Sebastian Richter and Michael Bestehorn — Department of Theoretical Physics, BTU, 03044, Cottbus, Germany

We investigate the dynamics of a two-dimensional liquid film on a horizontal substrate with free and deformable surface. The system is subjected to a time-periodic gravitation field in normal or lateral direction. We present a finite-difference method on staggered-grids for the full incompressible Navier-Stokes equations. To avoid surface tracking and to reduce the necessary interpolations to a minimum, the time-dependent free surface is mapped to a constant rectangular region using the non-linear transformation $z = h(x,t) \cdot \tilde{z}$ of the vertical coordinate. Taking the continuity equation into account, a sparse linear system for the pressure, whose solution fulfills momentum and mass conservation, can be computed directly from the discretized Navier-Stokes equations allowing us to refrain from applying pressure corrections. We compare our findings to those of a simplified model studied in [1] and [2]. Vertical excitations generate the classic Faraday waves and lateral forces engender the formation of coarsening droplets. A preferred direction of motion of the drops and a non-vanishing mean flow rate is observed for lateral excitations that break the horizontal mirror symmetry $x \to -x$. Our results show good agreement with the model.

[1] M. Bestehorn, "Laterally extended thin liquid films with inertia under external vibrations", Phys. Fluids 25, 114106 (2013)
[2] S. Richter and M. Bestehorn, "Thin-Film Faraday patterns in three dimensions", Eur. Phys. J. Special Topics 226, 1253 (2017)

DY 15.5 Tue 11:00 H3

Simulation of surface evolution beyond the small gradient approximation — •Christoph Kabelitz and Stefan Jakob Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

Apart from three-dimensional and discrete models the evolution of surfaces is usually described by spatially two-dimensional PDEs. These models are often derived from small gradient approximations, but the studied surfaces do not fulfill this requirement in all cases. We will explain how to overcome the small gradient approximation. Therefore, we will introduce a method to simulate the evolution of surfaces with respect to local geometric properties. In contrast to traditional PDEs, the resulting geometric PDEs do not depend on the parametrization of the surface [1]. This allow us to simulate surface evolution not only on almost flat surfaces but also on more complex shaped objects. For small gradients the studies of simple model equations show similar re-

sults compared to the related PDEs (like the Kuramoto-Sivashinsky equation [2, 3]). For large gradients the results differ fundamentally.

[1] M. Marsili et al, Rev. Mod. Phys., 68, 963 (1996).

[2] Y. Kuramoto and T. Tsuzuki, Progress of Theoretical Physics, 55, 356 (1976).

[3] G. Sivashinsky, Acta Astronautica, 4, 1177 (1977).

DY 15.6 Tue 11:15 H3

Pattern formation in salt playa — •Jana Lasser — Max Planck Institut für Dynamik und Selbstorganisation, Göttingen

Salt pans are geological sinks where evaporation outweighs precipitation. As a result, a continuous salt crust forms, which expresses iconinc hexagonal ridge patterns with a diameter of roughly one meter. We model the process driving the emergence of these patterns as result of an instability in a dynamical process, taking place in the ground below the patterns: Here, the subsurface is composed of a porous medium saturated with salty water. As water evaporates through the surface, a salinity gradient builds below the surface and is prone to a buoyancy-driven convective instability. With this advection-diffusion model, we can explain the onset of convection as well as the length scale of the patterns. We show evidence from experiments, numerical simulations and direct field observations, confirming that convection takes place in the underground, and that convection cells are co-located with the patterns visible on the surface.

15 min. break

DY 15.7 Tue 11:45 H3

Single-Mode Turbulence in Pattern-Forming Protein Systems — •Jonas Denk, Jacob Halatek, Fridtjof Brauns, Korbinian Pöppel, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Germany

Protein pattern formation often relies on proteins that cycle between a cyctosolic bulk and a membrane at which they undergo molecular interactions. On a flat membrane, this cycling can lead to intriguing protein patterns including spiral waves as well as more irregular dynamics such as chemical turbulence. While theoretical approaches have been able to reproduce various experimentally observed protein patterns, the underlying mechanisms for pattern selection remain poorly understood. Motivated by the bacterial Min protein system, we present a spatially reduced reaction-diffusion model to study pattern selection in protein systems with bulk-membrane coupling. Remarkably, we find that already a single-mode instability can lead to turbulent dynamics at the onset of pattern formation. Further away from this onset, we observe a transition from turbulent to coherent patterns, which can be explained on the basis of diffusively coupled local equilibria. Our study yields insights into a novel route to chaos for a widespread class of mass-conserving reaction-diffusion systems with bulk-boundary coupling.

DY 15.8 Tue 12:00 H3

Transition to Chaos: From Small to Large Domains in the Nikolaevskiy Model — •Simon Hartmann, Steffen Richters-Finger, and Stefan J. Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Straße 9, 48149 Münster

We investigate the dynamics and the transition to spatiotemporal chaos observed in the partial differential equation known as Nikolaevskiy equation in one and two spatial dimensions while applying periodic boundary conditions. In contrast to the generic chaotic solution in large domains, the model exhibits rich possibilities for different chaotic and non-chaotic dynamics if the considered domain size is constrained to only a few characteristic wavelengths. Extending the work by Tanaka [1], we provide an in-depth numerical analysis including maps of several parameter subspaces and results from the numerical continuation of many types of regular dynamics.

[1] Tanaka D., J. Phys. Soc. Jpn., 74, 2223 (2005).

DY 15.9 Tue 12:15 H3

Nonlinear analysis of dissipative systems with a conservation law — •Tobias Frohoff-Hülsmann[1] and Uwe Thiele[1,2] — [1]Institute of Theoretical Physics, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster — [2]Center of Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Corrensstr. 2, 48149 Münster

We investigate the coupled dynamics of a conserved and a non-conserved order parameter field using the generic example of a Cahn-Hilliard equation coupled to a Swift-Hohenberg equation. Uncoupled, both equations have a gradient dynamics structure and we employ couplings that may preserve or violate this structure. In both cases, the coupled system can show short- and long-scale instabilities. We analytically examine the types of linear instability and the weakly nonlinear behaviour deriving amplitude equations which are generically influenced by the conservation law. The weakly nonlinear results are compared to fully nonlinear bifurcation diagrams obtained with numerical path continuation. Finally, we discuss the generic consequences of a conservation law in variational and nonvariational systems.

DY 15.10 Tue 12:30 H3

Pattern formation of a coupled Turing-polarity model — •Francine Kolley[1], Peter Gross[1], K Vijay Kumar[2], and Stephan W Grill[1] — [1]BIOTEC, TU Dresden, Germany — [2]ICTS, Bangalore, India

Pattern formations are ubiquitous phenomena in nature. It is the ability of non-equilibrium systems to form stable, spatially non-homogeneous states. Such non-equilibrium patterns can emerge via a large class of distinct mechanisms.
Our aim is to couple two different mechanisms, Turing patterns and polarity patterns.
Turing systems are typically described using a diffusion term, which enables to spread out over the space and a reaction term, which couples two different species. These two species can establish Turing patterns under the condition of short-ranged activation and long-ranged inhibition.
In comparison to Turing systems, a central feature of polarity models is mass conservation. As a consequence, the patterned state generally has a singular domain. Furthermore, polarity models can show multistability, where the homogeneous state and the patterned state are both stable to perturbations.
We construct a model that can be gradually shifted from a pure Turing system to a pure polarity system. We investigate the pattern formation properties of this model, with a particular emphasis on the region where the Turing mode and the polarity mode compete.

DY 15.11 Tue 12:45 H3

Nonlinear patterns shape their domain on which they live — •Mirko Ruppert[1], Falko Ziebert[2] und Walter Zimmermann[1] — [1]Theoretical Physics I, University of Bayreuth, Germany — [2]Institute for Theoretical Physics, Heidelberg University, Germany

We investigate nonlinear pattern formation on a finite domain with fixed area but flexible borders. The self-consistent interplay between the stationary stripe pattern of a Swift Hohenberg model and the domain boarders, described by a phase field, may reshape the domain. With increasing amplitude of the stripe pattern the nearly circular domain for a small pattern amplitude deforms with increasing amplitude into an elliptical shaped domain. The behavior of this coupling resembles experimental observations made for vertically vibrated liquid drops. We also couple the Cahn-Hilliard model to a phase field, where the demixing process of a binary emulsion deforms the domain shape.

DY 15.12 Tue 13:00 H3

Boundary driven oscillations in *Dictyostelium discoideum* — •Torsten Eckstein, Estefania Vidal-Henriquez, and Azam Gholami — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Dictyostelium discoideum amoeba aggregate if deprived of nutrients, producing wave patterns of a chemo attractant called cyclic adenosine monophosphate (cAMP). To successfully produce waves, the role of degradation of cAMP by phosphodiesterase is fundamental, preventing the accumulation of cAMP and producing the gradients necessary for cell detection. The knockout mutant pdsA$^-$ can not produce the most active type of phosphodiesterase and therefore does not show pattern formation under normal circumstances. Using a microfliuidic channel, we show how an advective flow can partially recover signaling in this system. Above a minimum flow velocity decaying waves are induced, with a decay length that scales with the applied flow speed. After stopping the advecting flow, the cells continue to signal, showing normal structures and aggregation, although with a wave period much higher than in wild type cells. Extensive numerical simulations showed that these waves have a boundary driven origin, where the lack of cAMP in the upstream flow destabilizes the system. We explored the parameter region where these waves exist and their properties, with good agreement with our experimental observations. The results here presented provide experimental confirmation of the destabilizing effect

of the upstream boundary in an otherwise stable reaction-diffusion system.

DY 16: Quantum Dynamics, Decoherence and Quantum Information

Time: Tuesday 10:00–11:30 Location: H6

DY 16.1 Tue 10:00 H6

The dynamics of the Lindblad equation when including feedback from the environment — •Bernd Michael Fernengel and Barbara Drossel — Hochschulstraße 6, 64289 Darmstadt

The Lindblad equation describes the time evolution of an open quantum system when the environment relaxes fast. In addition to the von-Neumann term * describing the unitary time evolution according to the Schroedinger equation * the Lindblad equation takes into account stochastic transitions between different states. It assumes that the environment is not changed as the state of the system changes.

We abandon this last assumption and allow for an (instantaneous) feedback of the (mixed) state of the ensemble onto itself via the environment. One way to realize this would be to have several systems coupled to the same environment. This leads to a time evolution equation that is nonlinear in the density matrix. By using the example of a two-level system, we show explicitly that various types of instabilities and bifurcations can occur.

DY 16.2 Tue 10:15 H6

Lindblad equation for thermal environments beyond the rotating-wave approximation — •Tobias Becker, Lingna Wu, and André Eckardt — Max Planck Institute for the Physics of Complex Systems, Dresden

Many problems addressing open quantum systems (for weak system-bath coupling) start from a master equation in Lindblad form. In particular, it is needed for quantum trajectory simulations. For thermal environments, such a Lindblad-type master equation can be derived starting from the Redfield-equation (Born-Markov approximation) by applying a rotating-wave approximation. However, this approximation requires extremely weak system-bath coupling, which is small compared to the level splitting in the system. Here, we describe an alternative approximation to the Redfield equation, which also leads to a master equation in Lindblad form. It is valid also for larger system-bath coupling. We test our results using the example of a system of interacting bosons in a double well coupled to an Ohmic bath.

DY 16.3 Tue 10:30 H6

Entanglement via dissipation in a nonlinear circuit QED system — •Dominik Maile[1,2], Sabine Andergassen[1], Wolfgang Belzig[2], and Gianluca Rastelli[2] — [1]Eberhard Karls University, Tübingen, Germany — [2]University Konstanz, Konstanz, Germany

We discuss a superconducting nanoscale circuit formed by two microwave cavities coupled via a Josephson junction and a joint capacitance to the ground. In addition, the Josephson junction is shunted by a resistance and one plate of the capacitor is in series with a resistance connected to the ground. Such a configuration leads to dissipation in the relative phase difference across the Josephson junction and in the total charge of the two capacitances in parallel [1,2]. We show that, in the steady state, the resonators are in an entangled state and calculate the logarithmic negativity as a measure of entanglement in the harmonic regime. We find that the entanglement grows by increasing both dissipative coupling strengths via simultaneous squeezing of the fluctuations of the total charge and the relative phase difference. Due to the dissipative interaction, the system is not in a pure state. However, in the limit of large squeezing we compare the entanglement generated via dissipation with the one of an effective pure two-mode squeezed state. Increasing the coupling strength between the two oscillators via the Josephson energy also leads to a rise of the entanglement. Here the system enters the nonlinear coupling regime. We analyze the effect of such nonlinear interaction perturbatively.

[1] G. Rastelli, New Journal of Physics 18, 053033 (2016)
[2] D. Maile, et al. PRB 97, 155427 (2018)

DY 16.4 Tue 10:45 H6

Dephasing and relaxation of topological states in extended quantum Ising models — •Hannes Weisbrich, Wolfgang Belzig, and Gianluca Rastelli — Universität Konstanz

Inspired by recent progress in coupled arrays of qubits, we study the dephasing and relaxation dynamics of topological states in an extended class of quantum Ising chains of finite length [1]. We assume a local dephasing interaction of each spin with a local thermal bath, from which we derive a Lindblad equation. This kind of interaction preserves the parity in the system [2]. We demonstrate a correlation between the decoherence in the manyfold ground state subspace and the topology in the spin chain, characterized by a winding number g. In particular, in the topological regime and at low temperature, the decoherence rates can be exponentially suppressed. For the simple case of the transverse Ising model (g=1) this simply corresponds to the exponentially small overlap of the two localized Majorana zero energy modes of the equivalent Kitaev chain. We generalize this result in a chain with a three body, next nearest neighbor interaction (with g=2) in which the ground state subspace is fourfold degenerate with two ground states in each parity sector (even and odd), namely with four Majorana modes. For the second model, we analyze the decay rates and the probability of occupation of the different ground states as a function of the initial excited state.

[1] H. Weisbrich, W. Belzig, G. Rastelli (to be submitted);
[2] H. Weisbrich, C. Saussol, W. Belzig, G. Rastelli, Phys. Rev. A 98, 052109 (2018).

DY 16.5 Tue 11:00 H6

Engineering thermal reservoirs for ultracold dipole-dipole-interacting Rydberg atoms — David Schönleber, Chris Bentley, and •Alex Eisfeld — MPI-PKS Dresden

We consider an open quantum system of ultracold Rydberg atoms. The system part consists of resonant dipole-dipole-interacting Rydberg states. The environment part is formed by 'three-level atoms': each atom has a ground state, a short-lived excited state, and a Rydberg state that interacts with the system states. The two transitions in the environment atoms are optically driven, and provide control over the environment dynamics [1]. Appropriate choice of the laser parameters allows us to prepare a Boltzmann distribution of the system's eigenstates. By tuning the laser parameters and system-environment interaction, we can change the temperature associated with this Boltzmann distribution, and also the thermalization dynamics [2]. The correct parameters are obtained via machine-learning techniques [3]. Our method provides novel opportunities for quantum simulation of thermalization dynamics using ultracold Rydberg atoms.

[1] Phys. Rev. Lett. 114 123005 (2015) [2] New J. Phys. 20, 013011 (2018) [3] J. Phys. B 51, 205003 (2018)

DY 16.6 Tue 11:15 H6

Thermally assisted Thouless pumping in the Rice-Mele model — •Luca Arceci[1], Angelo Russomanno[2], and Giuseppe Santoro[1,2] — [1]SISSA, Via Bonomea 265, I-34136 Trieste, Italy — [2]International Centre for Theoretical Physics (ICTP), P.O. Box 586, I-34014 Trieste, Italy

In the present talk, we investigate how topological quantum pumping on the Rice-Mele model may be affected by interaction with a Caldeira-Leggett thermal bosonic reservoir. Remarkably, we find that a bath at a low enough temperature can partially counteract non-adiabatic effects that lead to deviations from perfect charge quantization. Indeed, in the limit of infinite pumping cycles and for our choice of system-bath interaction, we find that the charge pumped in the dissipative case can be closer to the integer value than the one coming from a perfectly coherent evolution. We will show that this interesting effect can be viewed in the Floquet framework: with respect to the unitary case, the low temperature bath brings to a higher population of the lowest energetic Floquet band, which is the responsible for quantized pumping. Despite being still far from correctly modelling noise in real systems, this study proves that in principle dissipation can improve the performances of devices realizing quantum Thouless pumping.

DY 17: Statistical Physics (General) I

Time: Tuesday 10:00–12:45 Location: H19

DY 17.1 Tue 10:00 H19

Fluctuations and correlation functions of occupation measures in single-file diffusion — •Alessio Lapolla and Aljaz Godec — Mathematical Biophysics Group, Max Planck Institute for Biophysical Chemistry, Goettingen, Germany

Dynamical processes in statistical physics are predominantly Markovian, at least within a sufficiently high-dimensional setting. However, single-particle experiments in fact probe functionals of lower-dimensional projected dynamics, which typically turns out to be non-Markovian. While the statistical behavior of functionals of trajectories of Markov processes is meanwhile rather well understood, much less is known about the respective behavior in non-Markovian systems. We will present rigorous results for fluctuations and two-tag correlations of bounded additive functionals of ergodic Markov processes having a diagonalizable propagator. Our results relate the statistics of functionals on arbitrary time-scales to the relaxation eigenspectrum. As an application, we will present exact results for one- and two-tag local times in single-file diffusion (SFD), which is central to several phenomena, i.e. the transport in biological channels. In SFD individual particles diffuse in a narrow, effectively one-dimensional channel, which prevents their crossing. Tagging the trajectory of a particular particle corresponds to a projection to a one-dimensional system and introduces a persistent memory. Our analytical results unveil the intricate meaning of such a projection-induced memory on a trajectory level and allow for a detailed analysis of related experiments.

[1] Alessio Lapolla and Aljaž Godec *New J. Phys.* **20** 113021, 2018

DY 17.2 Tue 10:15 H19

Universal Finite-Size Scaling for Kinetics of Phase Separation in Multicomponent Mixtures — Suman Majumder[1], •Subir K. Das[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany — [2]Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore 560064, India

From Kawasaki-exchange Monte Carlo simulations of the q-state Potts model, we present results for the kinetics of phase separation in multicomponent mixtures, for $q \leq 10$, in space dimension $d = 2$. A particular focus has been on the quantification of finite-size scaling functions for various values of q and quench depths. For a range of final quench temperatures, our analyses, via finite-size scaling and other state-of-the-art methods, show that the growth follows the Lifshitz-Slyozov behavior, expected for a diffusive mechanism, irrespective of the number of components. We show that the growth for different q values and quench temperatures, in finite systems, can be described by a universal scaling function with a nonuniversal metric factor, originating from the differences in the amplitudes. We also demonstrate the morphological and kinetic equivalence between a q-component equal proportion mixture and an off-critical binary mixture, in the framework of the Ising model, with relative concentration of the minority component in the latter being $x_c = 1/q$.

DY 17.3 Tue 10:30 H19

Effective temperatures in equilibrium: ring statistics in 2D-silica — Projesh Kumar Roy and •Andreas Heuer — Institut f. Phys. Chemie, WWU Münster

The thermodynamic properties of subsystems in strong interaction with the neighborhood can largely differ from the standard behavior. For example the energy distribution of a harmonic dumbbell in a solvent can be described as if it would experience a broad distribution of temperatures, albeit with the correct average temperature [1]. Here we analyse for the case of 2D-silica [2] the energy distribution for rings of a given size via computer simulations [3]. It turns out that the observed energy distribution of also displays non-standard behavior. However, the observed energy distribution is related to a single strongly reduced temperature as compared to the temperature of the heat bath. This effective temperature approaches the temperature of the heat bath for larger ring sizes. From a systematic analysis of the 1D Ising model and an analytically solvable model we suggest that these observations reflect the presence of strong local energy correlations [4].

[1] P.D. Dixit, Phys. Chem. Chem. Phys.17, 13000 (2015).

[2] L. Lichtenstein, M. Heyde, and H.-J. Freund, J. Phys. Chem. C 116, 20426 (2012).

[3] P. K. Roy, M. Heyde, and A. Heuer, Phys. Chem. Chem. Phys. 20, 14725 (2018).

[4] P. K. Roy, A. Heuer, arXiv:1808.03869; Phys. Rev. Lett. (accepted)

DY 17.4 Tue 10:45 H19

Strong Coupling and non-Markovian Effects in the Statistical Notion of Temperature — •Camilo Alfonso Moreno and Juan Diego Urbina — Institut für Theoretische Physik, Universität Regensburg, Germany

We investigate the emergence of temperature T in the system-plus-reservoir paradigm starting from the fundamental microcanonical scenario at total fixed energy E. As shown by Schwinger [1] for the regime of weak coupling γ between system and environment, $T(E)$ emerges from the saddle-point analysis that leads to the usual ensemble equivalence in the thermodynamic limit [2]. By extending these ideas for finite γ, in [3] we provide a consistent generalization of temperature $T(E, \gamma)$ in strongly coupled systems and we illustrate its main features for the specific model of Quantum Brownian Motion where it leads to consistent microcanonical thermodynamics. Interestingly, we show that while this $T(E, \gamma)$ is a monotonically increasing function of the total energy E, its dependence with γ is a purely quantum effect drastically different for Markovian and non-Markovian regimes. We also derive a generalization of the idea of equivalence of ensembles for systems with finite coupling and discuss possible issues when the observables are not smooth and must be taking into account in the saddle-point analysis.

[1] P. C. Martin, J. Schwinger, *Phys. Rev* **6**, 115 (1959).
[2] N. J. Morgenstern, *Quantum Statistical Field Theory* (2017)
[3] C. A. Moreno, J. D. Urbina, *arXiv:1811.12110*, (2018).

DY 17.5 Tue 11:00 H19

Isotropic-anisotropic phase transition in a three-dimensional lattice model of sticky rods — •Paul Quiring, Miriam Klopotek, and Martin Oettel — Institute for applied Physics, Theoretical and Computational Soft Matter/Nano-Science and Experimental Colloidal Physics, Tübingen, Germany

We investigate the isotropic-anisotropic phase transition in a three-dimensional lattice model of 1x1xL-sized hard rods with nearest-neighbor attractions using grand-canonical Monte Carlo simulations. We find that the topology of the phase diagram strongly depends on the rod length L.

For higher temperatures and L>4, we generally find a very weak first order isotropic-nematic transition as in the corresponding system with no attractions [1]. There is no appreciable widening for increasing attractions. For L=8 and decreasing temperature, this transition line ends in a quasi-tricritical point, below which there is a first-order transition between an isotropic vapor and a nematic liquid.

For L=5, the critical point for the liquid-vapor transition between isotropic states is not affected. The nematic order is of "layered-disordered" type, i.e. one of the three directions is suppressed. The line of isotropic-nematic transitions presumably ends in a critical endpoint on the liquid side of the binodal.

[1] A. Gschwind, M. Klopotek, Y. Ai und M. Oettel, "Isotropic-nematic transition for hard rods on a three-dimensional cubic lattice", Physical Review E, Bd. 96, Nr. 1, S. 012 104, 2017.

15 min. break

DY 17.6 Tue 11:30 H19

The Ising model on finite projective geometries — •Kai Klede and Klaus Mecke — Institut für Theoretische Physik 1, FAU Erlangen-Nürnberg

Various attempts to reconcile quantum field theories with general relativity have not yet led to a breakthrough in the construction of a unified theory of quantum gravitation. We investigate a fundamentally new approach to quantum spacetime, using finite projective geometries, that inherently incorporate finite features in the model of spacetime. In order to understand this geometry better, the Ising Model is studied on two dimensional finite projective spaces, over finite fields of prime order. I will discuss in particular numerical results for the critical be-

havior, suggesting a notion of system size, proportional to the square root of the field order.

DY 17.7 Tue 11:45 H19

The phases of a 2D lattice system of hard rods 'through the eyes' of unsupervised and generative machine-learning algorithms — •Miriam Klopotek, Shang-Chun Lin, Cristoph Mony, Paul Quiring, and Martin Oettel — Institute for Applied Physics, University of Tübingen, Germany

There has been a recent burst of effort from the statistical physics community to apply machine learning algorithms to workhorse lattice spin models, e.g. often the Ising, XY, but also other variants [1,2]. We examine how unsupervised and generative machine learning algorithms 'interpret' raw configurational data in a different model that is very simple in construction, yet nontrivial with respect to its spatial structure and phases. It entails global and local orientational ordering, anisotropies, both continuous transitions and phase coexistence, and is non-fully-packed [3]. The neural-network architectures we test are convolutional autoencoders, variational autoencoders, as well as generative adversarial networks. We pay special attention to the internally-learned, 'boiled-down' representation of the data – the *latent space* variables – which correlate with the order parameters [2].

[1] Carrasquilla and Melko, *Nat. Phys.* **13**, 431 (2017). Hu, Singh and Scalettar, *PRE* **95**, 062122 (2017). Ch'ng, Vazquez, and Khatami, *PRE* **97**, 013306 (2018)., *etc.*
[2] S. Wetzel., *PRE* **96**, 022140 (2017).
[3] Longone, Linares, and Ramirez-Pastor, *JCP* **132**, 184701 (2010). Mortazavifar and Oettel, *PRE* **96**, 032608 (2017).

DY 17.8 Tue 12:00 H19

Discovering physical concepts with neural networks — •Raban Iten, Tony Metger, Henrik Wilming, Lidia del Rio, and Renato Renner — Institute for Theoretical Physics, ETH Zürich, 8093 Zürich, Switzerland

We introduce a neural network architecture that models the physical reasoning process and that can be used to extract simple physical concepts from experimental data without being provided with additional prior knowledge. We apply the neural network to a variety of simple physical examples in classical and quantum mechanics, like damped pendulums, two-particle collisions, and qubits. The network finds the physically relevant parameters, exploits conservation laws to make predictions, and can be used to gain conceptual insights. For example, given a time series of the positions of the Sun and Mars as observed from Earth, the network discovers the heliocentric model of the solar system - that is, it encodes the data into the angles of the two planets as seen from the Sun. Our work provides a first step towards answering the question whether the traditional ways by which physicists model nature naturally arise from the experimental data without any mathematical and physical pre-knowledge, or if there are alternative elegant formalisms, which may solve some of the fundamental conceptual problems in modern physics, such as the measurement problem in quantum mechanics.

DY 17.9 Tue 12:15 H19

Low-energy physics of the bilinear-biquadratic spin-1 chain — •Moritz Binder and Thomas Barthel — Department of Physics, Duke University, Durham, North Carolina 27708, USA

The bilinear-biquadratic spin-1 chain features various interesting quantum phases, including the Haldane phase, a dimerized phase, and an extended critical phase. Here, we apply an efficient density matrix renormalization group (DMRG) algorithm utilizing infinite boundary conditions [1] to compute precise dynamic spin structure factors for a comprehensive set of points in the phase diagram. Analyzing both dynamic spin and quadrupolar correlations, we gain detailed insights into the nature of low-lying excitations of the model. We compare our results to Bethe ansatz solutions at the SU(3)-symmetric ULS point and the TB point as well as at the pure biquadratic point, which can be mapped to an anisotropic spin-1/2 XXZ chain in the gapped Néel phase. In the Haldane phase, we relate our results to the approximate description in terms of the non-linear sigma model.

[1] M. Binder and T. Barthel, Phys. Rev. B **98**, 235114 (2018).

DY 17.10 Tue 12:30 H19

Multiscale model for heterogeneous catalysis in open-cell metal foam structures — •Sebastian Mühlbauer, Severin Strobl, and Thorsten Pöschel — Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg

Heterogeneous catalysis in metallic or ceramic foam structures represents a very promising alternative to catalysis in packed beds or monoliths. Due to high porosity, specific surface and tortuosity, these structures provide excellent mass transport properties at moderate pressure drops. To investigate the reaction rate in such open-cell foam structures in the mass transfer limited regime, we develop a particle based simulation software. We combine an isotropic, lattice-free variant of Stochastic Rotation Dynamics with specialized boundary condition capable of modeling inlet and outlet for reactive flow. The foam structure itself is modeled as an inverse sphere packing, which is described via constructive solid geometry.

Using the developed simulation tool, we first investigate the flow through single unit cells for a wide range of parameters. The gathered results are then condensed to relations for pressure drop and reaction rate, which can be validated based on experimental data. Exploiting the derived relations, we follow a multiscale approach enabling us to investigate reactive flow through complex porous metal foam structures on macroscopic scale. We apply this multiscale model to find optimum foam structures which, for example, minimize flow resistance, while maximizing the reaction rate in a macroscopic catalytic converter.

DY 18: Fluid physics and turbulence

Time: Tuesday 10:00–13:00 Location: H20

Invited Talk DY 18.1 Tue 10:00 H20

Bursting, amplitude explosions and mixed mode oscillations at the onset of shear flow turbulence — •Björn Hof[1], Chaitanya Paranjape[1], Yohann Duguet[2], Vasudevan Mukund[1], and Nazmi B Budanur[1] — [1]IST Austria — [2]LIMSI-CNRS

In pipe and channel flows turbulence appears abruptly and the dynamics is immediately high dimensional. Where exactly turbulence originates from and how the turbulent patches characteristic for low Reynolds number turbulence develop has remained an open question for over a century. I will here discuss the different stages of the transition process starting from spatially localized exact coherent structures. In particular I am going to highlight the interplay between the fast fluctuation time scale and the slow recovery of shear, inherent to these structures. Following an explosive increase in fluctuation amplitude, a sharp rise in the attractor dimension is observed and subsequently a boundary crisis to transient chaos. This transition scenario results in localized turbulent transients that through interaction become sustained at a directed percolation phase transition.

DY 18.2 Tue 10:30 H20

Annihilation of Point Defect Pairs in Fluid Films — •Amine Missaoui[1], Kirsten Harth[1,2], and Stannarius Ralf[1] — [1]Otto von Guericke University Magdeburg, Inst. of Physics, ANP, Magdeburg, Germany. — [2]Physics of Fluids and Max Planck Center for Complex Fluid Dynamics, University of Twente, Enschede, The Netherlands

Liquid crystals (LC) are one of the most valuable systems for studying the coarsening dynamics of topological defects. Disclinations in LC, pointlike defects, can be created and observed easily. They are excellent models to study fundamental properties of defect interactions, which are relevant in a wide range of research fields like cosmology or particle physics. In contrast to experiments in nematic LCs, which are 3D and much more complex, freely suspended smectic C films behave like quasi 2D polar nematics and are thus an ideal model system for studying quasi 2D systems.

We study defect annihilation in free-standing SmC freely suspended films experimentally. We prepare isolated defect pairs and we analyze their annihilation dynamics. The dynamics are strongly influenced by the orientation of the -1 defect with respect to the connecting axis, disorientation induces an orbital motion, dancing of the defects during the approach.

DY 18.3 Tue 10:45 H20

Long-wave analysis of liquid meniscus driven by surface acoustic waves — •Kevin David Joachim Mitas[1], Ofer Manor[3], and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm Klemm Straße 9, D-48149 Münster, Germany — [2]Center of Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Corrensstr. 2, D-48149 Münster, Germany — [3]Department of Chemical Engineering. Technion - Israel Institute of Technology, Haifa 32000, Israel

The behaviour of a meniscus of a partially wetting Newtonian liquid that is transfered from a bath onto a moving plate is well studied. We study the related system of a meniscus that is driven by a Rayleigh surface acoustic wave (SAW) propagating in the plate. This Landau-Levich-type problem is modeled by a thin-film equation that combines SAW driving [1] with the standard long-wave description for partially wetting liquids [2]. In our analysis, we first analyse the occurring transitions using the numerical path-continuation package pde2path [3] to obyain bifurcation diagrams for one-dimensional steady profiles and also discuss the corresponding stationary velocity profiles. Next, we briefly discuss time-periodic states corresponding to the deposition of line patterns. Finally, we present results for two-dimensional steady profiles that emerge beyond a transversal contact line instability. [1] M. Moronov et al., *Fluid Mech.*, 810:307–322, 2017; [2] M. Galvagno et al., *Phys. Rev. Lett.*, 112:137803, 2014; [3] H. Uecker et al., *Numer. Math. Theor. Meth. Appl.*, 7(1):58–106, 2014.

DY 18.4 Tue 11:00 H20

Investigation of different transition phenomena on airfoils by means of infrared thermography and PIV — •Enno Bösenberg, Tom T. B. Wester, Dominik Traphan, Gerd Gülker, and Joachim Peinke — ForWind, Institute of Physics, University of Oldenburg, Oldenburg, Germany

In fluid dynamic research phenomena like laminar separation bubble and transition in the boundary layer are known to be sensitive to the inflow and can change the entire flow topology. Consequently, they can induce changes in loads increasing fatique of e.g. wind turbines.

Due to a thin boundary layer, the transition zone is difficult to observe. Best practice methods, like pressure taps or oil-film, require some form of preparation on airfoils.

Thermography has proven to be a quick and easy way of visualising aerodynamic effects on airfoils while requiring little to no preparation. Experiments have been made to identify the effects of transition, separation bubble and turbulent flow from thermal images of airfoils. Now we are comparing the high temporal and spatial resolution in flow measurement of particle image velocimetry (PIV) to the surface-bound measuring technique of thermography.

Varying wind velocities, during combined triggered PIV and high speed thermographic measurements, enable us to assess the spatial and temporal accuracy of said events in thermography. First results suggest a high correlation with PIV.

DY 18.5 Tue 11:15 H20

Transitions between large-scale flow states in turbulent 3D Kolmogorov flow — •Cristian C Lalescu and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen

For most turbulent flows in nature, the idealization of statistical homogeneity and isotropy only applies to the small scales. The large scales are typically non-universal with pronounced inhomogeneities resulting from walls, large-scale driving etc. This motivates the investigation of the large-scale structure, turbulent fluctuations as well as their interaction in a canonical flow.

Here we present results on a generalized turbulent Kolmogorov flow in three-dimensional periodic domains with aspect ratios larger than one. The flow is forced on a single Fourier mode and is subject to large-scale friction. The flow develops large-scale vortex patterns similar to two-dimensional Kolmogorov flow, even in the presence of intense three-dimensional small-scale fluctuations. We characterize transitions between different large-scale flow states as the large-scale friction is modified, including a regime reminiscent of noise-suppressed hysteresis. In addition to the large-scale flow features, we address the question of small-scale isotropy in the presence of large-scale anisotropies in this flow. Our results help to clarify the role of fluctuations for transitions in fully developed turbulence.

15 min. break

DY 18.6 Tue 11:45 H20

Power-law scaling of friction in pipe flow — •Jose M. Lopez, Davide Scarselli, Balachandra Suri, and Bjoern Hof — Institute of Science and Technology (IST), Klosterneuburg, Austria

We present a study of the friction factor scaling for pipe flow at moderate Reynolds numbers ($5000<Re<120\,000$) in experiments and highly resolved direct numerical simulations. The experimental and numerical data are in excellent agreement and we find that for $Re<80\,000$ they do not follow the Karman-Prandtl friction relation. Instead the friction factor precisely follows the Blasius power law. This power law scaling can also be derived based on Kolmogorov's first hypothesis (assuming local isotropy) in line with an earlier study. Finally, we will show that the deviation of the friction factor from the power law scaling ($Re>80\,000$) is related to the increasing dominance of the large scale motions in the logarithmic layer.

DY 18.7 Tue 12:00 H20

Nonlinear mode decomposition and optimal iterative estimation of Koopman modes — •Oliver Kamps and Tim Kroll — Center for Nonlinear Science, University of Münster

Complex systems composed of a large number of degrees of freedom can often be described on the macroscopic level by only a few interacting modes or coherent structures. In general many turbulent flows seem to be composed of a few coherent structures and it might be possible to find a low dimensional representation of the flow. This has to be done in most cases by means of data analysis methods since it is not possible to derive the low dimensional model from the basic equations of the complex system.

We present a nonlinear decomposition method that is able to extract coherent structures and their dynamics from data of turbulent flow fields. We apply this method to reversal dynamics in convection and to a flow past a cylinder in order to derive low dimensional representations of the systems. We also discuss the relation of our method to Koopman operator theory and dynamic mode decomposition and show how a special case of the presented method can be used to estimate Koopman modes and their dynamics.

DY 18.8 Tue 12:15 H20

Laboratory Study of the Bottleneck Effect in ultra-strong Turbulence — •Christian Küchler[1], Gregory P. Bewley[2], and Eberhard Bodenschatz[1,2,3] — [1]Max Planck Institute for Dynamics and Self-Organization — [2]Cornell University, Ithaca — [3]Georg August University Göttingen

The turbulent flows characteristic of the atmosphere as well as many engineering problems, are intrinsically a multi-scale phenomenon. While the large-scale motions depend on the turbulence forcing mechanism, and the small scales are dominated by viscosity, the intermediate scales are believed to depend only on the scale-to-scale energy transfer of kinetic energy. In this inertial range, the turbulence is suspected to follow universal laws, e.g. Kolmogorov's 1941 scaling of the energy spectrum $E(k) \sim k^{-5/3}$. However, deviations from this scaling are commonly observed, possibly revealing more complicated energy transfer mechanisms. We present the first laboratory study of one of these effects, namely the bottleneck effect - a pileup of energy at the transition from inertial to dissipative flow scales. In particular we show the dependence of this phenomenon on the turbulence intensity measured by the Taylor-scale Reynolds number R_λ. For this we devised a technique to examine energy spectra plagued by non-flat frequency responses of the hot-wire anemometer we use to measure flow speed. This is made possible by the unique mosaic active grid in the Variable Density Turbulence Tunnel. The active grid also permits the creation of $R_\lambda > 5000$, which is unmatched by any well-controlled laboratory flow with experimentally resolvable dissipative scales.

DY 18.9 Tue 12:30 H20

Turbulence in precessing flows — •Andreas Tilgner and Oliver Goepfert — Institut für Geophysik, Universität Göttingen

There are several geophysical and astrophysical applications for which precession driven flows are of relevance. For example, the rotation axis of the Earth is precessing and this induces a flow in the liquid iron core of the Earth which may be at the origin of the Earth's magnetic field. The problem of tidal flows is closely connected to precession driven flows. In both cases, we are faced with a rotating fluid exposed to a time periodic forcing. The talk will describe the known routes to instability and turbulence, among which figure triad resonances which excite inertial waves. Precession driven flows may thus be a good

model system to study wave turbulence of inertial waves. During the search for a wave turbulent state, a different and much simpler state emerged, consisting mainly of a single vortex.

DY 18.10 Tue 12:45 H20

Drop dynamic due to condensation and evaporation in a thin Rayleigh-Bénard cell — •Stephan Weiss[1], Prasanth Prabhakaran[1,2], Alexei Krekhov[1], and Eberhard Bodenschatz[1,3] — [1]Max Planck Institute f. Dynamics and Self-Organisation, Göttingen — [2]Michigan Tech, Houghton, MI, USA — [3]Georg-August University, Göttingen

We report on condensation phenomena in a thin horizontal cell, heated from below and cooled from above, i.e., the well known Rayleigh-Bénard setup. We use Sulphur Hexaflouride (SF_6) as the working fluid with the pressure and temperatures of the plates set such that the bottom plate is above and the top plate below the liquid-vapor transition temperature of SF_6. As a result liquid condenses at the top plate forming a thin layer. This layer undergoes a Rayleigh-Taylor like instability, resulting in the formation of drops that arrange themselves into a hexagonal pattern. At sufficient strong heating from below, the drops are stable and are prevented from touching the bottom plate due to pressure caused by evaporation of the liquid at the bottom of the drops, similar to levitating Leidenfrost drops. When the amount of liquid in the cell is increased in the experiment, e.g., by increasing the pressure, the drops increase in size and form larger domains - puddles. Above a critical size, these puddles undergo another instability leading to the formation of wholes (chimneys) inside the liquid domain. The larger the liquid domain, the more such chimneys occur.

DY 19: Complex Systems

Time: Tuesday 11:45–13:00 Location: H6

DY 19.1 Tue 11:45 H6

Nodal modeling of a Vuilleumier refrigerator — •Raphael Paul, Abdellah Khodja, and Karl Heinz Hoffmann — Technische Universität Chemnitz, Institut für Physik, 09107 Chemnitz, Germany

Conventional cooling units of light and medium duty refrigerator trucks are commonly powered via the truck's electrical system, or by an auxiliary combustion engine. This raises the vehicle's overall fuel consumption and pollutant emissions. An innovative, sustainable approach to attenuate these disadvantages is to use a specially designed Vuilleumier refrigerator for mobile waste heat recovery. The aim is harnessing the residual exergy of the truck engine's exhaust gas for cargo cooling. In this contribution, a nodal simulation model is presented, which can be used for design optimization of a respective Vuilleumier refrigerator. The model is predicated on the concept of endoreversible thermodynamics. The bulk of the Vuilleumier machine is decomposed into a network of reversible subsystems with irreversible interactions. The formulation of conservation laws and interactions is based on fluxes of heat, mass, and enthalpy. The regenerators, however, are treated using a finite volume approach with central flux scheme. For an exemplary set of design parameters and operational conditions, preliminary simulation results and accordingly predictions for refrigerator performance measures are presented.

DY 19.2 Tue 12:00 H6

Perturbation characteristics of power grid models under stochastic power input — •Matthias Wolff, Pedro Lind, and Philipp Maass — Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück

A higher percentage of electrical power provided by renewable energy sources is accompanied by increasing fluctuations in the power generation. This can have a negative effect on the frequency stability on different time scales ranging from sub-seconds to seasons. There are already studies that address the impact of these fluctuations on short time scales [1,2] as well as in the steady state limit [3].

We provide an extension of these studies by comparing different power grid realizations under a perturbation of the frequency and the power injection. The fluctuating power input is estimated from transforming wind velocities measured at a research platform located in the north sea (FINO1). Our stability analysis includes different treatments of the consumers, different voltage levels, as well as structural properties like internal nodes and the related Kron reduction.

It is shown that the results vary strongly, depending on the modeling level of the grid [4]. Not only the stability assessment can change but also the location of weak spots in the grid.

[1] S. Auer *et al.*, Chaos **27**, 127003 (2017).
[2] K. Schmietendorf *et al.*, Eur. Phys. J. B **90**, 222 (2017)
[3] C. Schiel *et al.*, Sci. Rep. **7**, 11562 (2017)
[4] M. F. Wolff *et al.*, Chaos **28**, 103120 (2018).

DY 19.3 Tue 12:15 H6

WKB-type-of approximation for probabilistic description of rare events in reaction systems — •Andreas Mühlbacher and Thomas Guhr — Fakultät für Physik, Universität Duisburg-Essen

We calculate the probabilities to find systems of reacting particles in states which largely deviate from typical behavior. The rare event statistics is obtained from the master equation which describes the dynamics of the probability distribution of the particle number. We transform the master equation by means of a generating function into a time-dependent "Schrödinger equation". Its solution is provided by a separation ansatz and a WKB-approximation for the stationary part. The classical equations of motions are formulated. We calcutate the probabilities employing a saddle-point approximation. Hereby, we switch from a deterministic to a probabilistic description which has important repercussions on the system dynamics. We present a method to calculate the rare event statistics for systems where the dynamics cannot be entirely analyzed in an analytical manner. The method is applied to a set of different examples.

DY 19.4 Tue 12:30 H6

Contracting projected entangled pair states is average-case hard — •Jonas Haferkamp, Dominik Hangleiter, Jens Eisert, and Marek Gluza — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

An accurate calculation of the properties of quantum many-body systems is one of the most important yet intricate challenges of modern physics and computer science. In recent years, the tensor network ansatz has established itself as one of the most promising approaches. In higher dimensions, however, a connection to the field of computational complexity theory has shown that the accurate normalization of the two-dimensional tensor networks called projected entangled pair states (PEPS) is #P complete. Therefore, an efficient algorithm for PEPS contraction would allow to solve exceedingly difficult combinatorial counting problems, which is considered highly unlikely. Due to the importance of understanding two- and three-dimensional systems the question currently remains: Are the known constructions typical of states relevant for quantum many-body systems? In this work, we show that an accurate evaluation of normalization or expectation values of PEPS is as hard to compute for typical instances as for special configurations of highest computational hardness.

DY 19.5 Tue 12:45 H6

Laminar chaos in nonlinear delayed Langevin equations — •David Müller, Andreas Otto, and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Due to environmental fluctuations, delays in nature are typically not constant but rather time-varying. Time-varying delays can be divided into different classes, which lead to different types of dynamics in the delay system [1,2]. Laminar chaos, for example, is a recently discovered type of chaotic dynamics, which arises in systems with a so-called *dissipative delay* [3]. It is characterized by nearly constant laminar phases, which are periodically interrupted by burst-like transitions. The intensity levels of these phases are connected by an iterated map, which can be derived from to the nonlinearity of the delay equation.

In this talk, we analyze laminar chaotic dynamics in the presence of noise. We derive robust features of laminar chaos, which persist even for relatively large noise strengths, where it is difficult to classify the time-series visually as laminar chaos. These features are exploited to provide a toolbox for the detection and the analysis of laminar

chaos in experimental time-series, where noise is always present. We demonstrate that the nonlinearity of the delay equation and certain properties of the time-varying delay can be reconstructed easily, even for relatively strong noise.

[1] Otto, Müller, and Radons, Phys. Rev. Lett. 118, 044104 (2017).
[2] Müller, Otto, and Radons, Phys. Rev. E 95, 062214 (2017).
[3] Müller, Otto, and Radons, Phys. Rev. Lett. 120, 084102 (2018).

DY 20: Active Matter B (joint session DY/CPP)

Time: Tuesday 14:00–15:45 Location: H3

DY 20.1 Tue 14:00 H3

Collective behavior of active colloids in confined viscoelastic fluids — •N Narinder[1], Mahsa Sahebdivani[1], Juan Ruben Gomez-Solano[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Instituto de Física, Universidad Nacional Autónoma de México, México.

The natural habitat of microorganisms is complex not only in geometrical aspects but also in the sense that it is viscoelastic [1]. The fundamental question to address is what prime role such sophisticated surroundings play. To uncover this, we experimentally study the motion of light activated Janus particles in a viscoelastic fluid inside hard wall circular confinements. Unlike a Newtonian liquid [2], we observe that particles in viscoelastic fluids [3] experience an elastic repulsion from the walls which strongly depends on their activity and the elasticity of the surrounding fluid. Furthermore, strongly confined many-particle system inside circular pores exhibits a transition from liquid-like to a well-organized crystal-like behavior upon increasing the activity of particles. A further increase in activity liquifies the system and thus a reentrant liquid-like behavior is observed.

[1] J. Elgeti, R. G. Winkler, and G. Gompper, Rep. Prog. Phys. 78, 056601 (2015).
[2] G. Volpe, I. Buttinoni, D. Vogt, H. Kümmerer and C. Bechinger, Soft Matter 7, 8810 (2011).
[3] N. Narinder, C. Bechinger, and J. R. Gomez-Solano, Phys. Rev. Lett. 121, 078003 (2018).

DY 20.2 Tue 14:15 H3

Two-step melting in two-dimensional active matter — Juliane Klamser[1], •Sebastian Kapfer[2], and Werner Krauth[1] — [1]Laboratoire de Physique Statistique, Département de physique de l'ENS, Ecole Normale Supérieure, Paris, France — [2]Theoretische Physik 1, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

Phase transitions in active matter offer a window to study the elusive critical phenomena outside equilibrium and have taken the center stage of studies in modern statistical physics. We present a kinetic Monte Carlo model of interacting active particles which can be connected to the equilibrium phase diagram. Using extensive numerical simulations, we show that this active model exhibits a rich phase behavior, including liquid-gas coexistence (motility induced phase separation) and the first ever evidence of two-stage melting via solid-hexatic-liquid outside equilibrium.

DY 20.3 Tue 14:30 H3

Self-organized large-scale order in active fluids — Martin James[1,2], Dominik Suchla[1,2], and •Michael Wilczek[1] — [1]Max-Planck-Institut für Dynamik and Selbstorganisation, Göttingen — [2]Georg-August-Universität Göttingen

Active fluids, such as dense suspensions of bacteria or microtubules and molecular motors, display a fascinating range of dynamical states. Active stresses exerted by the individual agents, along with their hydrodynamic interactions, generically lead to the emergence of mesoscale vortex patterns reminiscent of two-dimensional turbulence. In this presentation, we discuss how ordered flows emerge in a minimal continuum model of active fluids. In particular, we focus on a novel type of turbulence-driven pattern formation: a self-organized, dynamic vortex crystal. Crucially, this state emerges from an extended disordered transient characterized by an upscale energy transfer. Exploring the transition from active turbulence to the vortex crystal state with a focus on the role of fluctuations and system size, we find surprising analogies to classical phase transitions. For example, we observe locally ordered crystal domains, which share similarities with magnetic domains in ferromagnetic materials, separated by turbulent boundaries. Our results therefore explore one route to self-organization in active flows.

DY 20.4 Tue 14:45 H3

Dynamics of confined phoretic colloids — •Prathyusha Kokkoorakunnel Ramankutty, Suropriya Saha, and Ramin Golestanian — Max Planck Institue for Dynamics and Self Organization, Am Fassberg 17, Gottingen, Germany

Phoretic colloids are known to form clusters by mechanisms similar to those in black holes formed by long ranged gravitational forces. The long ranged interactions are driven by phoretic response of one colloid to the chemical field generated by others. We investigate the dynamics of uniformly coated colloidal assembly in a confined geometry using Brownian dynamics simulation. In steady state, the colloids self assemble to form a cluster and exhibits slow spontaneous fluctuations. The interesting cluster dynamics is studied as a function of number of particles and strength of phoretic interaction. The mean square displacement shows distinct plateaus indicating cage breaking dynamics.

DY 20.5 Tue 15:00 H3

Continuum model for active polar fluids with density variations — •Vasco M. Worlitzer[1], Avraham Be'er[2], Gil Ariel[3], Markus Bär[1], Holger Stark[4], and Sebastian Heidenreich[1] — [1]Department of Mathematical Modelling and Data Analysis, Physikalisch-Technische Bundesanstalt, 10597 Berlin, Germany — [2]Zuckerberg Institute for Water Research, The Jacob Blaustein Intitutes for Desert Research, Ben-Gurion University, Sede Boqer Campus, Midreshet Ben-Gurion, Israel — [3]Department of Mathematics, Bar-Ilan University, Ramat Gan, Israel — [4]Institute of Theoretical Physics, Technical University of Berlin, 10623 Berlin, Germany

Bacterial suspensions are intriguing examples for active polar fluids which exhibit large scale collective behavior from mesoscale turbulence to vortex lattices. For dense bacterial suspensions an effective fourth-order polar field theory was introduced modelling the collective dynamics in agreement with experimental findings [1,2]. However, in recent experiments of Bacillus subtilis suspensions anomalous velocity statistics and density variations are found which are not captured by the theory. In our contribution, we present a phenomenological theory for an active polar fluid with density and swimmer-velocity variations. We show that these variations result in an anomalous velocity statistics as observed in recent experiments [3].

[1] J Dunkel, S Heidenreich, K Drescher, HH Wensink, M Bär and RE Goldstein, Phys. Rev. Lett. 110 (2013) 228102. [2] S Heidenreich, J Dunkel, SHL Klapp and M Bär, Phys. Rev. E 94 (2016) 020601(R). [3] SD Ryan, G Ariel, A Be'er, Biophys J. (2016) 247.

DY 20.6 Tue 15:15 H3

Systematic extension of the Cahn-Hilliard model for motility-induced phase separation — Lisa Rapp, •Fabian Bergmann, and Walter Zimmermann — Universität Bayreuth, Germany

We consider a continuum model for motility-induced phase separation (MIPS) of active Brownian particles [J. Chem. Phys. **142**, 224149 (2015)]. Using a recently introduced perturbative analysis [Phys. Rev. E **98**, 020604(R) (2018)], we show that this continuum model reduces to the classic Cahn-Hilliard (CH) model near the onset of MIPS. This makes MIPS another example of the so-called active phase separation. We further introduce a generalization of the perturbative analysis to the next higher order. This results in a generic higher order extension of the CH model for active phase separation. Our analysis establishes the mathematical link between the basic mean-field MIPS model on the one hand, and the leading order and extended CH models on the other hand. Comparing numerical simulations of the three models, we find that the leading order CH model agrees nearly perfectly with the full continuum model near the onset of MIPS. We also give estimates of the control parameter beyond which the higher order corrections become relevant and compare the extended CH model to recent phenomenological models.

DY 20.7 Tue 15:30 H3

Spatially periodic patterns succeed active phase separation — •Lisa Rapp, Fabian Bergmann, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth

We investigate a model equation for a conserved order-parameter field that covers as special cases the conserved Swift-Hohenberg model and the extended Cahn-Hilliard model for active phase separation. This model shows a primary bifurcation from a homogeneous state to large-scale phase separation - as typical for active phase separation [1,2]. We show here that with increasing distance from the primary bifurcation, however, a novel secondary bifurcation to spatially periodic patterns occurs. We explore these secondary periodic patterns in more detail including hysteresis and bistability/coexistence of patterns.

[1] F. Bergmann et al.: Phys. Rev. E 98, 020603(R) (2018)
[2] L. Rapp et al.: arXiv:1901.03203 (2019)

DY 21: Statistical Physics (General) II

Time: Tuesday 14:00–15:30 Location: H6

DY 21.1 Tue 14:00 H6

Ground state energy of noninteracting fermions with a random energy spectrum — •Hendrik Schawe[1], Alexander K. Hartmann[1], Satya M. Majumdar[2], and Grégory Schehr[2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Laboratoire de Physique Théorique et Modèles Statistiques, Université de Paris-Sud

We study the distribution of the ground states of a toy model for K noninteracting fermions. In the spirit of Derrida's random energy model, we assume the N energy levels ε_i to be independently, identically distributed according to $p(\varepsilon)$. The ground state energy is the sum of the K smallest energy levels. While the single energy levels are independent, correlations arise due to the ordering. We derive analytically a universal form for the limit of $N \to \infty$ only dependent on the small ε behavior of $p(\varepsilon)$, which reduces in the $K = 1$ case to the well-known Weibull distribution. Further, we confirm this analytical limiting form with numerical data not only in the main region of the distribution but also including the very rare event tails of probabilities much smaller than 10^{-100}. In this talk we will focus on the numerical calculations necessary to reach this precision.

DY 21.2 Tue 14:15 H6

On the derivation of the escape rate of giant classical magnetic spins via an adaptation of the very low damping method of Kramers for particles — •Declan Byrne[1], William Coffey[1], Yuri Kalmykov[2], and Serguey Titov[3] — [1]Department of Electronic and Electrical Engineering, Trinity College, Dublin 2, Ireland — [2]Laboratoire de Mathématiques et Physique, Université de Perpignan Via Domitia, 54, Avenue Paul Alduy, F-66860 Perpignan, France — [3]Kotel'nikov Institute of Radio Engineering and Electronics of the Russian Academy of Sciences, Vvedenskii Square 1, Fryazino, Moscow Region, 141190, Russian Federation

It is demonstrated how the original perturbative Kramers' method (starting from the phase space coordinates only) [H.A. Kramers, Physica 7, 384 (1940)] of determining the energy-controlled-diffusion equation for Newtonian particles with separable and additive Hamiltonians may be easily modified to yield the energy-controlled diffusion equation and thus the very low damping escape rate (including spin-transfer torque) for classical giant magnetic spins with two degrees of freedom. These have dynamics governed by the magnetic Langevin and Fokker-Planck equations and thus are generally based on non-separable and non-additive Hamiltonians. The derivation of the VLD rate directly from the (magnetic) Fokker-Planck equation in the space of polar angles of the magnetization following from the Kramers method is much simpler than those previously used which involve inter alia transformation to energy and phase variables as well as the properties of multiplicative noise.

DY 21.3 Tue 14:30 H6

Chiral 1D Floquet topological insulators beyond rotating wave approximation — Dante M. Kennes[1], •Niclas Müller[2], Mikhail Pletyukhov[2], Clara Weber[2], Christoph Bruder[3], Fabian Hassler[4], Jelena Klinovaja[3], Daniel Loss[3], and Herbert Schoeller[2] — [1]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen, 52062 Aachen, Germany and JARA - Fundamentals of Future Information Technology — [3]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056, Switzerland — [4]JARA-Institute Quantum Information, RWTH Aachen University, 52062 Aachen, Germany

We study one-dimensional (1D) Floquet topological insulators with chiral symmetry going beyond the standard rotating wave approximation. The occurrence of many anticrossings between Floquet replicas leads to a dramatic extension of phase diagram regions with stable topological edge states (TESs). We present an explicit construction of all TESs in terms of a truncated Floquet Hamiltonian in frequency space, prove the bulk-boundary correspondence, and analyze the stability of the TESs in terms of their localization lengths. We propose experimental tests of our predictions in curved bilayer graphene.

DY 21.4 Tue 14:45 H6

Mori-Zwanzig formalism for systems with time-dependent Hamiltonians* — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

The Mori-Zwanzig projection operator formalism is a powerful method for the derivation of mesoscopic and macroscopic theories based on known microscopic equations of motion. It has applications in a large number of areas including dynamical density functional theory and spin relaxation theory. In its present form, however, the formalism cannot be directly applied to systems with time-dependent Hamiltonians. Such systems are relevant in a lot of scenarios like, for example, NMR or driven soft matter.

We derive a generalization of the present Mori-Zwanzig formalism that is able to treat time-dependent Hamiltonians in both classical and quantum systems. Moreover, we develop a variety of approximation techniques that enhance the practical applicability of our formalism. Our method is demonstrated for the important case of spin relaxation in a time-dependent external magnetic field. The Bloch equations are derived together with microscopic expressions for the relaxation times. **Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

DY 21.5 Tue 15:00 H6

Influence of spin-orbit and spin-Hall effects on the spin Seebeck current beyond linear response — •Levan Chotorlishvili — Karl-Freiherr-von-Fritsch Str. 3 D-06120 Halle

We study theoretically the spin transport in heterostructures consisting of a ferromagnetic metallic thin film sandwiched between heavy-metal and oxide layers. The spin current in the heavy metal layer is generated via the spin Hall effect, while the oxide layer induces at the interface with the ferromagnetic layer a spin-orbital coupling of the Rashba type. Impact of the spin Hall effect and Rashba spin-orbit coupling on the spin Seebeck current is explored with a particular emphasis on nonlinear effects. Technically, we employ the Fokker-Planck approach and contrast the analytical expressions with full numerical micromagnetic simulations. We show that when an external magnetic field is aligned parallel (antiparallel) to the Rashba field, the spin-orbit coupling enhances(reduces) the spin pumping current. In turn, the spin Hall effect and the Dzyaloshinskii-Moriya interaction are shown to increase the spin pumping current.

DY 21.6 Tue 15:15 H6

Solving the quantum dimer and six vertex models one electric field line at a time — Inti Sodemann[1], Jonah Herzog-Arbeitman[2], and •Sebastián Felipe Mantilla Serrano[1] — [1]Max Planck Institute for the Physics of Complex Systems Dresden, Germany — [2]Princeton University, Princeton, USA

The phase diagram of the quantum dimer model in the square lattice has recently been challenged by Monte Carlo studies that question the existence of a resonant plaquette state neighboring the Rokhsar-Kivelson point (Phys. Rev. B 90, 245143 (2014) and Phys. Rev. B 98, 064302 (2018)). This model can be viewed as a U(1) lattice gauge the-

ory with a finite density of fluctuating electric field lines. Here we take a different line of attack on this model and on the related six-vertex model (6VM), by exploiting the global conservation law of the number of electric field lines, which allows us to study an isolated fluctuating electric field line. In the case of the 6VM we map it onto the spin 1/2 XXZ chain which can be solved exactly. For the QDM the problem maps onto a two-leg spin 1/2 ladder which we solve using numerical exact diagonalization. Our findings are consistent with the existence of three distinct phases including a Luttinger liquid phase which is the 1D precursor to the fully 2Dplaquette phase. The uncanny resemblance of our single electric field line problem and the classic 2Dproblem suggests that much of the behaviour of the latter might be understood by thinking of it as a closely packed array of quasi-1D electric field lines which by themselves are undergoing non-trivial phase transitions

DY 22: Critical Phenomena and Phase Transitions

Time: Tuesday 14:00–15:30 Location: H19

DY 22.1 Tue 14:00 H19

The hardness of finding ground states with simulated annealing. For Ising spin Glasses in a field. — •Hauke Fajen and Alexander K. Hartmann — Institut für Physik, University of Oldenburg, Germany

We investigated the behavior of simulated annealing for Ising spin glasses (2d planar and 3d) with and without magnetic field. Ising Spin glasses are Ising systems that introduce disorder with randomly chosen antiferromagnetic and ferromagnetic couplings, that leads to higher complexity. Simulated annealing is a process for finding the ground state of a system. For this purpose, the system is simulated with a usual Monte Carlo method at a finite temperature which is more or less slowly decreased. To evaluate the *hardness* we are looking at the time to find a ground state with a certain probability for the optimal ratio of annealing time to restarts of the annealing. We are studying whether simulated annealing has a different hardness for a planar system without magnetic field and other cases like 3d grids systems. In particular, we are interested in the influence of a magnetic field on the hardness of a realization.

DY 22.2 Tue 14:15 H19

Two- and three-point functions at criticality: Monte Carlo simulations of the improved three-dimensional Blume-Capel model — •Martin Hasenbusch — Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, D-69120 Heidelberg, Deutschland

We compute two- and three-point functions at criticality for the three-dimensional Ising universality class. To this end we simulate the improved Blume-Capel model at the critical temperature on simple cubic lattices of a linear size up to $L = 1600$. As check also simulations of the spin-1/2 Ising model are performed. We find $f_{\sigma\sigma\epsilon} = 1.051(1)$ and $f_{\epsilon\epsilon\epsilon} = 1.533(5)$ for operator product expansion coefficients. These results are consistent with but less precise than those recently obtained by using the bootstrap method. An important ingredient in our simulations is a variance reduced estimator of N-point functions. Finite size corrections vanish with $L^{-\Delta_\epsilon}$, where L is the linear size of the lattice and Δ_ϵ is the scaling dimension of the leading Z_2-even scalar ϵ.

DY 22.3 Tue 14:30 H19

Phase diagram of lattice bosons with cavity-mediated long-range interactions with uncorrelated disorder — Chao Zhang and •Heiko Rieger — Theoretical Physics, Saarland University, Campus E2 6, Saarbrücken, 66123, Germany

Recent experiments with ultra-cold atoms in an optical lattice have realized cavity-mediated global range and observed the emergence of a supersolid and a density wave phase in addition to Mott insulator and superfluid phases. Here we consider theoretically the effect of uncorrelated disorder on the phase diagram of this system and study the two-dimensional Bose-Hubbard model with global range interactions and uncorrelated diagonal disorder. With the help of quantum Monte Carlo simulations using the Worm algorithm, we determine the phase diagram of this model. We show that two kinds of Bose glass phases exist: one with and one without density wave order and discuss the nature of the various phase transitions that occur.

DY 22.4 Tue 14:45 H19

Quantum critical scaling and holographic bound for transport coefficients near Lifshitz points — •Gian Andrea Inkof[1], Joachim Küppers[1], Julia Link[1], Blaise Goutéraux[2], and Jörg Schmalian[1,3] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]CPHT, École Polytechnique, 91128 Palaiseau Cedex, France — [3]Institute for Solid State Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The present study uses scaling arguments and holography to investigate universal bounds appearing in strongly coupled QFT. The analysis focuses on the critical regime of anisotropic graphene-like systems at charge neutrality. Through scaling techniques we state a generalization to the anisotropic case of both the shear-viscosity to entropy density ratio and the charge diffusivity bounds. In order to obtain scale dimensionless quantities, we take into account the electric transport for the former, while the structure of the latter is supposed to remain unchanged. We investigate the strongly coupled phase in a gravitational EMD model, where both translations and rotations are broken. The holographic computation suggests a relation between some entries of the η/s-tensor and the conductivities, similar to the one predicted with the scaling. From the IR critical geometry, we derive a recursion formula which allows us to analytically express the diffusion constants in terms of the square butterfly velocities. The proportionality factor turns out to be direction-independent, linear in the inverse temperature, and related to the anisotropic exponents of the dual field theory.

DY 22.5 Tue 15:00 H19

Nonequilibrium dynamics of the critical Casimir force — •Markus Gross[1,2], Andrea Gambassi[3], and Siegfried Dietrich[1,2] — [1]MPI für Intelligente Systeme, Stuttgart — [2]IV. Institut für Theoretische Physik, Universität Stuttgart — [3]SISSA - International School for Advanced Studies and INFN, Trieste, Italy

We discuss how the critical Casimir force, primarily investigated in equilibrium conditions, can be determined as function of time for a general Landau-Ginzburg model. We focus here on the conserved dynamics of a fluid in film geometry, described by the equations of the so-called 'model B'. Specifically, we analyze the nonequilibrium time-evolution following a rapid quench from an initial homogeneous high-temperature state to the critical temperature. Concerning the behavior at the walls bounding the film, we assume that the fluid order parameter (e.g., concentration or density) shows a strong preferential adsorption – a behavior which is typically observed in experiments. The resulting dynamics of the order parameter and the critical Casimir force are discussed within analytical as well as numerical approaches.

Ref.: M. Gross, A. Gambassi, S. Dietrich, Phys. Rev. E 98, 032103 (2018)

DY 22.6 Tue 15:15 H19

Analytic finite-size scaling functions in the anisotropic square-lattice Ising model — Hendrik Hobrecht and •Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

We present recent analytic results on finite-size scaling functions in the anisotropic square-lattice Ising model. We discuss different boundary conditions and analytically verify different finite-size scaling assumptions.

[1] Anisotropic scaling of the two-dimensional Ising model I: The torus, H. Hobrecht and A. Hucht, arXiv:1803.10155

[2] Anisotropic scaling of the two-dimensional Ising model II: Surfaces and boundary fields, H. Hobrecht and A. Hucht, arXiv:1805.00369

DY 23: Stochastic Thermodynamics

Time: Tuesday 14:00–15:30 Location: H20

DY 23.1 Tue 14:00 H20

Cycling tames power fluctuations near optimum efficiency — •Viktor Holubec[1,2] and Artem Ryabov[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany — [2]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, Praha, Czech Republic

According to the laws of thermodynamics, no heat engine can beat the efficiency of a Carnot cycle. This efficiency traditionally comes with vanishing power output and practical designs, optimized for power, generally achieve far less. Recently, various strategies to obtain Carnot's efficiency at large power were proposed. However, a thermodynamic uncertainty relation implies that steady-state heat engines can operate in this regime only at the cost of large fluctuations that render them immensely unreliable. Here, we demonstrate that this unfortunate trade-off can be overcome by designs operating cyclically under quasi-static conditions. The experimentally relevant yet exactly solvable model of an overdamped Brownian heat engine is used to illustrate the formal result. Our study highlights that work in cyclic heat engines and that in quasi-static ones are different stochastic processes.

[1] Viktor Holubec and Artem Ryabov, Phys. Rev. Lett. 121, 120601 (2018)

DY 23.2 Tue 14:15 H20

Phase transition in thermodynamically consistent biochemical oscillators — •Basile Nguyen[1], Udo Seifert[1], and Andre C. Barato[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart, Germany — [2]Department of Physics, University of Houston

Biochemical oscillations are ubiquitous in living organisms. In an autonomous system, not influenced by an external signal, they can only occur out of equilibrium. We show that they emerge through a generic nonequilibrium phase transition, with a characteristic qualitative behavior at criticality. The control parameter is the thermodynamic force which must be above a certain threshold for the onset of biochemical oscillations. This critical behavior is characterized by the thermodynamic flux associated with the thermodynamic force, its diffusion coefficient, and the stationary distribution of the oscillating chemical species. We discuss metrics for the precision of biochemical oscillations by comparing two observables, the Fano factor associated with the thermodynamic flux and the number of coherent oscillations. Since the Fano factor can be small even when there are no biochemical oscillations, we argue that the number of coherent oscillations is more appropriate to quantify the precision of biochemical oscillations. Our results are obtained with three thermodynamically consistent versions of known models: the Brusselator, the activator-inhibitor model, and a model for KaiC oscillations.

[1] B. Nguyen, U. Seifert and A. C. Barato, *J. Chem. Phys.* **149**, 045101 (2018)

DY 23.3 Tue 14:30 H20

Stochastic thermodynamics of self-oscillations: the electron shuttle — •Christopher W. Wächtler[1], Philipp Strasberg[2], Sabine H. L. Klapp[1], Gernot Schaller[1], and Christopher Jarzynski[3] — [1]Institute of Theoretical Physics, Berlin, Germany — [2]Complex Systems and Statistical Mechanics, Luxembourg, Luxembourg — [3]Institute for Physical Science and Technology, College Park, USA

Self-oscillation is a phenomenon studied across many scientific disciplines, including the engineering of efficient heat engines. We investigate an example of a nano-scale system exhibiting a transition towards self-oscillation, namely the single electron shuttle, from a thermodynamic perspective. To this end we employ different levels of description: The fully stochastic level, the mean-field level, and a perturbative solution. Investigating the dynamical behaviour we find that the perturbation theory works particularly well for small amplitudes of the self-oscillation. Consistent derivations of the laws of thermodynamics for this model system can be formulated at these levels. Although the stochastic nature of the system smears out the abrupt transition observed at the mean-field level, the probability density still shows signs of the Hopf bifurcation. Beyond the mean-field description, thermodynamic quantities lack such a corresponding abrupt transition. Nevertheless, the transition towards self-oscillation is also observed in the stochastic and perturbative description.

DY 23.4 Tue 14:45 H20

Hidden degrees of freedom and fluctuation theorems: An analytically solvable model — •Jannik Ehrich and Marcel Kahlen — Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

In some situations in stochastic thermodynamics not all relevant slow degrees of freedom are accessible. Consequently, one adopts an effective description involving only the visible parts of the system. This gives rise to an apparent entropy production that violates standard fluctuation theorems. We present an analytically solvable model illustrating how the fluctuation theorems are modified. Furthermore, we define an alternative to the apparent entropy production: the marginal entropy production which fulfills the fluctuation theorems in the usual form. We show that the non-Markovianity of the visible process is responsible for the deviations in the fluctuation theorems.

[1] M. Kahlen and J. Ehrich, J. Stat. Mech. (2018) 063204

DY 23.5 Tue 15:00 H20

Discrete delay as the limit of distributed memory – An explicit study of the limit from a thermodynamic perspective — •Sarah A. M. Loos, Simon M. Hermann, and Sabine H. L. Klapp — Institut für theoretische Physik, TU Berlin, Germany

Stochastic thermodynamics provides a consistent description of a wide class of Langevin systems [1,2], but the Markov assumption is often crucial [1,2]. While some non-Markovian systems have indeed been studied in great detail, the case of a *discrete* delay in a continuous control is still insufficiently understood [2,3]. This is especially true in the presence of nonlinear forces.

In this talk, I will discuss the possibility of describing delayed dynamics as the limiting case of a process with gamma-distributed memory kernel of decreasing width [4]. While the kernel indeed decays smoothly to a delta peak, generating a discrete delay, we find that the (thermo-)dynamical properties are in fact only recovered in the delta limit. We investigate a way out by introducing colored noise, which at the same time allows us to explicitly study the impact of measurement errors. In fact, we find a divergent total entropy production for the error-free case. Considering linear and nonlinear example systems, we also study work and heat [3] and their fluctuations.

[1] U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012).
[2] M. L. Rosinberg, T. Munakata, G. Tarjus, PRE **91**, 042114 (2015).
[3] S. A. M. Loos and S. H. L. Klapp, ArXiv:1806.04995 (2018).
[4] A. Longtin, Complex time-delay systems (Springer, 2010).

DY 23.6 Tue 15:15 H20

Entropy production in systems with distributed delay via Markovian embedding — •Simon M. Hermann, Sarah A. M. Loos, and Sabine H. L. Klapp — TU Berlin

We study overdamped systems with extended memory kernels at temperature $\mathcal{T}$ in the framework of stochastic thermodynamics [1-3]. The (distributed) delay renders the dynamics non-Markovian. As a consequence the time-reversed process appearing in the path integral representation of the entropy production is acausal [2] making a calculation of this key quantity highly nontrivial. This can be circumvented by a Markovian embedding technique [4]. In particular, we replace the memory term by a set of n auxiliary variables with heat baths at temperature $\mathcal{T}'$ coupled to the original one on a unidirectional ring. In this way, we construct a Markovian system that generates the same dynamics as the delayed system. If $\mathcal{T}' \neq 0$, the additional heat baths introduce correlations in the noise. Here we consider explicitly systems with different numbers of auxiliary variables, corresponding to different memory kernels and associated noise correlations. We calculate the heat and entropy production focusing on a non-linear (bistable) system. For an infinite number of auxiliary variables the kernel collapses onto a δ-distribution producing a system with discrete delay [3].

[1] U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012).
[2] M. L. Rosinberg et al., PRE **91**, 042114 (2015).
[3] S. A. M. Loos, S. H. L. Klapp, ArXiv: 1806.04995 (2018).
[4] F. M. Atay, ed. Complex time-delay systems. Springer, 2010.

DY 24: Spintronics (joint session TT/MA/DY)

Time: Tuesday 14:00–16:00 Location: H23

DY 24.1 Tue 14:00 H23

Long-lived chirality states in low-temperature strongly-coupled Rashba systems — •Philipp C. Verpoort, James R. A. Dann, Gareth J. Conduit, and Vijay Narayan — Department of Physics, University of Cambridge, J.J. Thomson Avenue, Cambridge CB3 0HE, UK

We observe ultra-slow magnetoresistance dynamics at sub-Kelvin temperatures in various systems that display strong Rashba spin-orbit coupling. These dynamics display a striking magnetoresistance curve that follows different traces depending on direction and speed of a magnetic field sweep. This novel effect cannot be explained by magnetisation or magnetocaloric effects. We suggest that the dynamics arise from detuning of the Fermi levels of the two Rashba bands and the slowness of their relaxation into equilibrium due to the suppression of inter-band scattering mechanisms that would be expected in conventional systems. Surprisingly, the relaxation timescale of this non-equilibrium state is 10 seconds so exceeds typical electronic relaxation timescales by several orders of magnitude, which makes this effect intriguing to study and relevant for potential applications in information processing.

DY 24.2 Tue 14:15 H23

Channel analysis of atomic Pd contacts by Andreev Reflections — •Martin Prestel[1], Torsten Pietsch[1,2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]now at: Carl Zeiss AG, 73447 Oberkochen, Germany

For the strong paramagnetic material palladium (Pd) theoretical calculations predicted a local magnetic ordering [1]. In transport measurements a strong non-monotonic magneto-transport behaviour as well as indications for Kondo resonances have been reported for atomic contacts in Pd [2]. To get a more detailed view of the nature of this magnetic ordering we want to investigate the transport channel distribution and their spin polarisation in such contacts. Therefore we add superconducting leads to apply the method of multiple Andreev reflections [3, 4, 5]. In this talk I will present first experimental superconducting current-voltage characteristics revealing superconducting proximity effect into Pd depending on the exact atomic configuration.
[1] Delin et al., Phys. Rev. Lett. 92, 057201 (2004)
[2] Strigl et al., Phys. Rev. B 94, 144431 (2016)
[3] Scheer et al., Nature 394, 154 (1998)
[4] Andersson et al., Physica C 367, 117-122 (2002)
[5] Martin-Rodero et al., Physica C 352, 67-72 (2001)

DY 24.3 Tue 14:30 H23

Quasiparticle cooling using a Topological insulator-Superconductor hybrid junction — •D. Bercioux[1,2] and P. Lucignano[3,4] — [1]Donostia International Physics Center, Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain — [3]CNR-SPIN, Monte S.Angelo, via Cinthia, I-80126 Napoli, Italy — [4]Dipartimento di Fisica "E. Pancini", Universitá di Napoli "Federico II", Monte S.Angelo, I-80126 Napoli, Italy

We investigate the thermoelectric properties of a hybrid junction realised coupling surface states of a three-dimensional topological insulator with a conventional *s*-wave superconductor. We focus on the ballistic devices and study the quasiparticle flow, carrying both electric and thermal currents, adopting a scattering matrix approach based on conventional Blonder-Tinkham-Klapwijk formalism [1]. We calculate the cooling efficiency of the junction as a function of the microscopic parameters of the normal region (*i.e.* the chemical potential etc.). The cooling power increases when moving from a regime of Andreev specular-reflection to a regime where Andreev retro-reflection dominates. Differently from the case of a conventional N/S interface [2], we can achieve efficient cooling of the normal region, without including any explicit impurity scattering at the interface, to increase normal reflection [3].
[1] Blonder, Tinkham & Klapwijk, Phys. Rev. B **25**, 4515 (1982).
[2] Bardas & Averin, Phys. Rev. B **52**, 12873 (1995).
[3] Bercioux & Lucignano, arXiv:1804.07170, EPJ ST, *in press* (2018).

DY 24.4 Tue 14:45 H23

Magnetism in atomic Gd contacts: Noise and transport measurements — •Marcel Strohmeier, Martin Prestel, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Materials with partially filled f shells bear interesting electronic and magnetic properties, wich have been intensively studied in bulk. Yet, on the atomic scale they are still a widely unexplored topic. For gadolinium (Gd) first transport measurements and theoretical calculations on the influence of f electrons on the electronic transport have been carried out [1]. To get a deeper insight into the magnetic ordering at the atomic scale we use the mechanically controllable break junction (MCBJ) technique at low temperatures to produce tunable atomic-size contacts. Here we present first measurements on magnetic transport behavior as well as shot noise measurements. Shot noise is known to reveal the exact channel configuration [2] and is even sensitive to spin polarization [3].
[1] Olivera et al., Phys. Rev. B 95, 075409 (2017)
[2] Kumar et al., Phys. Rev. Lett. 108, 146602 (2012)
[3] Burtzlaff et al., Phys. Rev. Lett. 114, 016602 (2015)

DY 24.5 Tue 15:00 H23

Magnetoconductance in Bi quantum well states: coupling of interfaces — •Doaa Abdelbarey and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover

Ultrathin epitaxial Bi films are governed by strongly spin-polarized bands that determine to a large extent their magneto-transport properties. Magneto-conductance of films grown epitaxially on Si(111) with a thickness of 10 to 100 bilayers (BL) was measured mostly at T= 8 K in magnetic fields up to 4T and with orientations both perpendicular and parallel to the surface plane. For B-fields normal to the surface weak anti-localization (WAL) was observed. Analysis within the theory by Hikami et al. [1] indicates strong coupling of the interfaces up to 50 BL, whereas above 80 BL two independently conducting channels were observed. For the in-plane B-field orientation, the magneto conductivity turned out to be anisotropic. Whereas for in-plane B-fields parallel to the current direction and for films up to 70 BL mainly weak localization is seen, it switches to WAL for larger thicknesses. For in-plane B-fields perpendicular to the current only WAL was observed irrespective of thickness. Both curves merge close to 100 BL, i.e. WAL becomes independent of B-field direction. These phenomena are explained within the framework of interface scattering, including superimposed effects of band structure and spin polarization due to the Rashba effect.
[1] Hikami S., et al., Prog. Theor. Phys. 63, 707 (1980)

DY 24.6 Tue 15:15 H23

Manipulating orbitals with magnetic fields — xionghua liu, •chun-fu chang, alexander komarek, steffen wirth, and liu hao tjeng — Max Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, 01187 Dresden, Germany

Magnetite (Fe_3O_4) is one of most controversially discussed materials in solid state physics due to its enigmatic Verwey transition, while being heavily studied as thin film for spintronic applications. Here, we report on our study of the Verwey transition under magnetic fields in Fe_3O_4 thin films on spinel substrates $Co_{2-x-y}Mn_xFe_yTiO_4$ and non-magnetic Mg_2TiO_4. The Verwey transition of these films is highly tunable and anisotropic with applied magnetic fields. The strong magnetostriction evidences an active spin-orbit effect of the Fe^{2+} (d^6) ions in Fe_3O_4 which allows one to manipulate the Fe^{2+} orbital occupation via magnetic fields. Remarkably, the high magnetic tunability of the Verwey transition results in a closed magnetoresistance (MR)-loop with an MR as large as 88% at 0.5 Tesla, which is up to 2 order larger than the reported values of Fe_3O_4 films.

DY 24.7 Tue 15:30 H23

Noise of charge current generated by a precessing itinerant ferromagnet — •Tim Ludwig[1], Igor S. Burmistrov[2,3,1,4], Yuval Gefen[5], and Alexander Shnirman[1,4] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]L.D. Landau Institute for Theoretical Physics RAS, Kosygina street 2, 119334 Moscow, Russia — [3]Laboratory for Condensed Matter Physics, National Research University Higher School of Economics, 101000 Moscow, Russia — [4]Institut für Nan-

otechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [5]Department of Condensed Matter Physics, Weizmann Institute of Science, 76100 Rehovot, Israel

We determine the zero frequency noise of charge current that is generated by a precessing small itinerant ferromagnet which is tunnel-coupled to two normal metal leads. We assume the leads to be in equilibrium with each other, i.e. neither voltage nor thermal bias is applied. In this situation, the average charge current vanishes. However, the noise of charge current remains. While at high temperatures, we obtain the standard thermal noise; for low temperatures we find the noise of charge current to be governed by the precession frequency of the magnetization and the angle between magnetization and precession axis. We propose that this result can be used in FMR-type experiments to gain additional information about the magnetization dynamics.

DY 24.8 Tue 15:45 H23

Time stable remanence in Dzyaloshinskii Moriya Interaction driven canted antiferromagnets — Namrata Pattanayak[1], AAkanksha Kapoor[1], Arun kumar Nigam[2], and •Ashna Bajpai[1] — [1]Indian Institute of Science Education and Research, Pune, India — [2]Tata Institute of Fundamental Research , India

We report remanence measurements conducted on a number of magnetic oxides which are Dzyaloshinskii-Moriya Interaction (DMI) driven canted antiferromagnets or weak ferromagnets (WFM). All these systems are also symmetry allowed piezomagnets (PzM). We consistently observe an ultra-slow magnetization dynamics with a counter-intuitive magnetic field dependence in these WFM or PzM. This ultra- slow magnetization dynamics manifests itself in the form of a time-stable remanence and appears exclusive to these WFM. Though the effect is tunable with nano scaling, it is intrinsic in nature as these features are also observed in bulk single crystal. We further demonstrate that the magnitude of this unique remanence can be significantly enhanced at the room temperature by encapsulation of these WFM inside carbon nanotubes. These results illustrate why encapsulation of these functional magnetic oxides within carbon nanotubes is interesting from fundamental point of view and it can lead to nano spintronic devices tunable by electric field, magnetic field and possibly by stress.

DY 25: Granular Matter / Contact Dynamics

Time: Wednesday 9:30–12:30 Location: H3

Invited Talk DY 25.1 Wed 9:30 H3

Why the desert is not flat — •Klaus Kroy — Institut für Theoretische Physik, Universität Leipzig, Brüderstraße 16, 04003 Leipzig

Windblown sand creates a distinct hierarchy of mobile landforms on Earth and other heavenly bodies [1], ranging from neat tapestries of ripples to vast fields of shifting dunes. I explain how they form, and what determines their characteristic shapes, sizes, and migration dynamics. This involves three crucial physical mechanisms: spontaneous turbulent symmetry breaking, breaking of scale invariance by an emergent mesoscale, and particle sorting. Collectively, they give rise to the notion of a forbidden wavelength gap that can only be inhabited by a peculiar structure, commonly known as megaripple but mechanistically better understood as as a mini-dune [2], which may be the predominant aeolian structure on Mars [3].

[1] A. G. Hayes: Dunes across the solar system, Science 360 (2018) 960.
[2] M. Lämmel, A. Meiwald, H. Yizhaq, H. Tsoar, I. Katra, and K. Kroy: Aeolian sand sorting and megaripple formation, Nature Physics 14 (2018) 759.
[3] D. C. Berman, M. R. Balme, J. R. Michalski, S. C. Clark, E. C. S. Joseph: High-resolution Investigations of Transverse Aeolian Ridges on Mars, Icarus 312 (2018) 247.

DY 25.2 Wed 10:00 H3

Hydrodynamics versus charged fractals — •Chamkor Singh and Marco Mazza — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, 37077, Göttingen, Germany

The growth of protoplanetary dust from sub-millimeter sized particles to much larger scales is not well understood. There is considerable debate about the role of electrostatic charging of grains in the aggregation process. Additional complexity arises due to the presence of complex hydrodynamic flow that couples to the aggregating grains. We study this growth process using massively parallel molecular dynamics simulations for the granular particles in combination with the hydrodynamic simulations for the interstitial flow. The results from a detailed cluster analysis are presented. Finally we propose an effective kinetic model for the charged grain aggregation inside interstitial flow.

DY 25.3 Wed 10:15 H3

Non-equilibrium steady states, coexistence and criticality in driven quasi 2D granular matter — •Thomas Schindler and Sebastian C. Kapfer — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen

Non-equilibrium steady states of vibrated inelastic frictionless spheres are in quasi-two-dimensional confinement via molecular dynamics simulations are presented. The phase diagram in the density-amplitude plane exhibits a fluid-like disordered and an ordered phase with threefold symmetry, as well as phase coexistence between the two. Moreover, there is a square bilayer state which is connected to the fluid by BKTHNY-type two-step melting with an intermediate tetratic phase. The critical behavior of the two continuous transitions is studied in detail. For the fluid-tetratic transition critical exponents of $\tilde{\gamma} = 1.73$, $\eta_4 = 0.25$, and $z = 2.05$ are obtained. The phase diagram topology is incompatible with any equilibrium free energy and features an anomalously diluted fluid in coexistence with the threefold cluster. A dynamical mechanism exists that brings about metastable traveling clusters and at the same time stable clusters with anisotropic shapes at low vibration amplitude.

DY 25.4 Wed 10:30 H3

Extending Differential Dynamic Microscopy (DDM) to X-ray imaging — •Manuel Baur and Matthias Schröter — Institute for Multiscale Simulation, FAU, Erlangen

We study a dense granular system in a water fluidized bed via X-ray radiography. The particles exhibit a 3D motion, which is not understood. Differential Dynamic Microscopy (DDM) is a well established technique to analyze the dynamics of dilute colloidal systems. We apply this method to X-ray imaging of a granular system. The physics behind the imaging is quite different; i.e. optical light scattering captured with a microscopy vs. X-ray attenuation according to Lambert-Beers law. We discuss to what extend this influences the analysis.

DY 25.5 Wed 10:45 H3

Granular Dotriacontapoles — Felix Braun, Stefan Hartung, •Ingo Rehberg, Reinhard Richter, and Andreas Weber — Universität Bayreuth

Granular matter is generally idealized as a material with pure contact interaction. Sometimes additional interactions have to be taken into account, e.g., for wet or polarizable granules. We present an experimental study of spherical particles [1] with dotriacontapole interaction.

[1] Dotriacontapoles - almost self-assembled. Stefan Hartung, Felix Sommer, Simeon Völkel, Johannes Schönke, Ingo Rehberg; arXiv:1809.08081; PRB, accepted.

DY 25.6 Wed 11:00 H3

Estimation of 3D force chains for packings of soft, nearly frictionless hydrogels spheres — •Diego Sancho Martínez[1], Ralf Stannarius[1], Ahmed Ashour[1], Torsten Trittel[1], Tilo Finger[1], Maja Illig[1], and Tamas Börzsönyi[2] — [1]1Institute of Physics, Otto von Guericke University, Magdeburg, Germany — [2]2Wigner Institute for Solid State Physics, Hungarian Academy of Sciences, Budapest, Hungary

Discharge of granular materials from hoppers has been extensively investigated in the past. Many factors affect the rheology of flow and discharge such as the shape of the hopper, the orifice geometry, or the characteristics of the granular material. We investigate soft and nearly frictionless hydrogels and compare them to hard spheres clogged in a 3D silo. By means of X-ray computed tomography, we determine the packing fractions and the contact numbers of soft and hard spheres. In addition, we estimate the force chains of hydrogel spheres randomly

packed in a container. These forces were calculated as a function of the deformation induced in the granular material, the force chains form due to the increasing pressure with increasing fill high. The Janssen law is not effective for the soft and nearly frictionless materials.

15 min. break

DY 25.7 Wed 11:30 H3

Dynamics of polygonal disks under vertical vibrations — •Simeon Völkel and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

In order to elucidate the assembly of hexagonal disks into a rotator-crystal-like state upon vertical vibrations, we investigate experimentally the dynamics of a single disk under different confining conditions.

The probability distribution of the angular velocity is found to contain three peaks, one originating from clapping and two from rotation due to precession. Furthermore, the translational and rotational degrees of freedom are coupled.

The time evolution of the translational and rotational part of the kinetic energy within one vibration cycle exhibits a phase shift depending on the container height, eventually leading to a qualitative change of the particle movement. This indicates the 'micro-' origin of the dependence of the collective behavior on the vertical confinement.

DY 25.8 Wed 11:45 H3

Structural similarity between dry and wet sphere packings — •Matthias Schröter[1,2], Simon Weis[3], and Gerd Schröder-Turk[3,4,5] — [1]Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [3]Institut für Theoretische Physik I, Friedrich-Alexander-Universität Erlangen-Nürnberg — [4]Maths & Stats, School of Engineering and Information Technology, Murdoch University, Perth, Australia — [5]Applied Maths, Research School of Physical Sciences & Engin., Australian National Univ., Canberra, Australia

The mechanical properties of granular materials change significantly in the presence of a wetting liquid which creates capillary bridges between the particles. Here we demonstrate, using X-ray tomographies of dry and wet sphere packings, that this change in mechanical properties is not accompanyied by structural differences between the packings. We characterize the latter by the average numbers of contacts of each sphere $\langle Z \rangle$ and the shape isotropy $\langle \beta_0^{2,0} \rangle$ of the Voronoi cells of the particles. Additionally, we show that the number of liquid bridges per sphere $\langle B \rangle$ is approximately equal to $\langle Z \rangle + 2$, independent of the volume fraction of the packing. These findings will be helpful in guiding the development of both particle-based models and continuum mechanical descriptions of wet granular matter.

DY 25.9 Wed 12:00 H3

Numerical investigation of shear-induced incipient particle motion on regular substrates — •Björn König[1], Othmane Aouane[1], Nikola Topic[2], Andreas Wierschem[2], and Jens Harting[1,3] — [1]Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Nürnberg, Germany — [2]Institue of Fluid Mechanics, Friedrich-Alexander-Universtät Erlangen-Nürnberg (FAU), Erlangen, Germany — [3]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

Incipient motion of particles is important in different natural and industrial processes. The aim of this work is the numerical simulation of the motion of a single spherical particle placed on a fixed regular substrate bed subjected to a laminar shear flow. The bed is a monolayer of quadratically arranged spheres of the same size as the top particle. Varying the distance between the substrate particles provides different exposure degrees of the single sphere to the flow. The numerical framework utilizes the lattice Boltzmann method (LBM) for the flow field coupled with the discrete element method (DEM) to solve the particle dynamics.

We first determine the critical conditions for incipient particle motion. Critical conditions are characterized by the dimensionless Shields number, describing the ratio of acting stress to the effective particle weight. Second we study the displacement of the single sphere over the substrate at super-critical conditions. The outcomes of the numerical simulations are benchmarked against experimental results.

DY 25.10 Wed 12:15 H3

Granular drag induced by oblique impact — Valentin Dichtl, Felix Rech, and •Kai Huang — Experimentalphysik V, Universität Bayreuth, Bayreuth, Germany

Considering granular medium as a complex fluid with a finite yield stress, an object moving inside has to locally unjam and mobilize the surrounding particles in order to step forward. Consequently, granular drag depends strongly on the local rheological behavior. Using a recently developed bi-static radar system capable of tracking a metallic object with a diameter down to a few millimeters, we monitor the trajectory of a projectile penetrating obliquely into a granular medium and characterize the velocity dependent granular drag in both vertical (along gravity) and horizontal directions. Recent advances in this particle tracking technique and the possibility of using it as a local rheometer for granular media will be discussed.

DY 26: Active matter I (joint session BP/CPP/DY)

Time: Wednesday 9:30–13:00 Location: H4

DY 26.1 Wed 9:30 H4

Self-assembled active systems - from individuals to a collective behaviour — •Aitor Martin-Gomez, Gerhard Gompper, and Roland G. Winkler — Forschungszentrum Juelich (ICS-2), Juelich, Germany

Active matter is comprised of agents which either convert internal energy or exploit energy from the environment to generate directed motion. Its associated out-of-equilibrium character is the origin of a number of fascinating phenomena. In particular, active systems with many internal degrees of freedom like filamentous, polymer-like structures are involved in various biological processes and exhibit novel conformational and dynamical properties. Moreover, the study of collective behavior emerging from the non-linear contributions of many individuals is an ongoing, open question. In conclusion, to shed light onto the effect of such active systems, or their passive counterparts embedded in an active environment, we perform analytical calculations combined to advanced computer simulations.

DY 26.2 Wed 9:45 H4

Light-dependent microbial motility induces pattern formation in confinement — •Alexandros Fragkopoulos[1], Johannes Frey[1], Flora-Maud Le Menn[1], Jeremy Vachier[1], Michael Wilczek[1], Marco Mazza[1,2], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization, D-37077 Göttingen, Germany — [2]Loughborough University, Loughborough LE11 3TU, United Kingdom

A collection of active swimmers can undergo complex dynamics due to hydrodynamic and steric interactions. For sufficiently concentrated suspensions, it is possible to form large-scale concentration patterns, where the active suspension separates into regions of high and low particle concentrations. Here we present that a collection of *Chlamydomonas reinhardtii* cells, a unicellular soil-dwelling microalgae and a model organism of puller-type microswimmers, form patterns of high and low cell density regions in confinement and under specific light conditions. We find that the motility of the cells differs significantly for different light intensities and cell densities, which regulate the pattern formation in such active suspensions. In addition, we observe that the emerged pattern follows the shape of the confinement that encloses the motile cells, which indicates that the boundaries enclosing the motile cells play a crucial role for pattern formation. Finally, by performing active Brownian dynamics simulations of active particles with the observed motility characteristics, we show that we can reproduce the experimentally observed patterns.

DY 26.3 Wed 10:00 H4

Active Matter Invasion into Capillaries — •Felix Kempf[1], Romain Mueller[2], Erwin Frey[1], Juila Yeomans[2], and Amin Doostmohammadi[2] — [1]Arnold Sommerfeld Center for Theoreti-

cal Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München - Theresienstr. 37, D-80333 München, Germany — [2]The Rudolf Peierls Centre for Theoretical Physics - Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, UK

Biological active materials such as bacterial biofilms and eukaryotic cells thrive in confined microspaces. Here, we numerically show that combining growth dynamics with their intrinsic activity active material can use confinement as a mechanical guidance to achieve distinct modes of collective invasion. We assess the dynamics of the growing interface and classify these collective modes of invasion based on the activity of the active substance. While at small and moderate activities the active material grows as a coherent unit, we find blobs of active materials collectively detaching from the cohort above an activity threshold in a process reminiscent of the intravasation in cancer cells. We further characterise the mechanical mechanisms of transition between different modes of invasion.

DY 26.4 Wed 10:15 H4

Collective Responses of Magnetic Swimmers in a Poiseuille Flow — •Fanlong Meng[1,2], Daiki Matsunaga[2], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Magnetotactic bacteria can be focused at the radial centre of a microfluidic channel under an external magnetic field, and found to form clusters if the external magnetic field is strong or the flow speed is large [1]. However, the underlying mechanism was missing. We show that the magnetic microswimmers (not only for magnetotactic bacteria, but also applicable to synthetic magnetic microswimmers) can form interesting large-scale clusters when the magnetic attractive interaction dominates thermal fluctuations. By applying analytic techniques and conducting Brownian dynamics simulation, we provide the critical conditions for clustering of magnetic microswimmers, which matches well with the experiment. Hydrodynamic interactions between the microswimmers are also incorporated as a generalisation. Understanding the physics of magnetic active matter will help advance the cause of studying matter out of equilibrium, and provides new insight for technological applications of synthetic magnetic microrobots (for drug delivery, solution stirring, etc.) with desired collective properties. References: [1] N. Waisbord, C. T. Lefèvre, L. Bocquet, C. Ybert, C. Cottin-Bizonne, Phys. Rev. Fluids, (2016) 1, 053203 [2] F. Meng, D. Matsunaga, R. Golestanian, Phys. Rev. Lett., (2018) 120, 188101

DY 26.5 Wed 10:30 H4

Hydrodynamic simulations of flagellated bacteria in polymer solutions and polymer networks — •Andreas Zöttl and Julia M Yeomans — University of Oxford, UK

Many cells in the human body have to move through dense complex fluids such as various cells in the extracellular matrix or bacteria in mucus. While the motion of swimming bacteria in simple Newtonian fluids can be well quantified using continuum low Reynolds number hydrodynamics, the presence of supramolecular elements such as biopolymers leads to a much more complex behavior. Although the presence of polymers generally lowers particle mobility, surprisingly, several experiments have shown that bacterial speeds increase in polymeric fluids, but there is no clear understanding why.

We perform extensive coarse-grained MPCD simulations of a bacterium swimming in explicitly modeled solutions of supramolecular model polymers of different lengths, stiffness and densities. We observe an increase of up to 60% in swimming speed with polymer density and show that this is a consequence of a non-uniform distribution of polymers in the vicinity of the bacterium leading to an effective slip. However, this alone cannot explain the large speed-up, but coupling to the chirality of the bacterial flagellum is essential. Finally we present results for swimming in crosslinked polymer networks where hydrodynamics is screened and speed enhancement is also observed.

DY 26.6 Wed 10:45 H4

Memory-induced persistent motion — •Bernhard Georg Mitterwallner, Laura Lavacchi, and Roland Netz — Institut für theoretisch Physik, Frei Universität Berlin, Berlin, Germany

We investigate the mean-square displacement (MSD) for random motion governed by the generalized Langevin equation for different two-scale memory-kernel models: In the first model, the memory kernel consists of a delta peak and a single exponential and in the second model of the sum of two exponentials. In particular, we investigate the scenario where the long-time exponential kernel contribution is negative. The competition between positive and negative friction contributions produces an enhanced transient ballistic regime in the MSD, which is relevant for biological motility and active matter systems.

15 minutes break.

Invited Talk DY 26.7 Wed 11:15 H4

Non-equilibrium dynamics in biological matter — •Christoph F Schmidt — Georg-August-Universität, Fakultät für Physik, Drittes Physikalisches Institut - Biophysik, Friedrich-Hund-Platz 1, 37077 Göttingen — Duke University, Department of Physics, 2316 French Family Science Center, 124 Science Drive, Durham, NC 27708, USA

Thermodynamic non-equilibrium is a defining feature of living systems on all levels of organization. Cells and tissues are built of active matter, dynamic materials with built-in force generators. Such materials self-organize in biological systems into well-ordered dynamic steady states, sustained by the dissipation of metabolic energy. The materials show striking collective phenomena on a mesoscopic scale. We used light microscopy to characterize the complex mechanical properties of and the motion and stress patterns in biological active matter, in particular the actin cortex, both in reconstituted model systems and in cells. I will introduce a method to detect and quantitate thermodynamic non-equilibrium in the dynamics of primary cilia of kidney epithelial cells using the principle of detailed balance.

DY 26.8 Wed 11:45 H4

Enhanced rotational diffusion of squirmers in viscoelastic fluids — •Kai Qi[1], Elmar Westphal[2], Gerhard Gompper[1], and Roland Winkler[1] — [1]Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Peter Grünberg Institute and Jülich Centre for Neutron Science, Forschungszentrum Jülich, D-52425 Jülich, Germany

Squirmers are generic models for biological microswimmers and synthetic self-propelled particles. Fluid-mediated interactions are essential for their swimming behavior, which can be strongly affected by the fluid viscoelasticity. Here, we perform mesoscale hydrodynamic simulations via the multiparticle collision dynamics (MPC) method for a spherical squirmer in a viscoelastic fluid, which is composed of MPC fluid particles and polymers. Polymers are either of phantom nature or self-avoiding. The concentration of monomers on the squirmer surface is enhanced by introducing a short-range attraction between the squirmer and polymers. This leads to a decrease of the rotational diffusion for a passive colloid in the presence of polymers. Self-propulsion reduces the monomer concentration on the surface and the squirmer's rotational diffusion is enhanced considerably, up to a factor 20 for phantom polymers. The actual change of the rotational diffusion D_r depends on the polymer length. An increasing polymer length reduces D_r^0 of the passive colloid, but D_r of the squirmer is enhanced. Both effects contribute to the obtained substantial increase of the ratio D_r/D_r^0.

DY 26.9 Wed 12:00 H4

Modelling coordinated motion in simplest multicellular animals — •Stephan Meschede[1] and Pawel Romanczuk[2] — [1]Department of Physics, Humboldt Universität zu Berlin — [2]Institute for Theoretical Biology, Department of Biology, Humboldt Universität zu Berlin

Placozoa, Trichoplax adhaerens, are structurally simplest known multicellular animals. Their bodies are flat and irregular, up to few milimeters in diameter and $10-15\mu m$ thick [1]. They consists of three layers, an upper and a lower epithelium enclosing a fiber cell layer. The Trichoplax body plan is completely decentralized without any hierarchical structure or a central nervous system. However, they are capable of amoeba-like, coordinated active motion on substrates through ciliary locomotion. We show that individual Trichoplax motion behavior can be modeled as a two-dimensional 'sheet' of active particles coupled through elastic forces, building upon previous models of cellular migration model proposed by Szabo et al [2]. We discuss the emergence of coordinated motion and the role of animal size and elastic coupling strength for the stochastic motility. Our aim is to understand how the self-organized active sheet dynamics shapes and constrains the motion behavior of these simple animals and their ability to navigate the

environment.

[1]: Miller, D. J., & Ball, E. E. (2005). Animal Evolution: The Enigmatic Phylum Placozoa Revisited. Current Biology, 15(1), 26-28.

[2]: Szabó, B. et al.(2006). Phase transition in the collective migration of tissue cells: Experiment and model. Phys. Rev. E, 74(6), 1-5.

DY 26.10 Wed 12:15 H4

Phase space geometry of reaction–diffusion systems — •Fridtjof Brauns, Jacob Halatek, and Erwin Frey — Arnold Sommerfeld Center for Theoret- ical Physics, Ludwig-Maximilians-Universität München, Germany

Self-organized pattern formation — typically studied in terms of spatially extended dynamical systems — is as ubiquitous in nature as it is difficult to deal with conceptually and mathematically. We build on the phase space geometric methods of Nonlinear Dynamics, using geometric structures like nullclines and fixed points, to develop a comprehensive theory for two-component mass-conserving reaction–diffusion systems — a paradigmatic model class for pattern formation, e.g. intracellular polarization. A dissection of space into (notional) compartments enables us to characterize the spatio-temporal dynamics based on the ODE phase space of local reactions. Diffusive coupling leads to mass redistribution between the compartments which, in turn, changes the local phase space properties.

We show that all aspects of pattern formation, from linear instability and excitability to the bifurcations of stationary patterns, can be extracted from the geometric features of the line of chemical equilibria in phase space. Furthermore, our analysis points towards a deep connection between the far from equilibrium reaction–diffusion dynamics to phase separation of binary mixtures near equilibrium, and thus offers a new perspective on phase separation far from equilibrium.

DY 26.11 Wed 12:30 H4

Diffusive dynamics of complex particles in active colloidal suspensions of motile algae — •Florian von Rüling and Alexey Eremin — Institute of Physics, Otto von Guericke Universität Magdeburg, Germany

We report experimental studies on the dynamics of complex passive particles in the presence of motile algae Chlamydomonas reinhardtii in thin capillaries. Employing video microscopy and particle tracking algorithm, the enhancement of the diffusion of elongated particles due to interactions with the microswimmers was explored. Depending on the number of motile algae, the translational and rotational diffusion constants of doublets of silica beads close to a solid boundary can be increased by several orders of magnitude in comparison to purely Brownian motion. At a high concentration of Chlamydomonas reinhardtii, the algae formed dense dynamic clusters at the lower capillary wall. In this state of the system, swimming and clustering algae interact with passive particles. Clustering algae can restrict both translational and rotational dynamics of the silica doublets. We explore the effect of the motion of algae in such active clusters on the dynamic of the passive silica doublets.

DY 26.12 Wed 12:45 H4

Self-propelled Dipolar Nanocubes — •Martin Kaiser[1], Sofia Kantorovich[1,2], Yeimy Martinez[3], and Annette Schmidt[3] — [1]University of Vienna, Austria — [2]Ural federal University, Russia — [3]Universität zu Köln, Germany

Microscopic active particles, including self-propelled cells, microorganisms and artificial swimming colloids, have gained a lot of attention due to their relevance in such important fields as biology, biomedicine, nanoscience and nanotechnology. The term "active" describes the ability of certain particles or units, to convert energy from their environment into motion, hence, kinetic energy.

In this study, we use active matter to create a new type of nanomotor, which is oriented by an applied magnetic field and propelled by an active particle. One of those units consists of a dipolar cube that can be directed due to its interaction with a magnetic field. A non-dipolar active particle attached to the cube, with a propulsion force directed into the cubes centre of mass, creates a field controlled swimming unit.

This scenario is investigated using molecular-dynamic simulations, setting the above described unit in an obstacle free environment while applying a constant magnetic field.

In collaboration with Dr. Schmidt from the University of Cologne, those nanomotors are also investigated experimentally.

DY 27: Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)

Time: Wednesday 9:30–12:45 Location: H14

Invited Talk DY 27.1 Wed 9:30 H14

Microstructural transitions and characterization of capillary suspensions — Sebastian Bindgen[1], Frank Bossler[2], Irene Natalia[1], and •Erin Koos[1] — [1]Department of Chemical Engineering, KU Leuven, Leuven, 3001, Belgium — [2]Institute for Mechanical Process Engineering, Karlsruhe Institute of Technology, Gotthard-Franz-Str. 3, 76131 Karlsruhe, Germany.

Suspensions can exhibit a wide range of rheological behaviors that are closely linked to both the bulk particle structure as well as the microstructure including direct particle contacts. Graph theory offers methods and parameters that can be used to analyze complex structures. This method is demonstrated using ternary liquid-liquid-solid systems, which exhibit a wide variety of different morphologies depending on the ratio of the three components. We analyze these networks using the coordination number and clustering coefficient. These parameters are compared to the measured storage and loss moduli.

These capillary suspension networks also exhibit atypical rheological behavior. For instance, a negative normal stress difference is observed from re-orientation of the flocs into the vorticity direction during shearing. Typically, systems with negative normal stress differences have either high volume concentrations and are shear thinning, or are shear thickening with very low particle concentrations. In contrast, the capillary suspensions we report here have a 25% solid concentration and are shear thinning; a combination that has never before been reported in literature.

DY 27.2 Wed 10:00 H14

Flow of silica rods in microfluidic channels — •Hansol Jeon[1] and Dirk Aarts[2] — [1]Max Planck Institute for dynamics and self-organization, Göttingen, Germany — [2]University of Oxford, Oxford, United Kingdom

This project presents the flow of dense liquid crystal phases of colloidal silica rods in microfluidic channels. We describe the synthesis of silica rods that exhibit three different phases (isotropic, nematic and smectic). Using microfluidic channels of novel designs, we observe the flow behaviour of silica rods in the channels by confocal microscopy. We then conduct image analysis to track the dyed rods and measure the flow profile. We compare the flow profiles with the theory and provide future outlook to this experiment.

DY 27.3 Wed 10:15 H14

Dynamics during the formation of an arrested protein phase separation studied using X-ray photon correlation spectroscopy — •Nafisa Begam[1], Anita Girelli[1], Anastasia Ragulskaya[1], Hendrik Rahmann[2], Kevin Lopata[2], Fabian Westermeier[3], Christian Gutt[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Universität Siegen, Germany — [3]Petra III, DESY, Germany

Phase separation in aqueous protein solutions is of primary interest in the field of many biological and chemical processes. It is observed that the glass line often interrupts the phase separation [1] and leads the solution to a dynamically arrested state which results in a drastic reduction of the microscopic relaxation rate. Kinetics of phase separation of such a system of bovine γ-globulin in the presence of polyethylene glycol studied using ultra-small angle X-ray scattering [2] shows an arrest for a quench to temperatures below $\sim 2.5°C$. Here, our goal is to study the dynamics of the solution while approaching such an arrested state. We have used X-ray photon correlation spectroscopy which provides the time evolution of dynamics in the form of two time correlation (TTC) functions. A systematic study of the evolving dynamics of protein solutions during arrest at different quench temperatures using TTC exhibits initially an exponential growth of the relaxation time and at the later stage, an ageing heterogeneous dynamics. This study

reveals a comprehensive picture of the protein dynamics that leads the solution to an arrested state. [1] Cardinaux et. al, *Phys. Rev. Lett.*, **99**, 118301, (2007) [2] S. Da Vela et. al, *Soft Matter*, **13**, 8756, (2017)

DY 27.4 Wed 10:30 H14

Electron-Atom duality in DNA-programmable assembly — •Martin Girard[1], Anindita Das[2,4], Shunzhi Wang[2,4], Jingshan Du[3,4], Byeongdu Lee[5], Chad A. Mirkin[2,4], and Monica Olvera de la Cruz[3,6] — [1]Max Planck Institute for Polymer Physics, Mainz, Germany — [2]Department of Chemistry, Northwestern University, Evanston, IL, USA — [3]Department of Material Science and Engineering, Northwestern University, IL, USA — [4]International Institute for Nanotechnology, Evanston, IL, USA — [5]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, IL, USA — [6]Department of Physics and Astronomy, Northwestern University, Evanston, IL, USA

A powerful method for designing colloidal crystals involves the use of DNA as a particle-directing ligand. With such systems, DNA-nanoparticle conjugates are considered programmable atom equivalents (PAEs), and design rules have been devised to engineer complex crystallization outcomes. Here, we report a new property of PAEs, a type of electron-atom duality. When reduced in size and DNA grafting density, PAEs can behave as electron equivalents (EEs) and move through lattices defined by larger PAEs. In such mixtures, the EEs roam through the crystals as electrons do in metals, holding the large PAEs in specific lattice sites. As the number of strands increases or the temperature decreases, the EEs localize yielding a transition from a metal to a compound. This concept of electron-atom-equivalent duality changes the way we think about colloidal systems and helps define new routes to metallic, intermetallic, and compound phases.

DY 27.5 Wed 10:45 H14

Interaction forces in model cement systems — •Simon Becker and Regine von Klitzing — Soft Matter at Interfaces, Institut für Festkörperphysik, TU Darmstadt

For the workability of concrete and cement as highly abundant construction materials the flow behaviour in the early stages of these materials is of special interest. This can be influenced using additives such as super plasticizers to decrease the viscosity of cement pastes, yielding an enhanced workability. A better understanding of the interactions on the nanoscopic level and the impact on the macroscopic rheology is of great importance in the development of higher performing additives.

The interaction between model particles is mapped via colloidal-probe atomic force microscopy (CP-AFM) in sphere-sphere geometry. Combining CP-AFM with optical microscopy allows to arrange colloidal particles coaxially and determine the interaction forces between these particles upon approach. Spherical silica beads with diameters in the micrometer range serve as model cement grains due to the restriction of the AFM technique to either spherical particles or particles with a defined roughness. The influence on the interaction forces of these model grains in presence of different pH and different salts such as KCl and $CaCl_2$ and their concentrations is investigated. Furthermore the change of the interaction between the model particles in presence of different concentrations of PCE is examined.

DY 27.6 Wed 11:00 H14

Computing the 3D Radial Distribution Function from Particle Positions: An Advanced Analytic Approach — •Bernd F. A. Kopera and Markus Retsch — Department of Chemistry, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth

The radial distribution function, g(r), is ubiquitously used to analyze the internal structure of particulate systems. However, experimentally derived particle coordinates are always confined to a finite sample volume. This poses a particular challenge on computing g(r): Once the radial distance, r, extends beyond the sample boundaries in at least one dimension, substantial deviations from the true g(r) function can occur. State of the art algorithms for g(r) mitigate this issue for instance by using artificial periodic boundary conditions. However, ignoring the finite nature of the sample volume distorts g(r) significantly. Here, we present a simple, analytic algorithm for the computation of g(r) in finite samples. No additional assumptions about the sample are required. The key idea is to use an analytic solution for the intersection volume between a spherical shell and the sample volume. In addition, we discovered a natural upper bound for the radial distance that only depends on sample size and shape. This analytic approach will prove to be invaluable for the quantitative analysis of the increasing amount of experimentally derived tomography data.

15 min. break

DY 27.7 Wed 11:30 H14

A classical density functional from machine learning and a convolutional neural network — •shangchun Lin and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen , Tübingen, Deutschland

We use machine learning methods to approximate a classical density functional. The functional *learns* by comparing the density profile it generates with that of simulations. As a study case, we choose the model problem of a Lennard Jones fluid in one dimension where there is no exact solution available and training data sets must be obtained from simulations. After separating the excess free energy functional into a "repulsive" and an "attractive" part, machine learning finds a functional in weighted density form for the attractive part. The density profile at a hard wall shows good agreement for thermodynamic conditions beyond the training set conditions. This also holds for the equation of state if it is evaluated near the training temperature.

DY 27.8 Wed 11:45 H14

Semi-dilute mixtures of circular and linear polymers - towards novel separation techniques — •Lisa B. Weiss[1], Christos N. Likos[1], and Arash Nikoubashman[2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna,Austria — [2]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

Linear polymers have been extensively studied in various concentration regimes, at rest and when exposed to a variety of flow fields. Recently, this interest extended to ring polymers, focusing on melts and dilute solutions. When diluted and at rest, rings show the same scaling behavior as chains, but when exposed to non-equilibrium conditions astonishing differences become apparent uniquely related to their topology. Furthermore, entangled rings show in equilibrium as well as when sheared marked differences compared to their linear counter part. However, the semi-dilute regime of pure ring polymer solutions and topological mixtures of rings and chains have been sparsely investigated so far. To resolve this, we simulate pure linear and ring polymer solutions and their mixtures around the overlap concentration at rest and under Hagen-Poiseuille flow. To correctly take into account hydrodynamic interactions, we employ the multi-particle collision algorithm. Mixtures of chains and rings show a distinct cross stream migration behavior at any investigated concentration, offering a promising route towards novel separation techniques. In particular, we observed a pronounced propensity of the rings to focus at the channel center while the chains populate the region close to the confining walls.

DY 27.9 Wed 12:00 H14

Ring polymers in confined geometries with mixed boundary conditions — •Zoryana Usatenko[1], Piotr Kuterba[2], and Joanna Halun[3] — [1]Institute of Physics, Cracow University of Technology, Cracow 30-084, Poland — [2]Jagiellonian University, Cracow 30-348, Poland — [3]Institute of Nuclear Physics PAN, Cracow 31-342, Poland

Investigation of a dilute solution of phantom ideal ring polymers and ring polymers with excluded volume interactions in a good solvent confined in a slit geometry of two parallel walls with mixed boundary conditions which corresponds to the case of one repulsive and the other one inert wall is performed. Besides, taking into account the Derjaguin approximation the investigation of a dilute solution of ring polymers confined in a solution of mesoscopic colloidal particles of big size with different radii and different adsorbing or repelling properties in respect for polymers is performed. The calculation of the dimensionless depletion interaction potentials, the depletion forces and the monomer density profiles were performed in the framework of the massive field theory approach at fixed space dimension $d<4$ up to one loop order. The density-force relation in the case of phantom ideal ring polymer chains is analyzed and the respective universal amplitude ratio is calculated. The obtained results indicate the interesting and nontrivial behaviour of ring polymers in confined geometries and give possibility better to understand the complexity of physical effects arising from confinement and chain topology, especially in the case of interaction of λ bacteriophages with E.coli bacteria cells.

DY 27.10 Wed 12:15 H14

Multi-scale simulations of polymeric nanoparticle fabrication through rapid solvent exchange — •Arash Nikoubashman[1], Nannan Li[2], and Athanassios Panagiotopoulos[2] — [1]Institut für

Physik, Johannes Gutenberg Universität Mainz, Mainz, Deutschland — [2]Department of Chemical and Biological Engineering, Princeton University, Princeton, USA

Tailored nanoparticles are increasingly sought after for many scientific and technological applications, such as optoelectronic devices and selective catalysts. However, both research and commercialization of these materials has been impeded by the lack of suitable fabrication techniques. One promising approach for overcoming this hurdle is flash nanoprecipitation, where (soft) nanoparticles are assembled through rapid micromixing of polymers in solution with a miscible poor solvent. This continuous process allows for high yields as well as precise control over particle size and morphology. We employed multiscale simulations of this process to understand its underlying mechanisms and to efficiently explore parameter space. We first performed explicit solvent molecular dynamics (MD) simulations of a bead-spring polymer model to study the microscopic properties of the fabrication process. Then, we fed the MD data into a kinetic Monte Carlo algorithm to reach macroscopic length- and timescales. We discovered that the nanoparticle size can be reliably tuned through the initial polymer concentration and the mixing rate. Further, we were able to fabricate a wide variety of structured colloids, such as Janus and core-shell particles, when polymer blends were used in the feed stream.

DY 27.11 Wed 12:30 H14

Molecular Simulation of Thermodynamic Properties with the Osmotic Equilibrium Approach: Accessing Activities in Complex Concentrated Liquid Phases — •Michael Bley[1,2], Magali Duvail[1], Philippe Guilbaud[3], and Jean-François Dufrêche[1] — [1]ICSM, CEA, CNRS, ENSCM, Univ Montpellier, BP 17171, F-30207 Bagnols-sur-Cèze, France — [2]Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder Str. 3, D-79104 Freiburg, Germany — [3]Nuclear Energy Division, Research Department on Mining and Fuel Recycling Processes (SPDS/LILA), CEA, BP 17171, F-30207 Bagnols sur Cèze, France

Thermodynamic properties such as activities of complex concentrated liquid phases are a key parameter for describing chemical equilibria by means of mass action law. The mass action law and the corresponding equilibrium constant provide a measure for the direction of any chemical equilibrium. The osmotic equilibrium approach has been developed for accessing activities for a huge bandwidth of complex liquid systems. Starting from Molecular Dynamics (MD) simulations of vapor-liquid interfaces using explicit polarization provides a direct access to the activity by comparing the mean amount of evaporated molecules of a given species in the vapor phase for a mixture and for the pure species, respectively. Obtained structures and thermodynamic properties showed a very good agreement with previous experimental and theoretical studies on various aqueous electrolyte solutions and organic solvent phases up to high solute concentrations.

DY 28: Dynamics of Multilayer Networks I (Focus Session SOE/DY/BP) (joint session SOE/DY/BP)

Recently, multilayer networks have been suggested to offer a better representation of the topology and dynamics of real-world systems in comparison with isolated one-layer structures. The prime objective of multiplex networks is to explore multiple levels of interactions where functions of one layer get affected by the properties of other layers. One of the most promising applications of the multilayer approach is the study of the brain, or technological interdependent systems, i.e., those systems in which the correct functioning of one of them strongly depends on the status of the others. The purpose of this focus session is to bring together researchers working on multilayer networks and to share recent ideas and results in the field. (The sessions Dynamics of Multilayer Networks I + II have been organized by Anna Zakharova and Sarika Jalan.)

Time: Wednesday 9:30–12:00 Location: H17

Topical Talk DY 28.1 Wed 9:30 H17

Inhibition induced explosive synchronization in multiplex network — •Sarika Jalan — Complex Systems Lab, IIT Indore, Indore 453552

To date, explosive synchronization (ES) is shown to be originated from either degree-frequency correlation or inertia of phase oscillators. Of late, it has been shown that ES can be induced in a network by adaptively controlled phase oscillators. We show that ES can occur in any network by appropriately multiplexing it with another layer. We devise an approach which leads to the occurrence of ES with hysteresis loop in a network upon its multiplexing with a negatively coupled (or inhibitory) layer. We discuss the impact of various structural properties of positively coupled (or excitatory) and inhibitory layer along with the strength of multiplexing in gaining control over the induced ES transition. This investigation is a step forward in highlighting the importance of multiplex framework not only in bringing novel phenomena which are not possible in an isolated network but also in providing more structural control over the induced phenomena.

Topical Talk DY 28.2 Wed 10:00 H17

Percolation on multi-layer networks — •Filippo Radicchi — Indiana University, Bloomington, Indiana, United States

In this talk, I will review some of my recent papers about percolation on multi-layer networks. I will first illustrate a theoretical approach consisting in a system of heuristic equations able to approximate the phase diagram of the ordinary percolation model for arbitrary multi-layer networks. Second, I will introduce and characterize the redundant percolation model, a genuine model for multi-layer networks where the addition of new layers boosts system robustness by creating redundant interdependencies among layers. Third, I will generalize the problem of optimal percolation from single-layer to multi-layer networks, and present several algorithms for finding approximate solutions to the problem. Finally, I will present a large-deviation approach to ordinary percolation able to shed light on the importance of fluctuations in the study of percolation on real-world multi-layer networks.

15 min. break

Topical Talk DY 28.3 Wed 10:45 H17

Mean field phase synchronization across multilayer networks in chimera states — •Ralph Gregor Andrzejak[1], Giulia Ruzzene[1], Kaspar Schindler[2], Eckehard Schöll[3], and Anna Zakharova[3] — [1]Dept. of Information and Communication Technologies, Univ. Pompeu Fabra, Barcelona, Spain — [2]Dept. of Neurology, Sleep-Wake-Epilepsy-Center, Inselspital, Univ. Bern, Switzerland — [3]Inst. für Theoretische Physik, Technische Univ. Berlin, Germany

Chimera states are an intriguing interplay of synchronous and asynchronous motion in networks of coupled oscillators. While chimera states were traditionally studied in one-layer networks, recent work studies interactions of chimera states across coupled layers in multilayer networks. We here review our recent work in which we applied different types of couplings between pairs of networks that individually show chimera states when there is no coupling between them. We show that these couplings across network layers can lead to generalized synchronization [1] and phase synchronization [2] between networks, while both layers continue to exhibit distinct chimera states. We show that these synchronization phenomena are in close analogy to those found for low-dimensional chaotic dynamics.

References: [1] Andrzejak, R. G., Ruzzene, G., & Malvestio, I. (2017). Generalized synchronization between chimera states. Chaos, 27(5), 053114.

[2] Andrzejak, R. G., Ruzzene, G., Malvestio, I., Schindler, K.,

Schöll, E., & Zakharova, A. (2018). Mean field phase synchronization between chimera states. Chaos, 28(9), 091101.

DY 28.4 Wed 11:15 H17

Weak multiplexing induces coherence resonance — •Nadezhda Semenova[1,2] and Anna Zakharova[3] — [1]Department of Physics, Saratov State University, Saratov, Russia — [2]FEMTO-ST / Optics Dept., Univ. Bourgogne Franche-Comté, Besançon Cedex, France — [3]Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Using the model of a FitzHugh-Nagumo system in the excitable regime, we study the impact of multiplexing on coherence resonance in a two-layer network [1]. We show that multiplexing allows for the control of the noise-induced dynamics. In particular, we find that multiplexing induces coherence resonance in networks that do not demonstrate this phenomenon in isolation. Examples are provided by deterministic networks and networks where the strength of interaction between the elements is not optimal for coherence resonance. In both cases, we show that the control strategy based on multiplexing can be successfully applied even for weak coupling between the layers. Moreover, for the case of deterministic networks, we obtain a counter-intuitive result: the multiplex-induced coherence resonance in the layer which is deterministic in isolation manifests itself even more strongly than that in the noisy layer.

[1] N. Semenova, A. Zakharova, Weak multiplexing induces coherence resonance, Chaos 28, 051104 (2018)

Topical Talk DY 28.5 Wed 11:30 H17

Relay synchronization in multiplex networks — •Inmaculada Leyva[1,2], Irene Sendina-Nadal[1,2], Ricardo Sevilla-Escoboza[3], and Victor Vera-Avila[3] — [1]Complex Systems Group & GISC, Universidad Rey Juan Carlos, Madrid, Spain — [2]Center for Biomedical Technology, Universidad Politécnica de Madrid, Madrid, Spain — [3]Centro Univ. de los Lagos, Universidad de Guadalajara, Jalisco, Mexico

The relay synchronization is observed when two dynamical units synchronize despite not being directly linked, due to the intermediation of a relay mismatched unit. In our work we have extended the concept of relay synchronization to the case of a multiplex network, showing that the intermediation of a relay layer can lead to inter-layer synchronization of a set of paired layers, both topologically and dynamically different from the transmitter. The phenomenon can be extended to indefinitely higher order relay configurations, provided a mirror symmetry is preserved in the multiplex. The coherent state is very robust to changes in the dynamics, topology, and even to strong multiplex disconnection.Our results provide a new path for starting the study of the role of symmetries in setting long distance coherence in real systems, specially in brain networks, where remote synchronization is of outstanding relevance for coordination between remote cortical areas.

DY 29: Many-body Quantum Dynamics

Time: Wednesday 9:30–13:00 Location: H19

Invited Talk DY 29.1 Wed 9:30 H19

Dynamical localization in Z_2 lattice gauge theories — •Dmitry Kovrizhin — Rudolf Peierls Centre for Theoretical Physics

We study quantum quenches in two-dimensional lattice gauge theories with fermions coupled to Z_2 gauge fields. Through the identification of an extensive set of conserved quantities we propose a generic mechanism of dynamical localization in the absence of quenched disorder, and provide diagnostics of this localization via a set of measures including entanglement measures, and out-of-time-order correlators. We discuss applications of our general phenomenology of disorder-free localization to dynamics of defects in Kitaev's toric code, and quantum quenches in Hubbard models.

DY 29.2 Wed 10:00 H19

Localization Dynamics on a Quantum Computer — •Adam Smith, Florian Mintert, Peter Haynes, Myungshik Kim, and Johannes Knolle — Imperial College London, London UK

Universal quantum computers are potentially an ideal setting for simulating collective quantum dynamics that is out of reach for classical digital computers. We use a state-of-the-art IBM quantum computer to study one of the paradigmatic examples of condensed matter physics – we simulate the effects of disorder and interactions on quantum particle transport. Our benchmark results show that the quality of the current machines is below what is necessary for quantitatively accurate continuous time dynamics of observables and reachable system sizes are small comparable to exact diagonalization. On the plus side, we are successfully able to demonstrate clear qualitative localization behaviour that matches the expected many-body localization physics in a number of different settings. New optimization protocols combined with a roadmap for the study of localization phenomena on IBM machines hold a lot of promise for what can be simulated on near-term universal quantum computers.

DY 29.3 Wed 10:15 H19

Thermalization and emergent hydrodynamics in long range spin models — •Alexander Schuckert[1] and Michael Knap[1,2] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Institute for Advanced Study, Technical University of Munich, 85748 Garching, Germany

While local equilibration of nonequilibrium initial states in spin models has been extensively studied both theoretically and experimentally, comparatively less is known about the global thermalization due to the long time scales that emerge from transport of conserved charges.

We study emergent hydrodynamics in long range spin chains with the recently developed Schwinger boson spin-2PI method. A focus is put on the intricate interplay between long-range interaction exponent and hydrodynamic tail exponent, which in short range models is only connected to the dimensionality. As a measure of thermalization, the emergence of fluctuation-dissipation relations between spin-spin correlation functions is studied.

Finally, we discuss how our results can be implemented in existing trapped ion and Rydberg atom experiments.

DY 29.4 Wed 10:30 H19

Time Dependent Variational Monte Carlo in real and imaginary time — •Mathias Gartner[1,2] and Robert E. Zillich[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Institute for Theoretical Physics, Johannes Kepler University Linz, Austria

The novel method of time dependent variational Monte Carlo simulations (t-VMC), by G. Carleo et al. [1], allows to simulate the time dynamics of quantum many-body systems. The method can also be used for imaginary time propagation which allows for optimizing parametrized ground state wavefunctions. It is shown that the imaginary time approach is suited to describe few-particle systems as well as bulk systems where up to 1000 particles in a periodic box are studied. The performed simulations demonstrate the possibility to efficiently optimize very generic trial wavefunctions, parametrized with up to a hundred parameters. For this purpose the well studied liquid ^{4}He serves as a test system for ground state optimization.

The current research focus lies on the simulation of real time dynamics of a bosonic model system with repulsive pair interaction undergoing a quench of the interaction strength. For this purpose a generic trial wavefunction that is felixible enough to descibe the dynamics of the strongly correlated system is developed. The results are compared to quench simulations employing the time dependent HNC-EL method.

[1] Scientific Reports **2**, 243 (2012)

DY 29.5 Wed 10:45 H19

Time evolution methods for matrix-product states — •Sebastian Paeckel[1], Thomas Köhler[1], Andreas Swoboda[2], Salvatore R. Manmana[1], Ulrich Schollwöck[2], and Claudius Hubig[3] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Departement of Physics and Arnold Sommerfeld Center for Theoretical Physics, LMU München — [3]Max-Planck-Institut für Quantenoptik Garching

Matrix-product states (MPS) have become the de facto standard for the investigation of one-dimensional quantum many body systems, also out-of-equilibrium. Various approaches have been introduced for com-

puting the time evolution of MPS, e.g., a time-dependent variational principle (TDVP) for MPS as well as matrix product operator (MPOs) representations of the time evolution operator. In this talk I review important developments and compare five commonly used methods applied to representative examples, including systems with long-ranged interactions or in 2D. These results give insights to the state-of-the-art treatment of MPS out-of-equilibrium and a guideline for which method to choose for a problem at hand.

Financial support via Research Unit FOR1807 (project P07) and SFB/CRC (project B03) from the Deutsche Forschungsgemeinschaft (DFG) is gratefully acknowledged.

DY 29.6 Wed 11:00 H19

Encoding quantum renormalization group transformations in artificial neural networks — Heiko Burau and •Markus Heyl — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden

Renormalization group methods are central tools for the description and understanding of equilibrium many-body systems. Far from equilibrium, however, they are facing challenges. Under the application of a renormalization group transformation typical initial conditions for quantum real-time dynamics can in many cases not be efficiently represented. In this work we show how such transformed initial states for systems of spin-1/2 degrees of freedom can be encoded generally in an artificial neural network. We apply this encoding for a strong-disorder renormalization group study of a disordered quantum Ising model and, in particular, its nonequilibrium real-time dynamics.

DY 29.7 Wed 11:15 H19

Observation of universal dynamics in a spinor Bose gas far from equilibrium — •Maximilian Prüfer[1], Philipp Kunkel[1], Helmut Strobel[1], Stefan Lannig[1], Daniel Linnemann[1], Christian-Marcel Schmied[1], Jürgen Berges[2], Thomas Gasenzer[1], and Markus K. Oberthaler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]Institut für Theoretische Physik, Universität Heidelberg

Far from equilibrium different scenarios on the way to equilibrium have been identified. Here, we present a new scenario featuring universal dynamics associated to the existence of non-thermal fixed points [1]. We access and study this regime experimentally for a Bose-Einstein condensate of ^{87}Rb in the F = 1 hyperfine manifold with ferromagnetic interactions. We quench an experimental control parameter, which leads to a build-up of excitations in the transversal spin. We identify a regime in the time evolution where the in-plane orientation of this spin becomes the relevant dynamical degree of freedom. Spatially resolved read-out allows the momentum resolved study of correlation functions which show rescaling in time and space - the dynamics is solely captured by a universal scaling function and associated exponents. We experimentally identify an emergent conserved quantity which is transported towards low momentum scales. By preparing different initial conditions we confirm that the non-thermal scaling involves no fine tuning of parameters.

[1] Prüfer, M. et al., Nature **563**, 217-220 (2018)

15 min break

DY 29.8 Wed 11:45 H19

Spin-models, dynamics and criticality with atoms in tilted optical superlattices — Anton Buyskikh[1], Luca Tagliacozzo[1], •Dirk Schuricht[2], Chris Hooley[3], David Pekker[4], and Andrew Daley[1] — [1]University of Strathclyde, Glasgow, UK — [2]Utrecht University, NL — [3]University of St Andrews, UK — [4]University of Pittsburgh, USA

We show that atoms in tilted optical superlattices provide a platform for exploring coupled spin chains of forms that are not present in other systems. In particular, using a period-2 superlattice in 1D, we show that coupled Ising spin chains with XZ and ZZ spin coupling terms can be engineered. We use optimized tensor network techniques to explore the criticality and non-equilibrium dynamics in these models, finding a tricritical Ising point in regimes that are accessible in current experiments. These setups are ideal for studying low-entropy physics, as initial entropy is *frozen-out* in realising the spin models.

DY 29.9 Wed 12:00 H19

Fingerprints of level repulsion in the work statistics of a mesoscopic grain — •Izabella Lovas[1,2] and Gergely Zarand[1] — [1]Budapest University of Technology and Economics, 1111 Budapest, Hungary — [2]Technische Universitat Munchen, D-85748 Garching, Germany

We investigate the out-of-equilibrium dynamics of non-interacting fermions in a generic mesocopic disordered grain, by combining numerical results with analytical considerations. We focus on the distribution of work, performed during quenches in different – orthogonal or unitary – random matrix ensembles, for a Fermi sea initial state. We analyze how this work statistics reflects the structure of particle-hole excitations, in particular, the level statistics of the underlying matrix ensemble.

We demonstrate that the initial Fermi sea shows a diffusive broadening during the quench, with the quench-velocity dependent diffusion coefficient reflecting the different level repulsion in the two ensembles. Turning to the full distribution of work, we find clear fingerprints of the rigidity of energy levels in the probability density function for slow quenches. Remarkably, the most important features of the work statistics can be captured by a classical Markovian description, taking into account only nearest neighbor level transitions of the fermions. Our results could be experimentally accessible by calorimetric measurements in mesoscopic settings.

DY 29.10 Wed 12:15 H19

Effective Hamiltonian theory of the geometric evolution of quantum systems — •Vlad Shkolnikov and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We present an effective Hamiltonian description of the quantum dynamics of a generalized Lambda system undergoing adiabatic evolution [1]. We assume the system to be initialized in the dark subspace and show that its holonomic evolution can be viewed as a conventional Hamiltonian dynamics in an appropriately chosen extended Hilbert space. In contrast to the existing approaches, our method does not require the calculation of the non-Abelian Berry connection and can be applied without any parametrization of the dark subspace, which becomes a challenging problem with increasing system size.

[1] V.O. Shkolnikov and Guido Burkard, arXiv:1810.00193

DY 29.11 Wed 12:30 H19

Non-equilibrium Fluctuation theorems for strongly-coupled, non-thermal environments — •Javier Cerrillo — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr 36 10623 Berlin

We propose a novel form of symmetry for the derivation of fluctuation theorems that only requires the assumption of an initial local thermal state of the subsystem of interest. Therefore, they do not rely on the usual concepts of microscopic time-reversibility and global thermal state involving the environment. Moreover, these theorems apply regardless of the Markovianity of the subsystem or of the strength of its coupling to the environment. In the context of laser cooling of trapped ions, experimentally confirmed deviations from weak-coupling thermalization can be treated with this perspective. These deviations are often detrimental for the thermodynamic function as we have shown with help of Floquet-Markov-based simulation methods, due to the appearance of polaronic, correlated dynamics between the subsystem and its environment.

DY 29.12 Wed 12:45 H19

Ultrafast switch in graphene — •Hamed Koochaki Kelardeh[1], Alexandra Landsman[1,2], Vadym Apalkov[3], and Mark Stockman[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Postech, Pohang, Republic of Korea — [3]Georgia State University, Atlanta, USA

We propose a switch made of graphene that acts on a one-fs scale and can controllably modulate the transient- induced photocurrent and carrier transport on the subcycle time scale (within one cycle of optical field). Few-cycle laser pulses generate a residual current, which is highly sensitive to the waveform of the driving laser. The residual current and charge transfer result from breaking the spatiotemporal symmetry of the system with few-cycle laser pulses. We investigate the carrier transport mechanism and criteria upon which we can manipulate its directionality and amplitude by the ellipticity, amplitude, and carrier-envelope phase of the pulse. For instance, we observe a change in current direction as a function of ellipticity when the polarization and the corresponding electron trajectories in the reciprocal space deform from linear to circular.

DY 30: Statistical Physics far from Thermal Equilibrium

Time: Wednesday 10:00–12:45 Location: H6

Invited Talk DY 30.1 Wed 10:00 H6

Fluctuations and responses in nonequilibrium fluids — •Matthias Krüger — Institut für Theoretische Physik, Georg-August-Universität Göttingen

Understanding systems far from equilibrium is of fundamental and technological interest. The linear response of systems mildly perturbed from equilibrium can be understood in terms of the well known fluctuation-dissipation-theorem (FDT). Further away from equilibrium, the situation is generally less clear, and is the topic of manifold ongoing investigations.

We derive a path-integral version of nonlinear response theory, which can be considered an extension of the FDT to nonlinear responses, and discuss the fundamental properties of such extensions in relation to the FDT itself, and also test it experimentally in a colloidal model system.

These path integral techniques can also be used to derive Langevin-descriptions for nonlinear fluids, necessary for understanding the motion of (driven) probe particles in (nonlinear) viscoelastic surroundings; Indeed, due to the nonlinear responses of viscoelastic solvents (such as shear thinning behavior), a driven colloidal particle can display pronounced nonequilibrium fluctuations already at slow driving speeds, as will be demonstrated using recent experimental data.

DY 30.2 Wed 10:30 H6

Transmission from reverse reaction coordinate mappings — •Niklas Martensen and Gernot Schaller — Institut für Theoretische Physik, Hardenbergstr. 36, Technische Universität Berlin, D-10623 Berlin, Germany

We point out that the transport properties of non-interacting fermionic chains that are tunnel-coupled to two reservoirs at their ends can be mapped to those of a single quantum dot that is tunnel-coupled to two transformed reservoirs. The parameters of the chain are mapped to additional structure in the spectral densities of the transformed reservoirs. For example, this enables the calculation of the transmission of quantum dot chains by evaluating the known transmission of a single quantum dot together with structured spectral densities. We exemplify this analytically for short chains, which allows to optimize the transmission. Tuning of the transmission allows to reach a non-Markovian transport regime that violates the thermodynamic uncertainty relation. In addition, we also demonstrate that the mapping can be performed numerically by computing the transmission of a Su-Schrieffer-Heeger chain.

[1] A. Nazir and G. Schaller, *The reaction coordinate mapping in quantum thermodynamics*, as a chapter of F. Binder, L. A. Correa, C. Gogolin, J. Anders, and G. Adesso (eds.), Thermodynamics in the quantum regime - Recent Progress and Outlook (Springer International Publishing), arXiv:1805.08307.

[2] N. Martensen and G. Schaller, *Transmission from reverse reaction coordinate mappings*, arXiv:1809.10529.

DY 30.3 Wed 10:45 H6

Thermoelectric performance of topological boundary modes — •Sina Böhling[1], Georg Engelhardt[2], Gloria Platero[3], and Gernot Schaller[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]Beijing Computational Science Research Center, Beijing, People's Republic of China — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain

We investigate quantum transport and thermoelectrical properties of a finite-size Su-Schrieffer-Heeger model, a paradigmatic model for a one-dimensional topological insulator, which displays topologically protected edge states. By coupling the model to two fermionic reservoirs at its ends, we can explore the non-equilibrium dynamics of the system. Investigating the energy-resolved transmission and the current, we find that these observables can be used to detect the topologically non-trivial phase.

In addition, we point out that the edge states can be exploited to design a refrigerator driven by chemical work or a heat engine driven by a thermal gradient, respectively. These thermal devices do not require asymmetric couplings and are topologically protected against symmetry-preserving perturbations. Their maximum efficiencies significantly exceed that of a single quantum dot device at comparable coupling strengths.

[1] S. Böhling, G. Engelhardt, G. Platero, and G. Schaller, *Thermoelectric performance of topological boundary modes*, Phys. Rev. B **98**, 035132 (2018)

DY 30.4 Wed 11:00 H6

The Quantum Otto Engine in Finite Time: Dynamics, Thermodynamics and Coherence — Michael Wiedmann, •Jürgen T. Stockburger, and Joachim Ankerhold — Ulm University, Institute for Complex Quantum Systems

We perform complete, exact dynamical simulations of the quantum Otto engine in terms of the full, interacting dynamics of the work medium and its two thermal reservoirs. In this context, the Otto cycle is defined by externally modulating the oscillation frequency of the work medium ("piston") and the coupling constants to the reservoirs ("valves"). We find that the work expended in operating the "valves" is far from negligible in this engine. Moreover, the system dynamics in cyclic operation displays non-thermal effects (squeezing, coherence), which should be taken into account in the finite-time thermodynamics of the Otto cycle.

15 min. break

DY 30.5 Wed 11:30 H6

Violation of Jarzynski Equality using catalysts — •Paul Boes[1], Rodrigo Gallego[1], Henrik Wilming[2], Nelly Ng[1], Markus Müller[3,4], and Jens Eisert[1] — [1]Freie Universität Berlin, Deutschland — [2]ETH Zürich, Schweiz — [3]IQOQI Wien, Österreich — [4]Perimeter Institute, Kanada

Fluctuation theorems are concerned with the probability distributions of work in a scenario where we measure the energy of a system in a Gibbs state, evolve it unitarily and then measure the energy again. In this setting, the second law states that it is impossible to extract work on average, while fluctuation theorems impose further constraints on the fluctuations of work. In this work, we study a generalization of this typical setup that additionally allows for the use of catalytic systems. In this setting, the usual second law continues to hold, however, fluctuation theorems can be violated. In particular, we show that it is possible to extract, for large systems, a finite amount of work per particle with a finite probability. This can be recast as the statement that the Jarzynski equality can be violated by an amount which diverges exponentially with the system size, at the cost of having to use increasingly large catalytic systems.

DY 30.6 Wed 11:45 H6

Field theory for interacting Brownian particles — •Rohit Jain[1] and Matthias Krüger[2] — [1]Institut für Theoretische Physik, 37077 Göttingen, Germany — [2]Institut für Theoretische Physik, 37077 Göttingen, Germany

We derive a field theory for interacting Brownian particles starting from the stochastic equation for the density operator [1], using different approximations [2]. This field theory, among other things, can be used to analyze stresses and forces in non-equilibrium scenarios [3]. We discuss and analyze several applications. For instance, with this approach, we calculate the time-dependent two-point correlation functions. We also discuss the relation of this approach with the existing ones, namely dynamical density functional theory, classical Ginzburg-Landau theory, and also with quantum field theories.

References: [1] D. S. Dean, J. Phys. A: Math. Gen., 29, L613 (1996). [2] D. S. Dean and M. Krüger, J. Chem. Phys. 146, 134507 (2017). [3] M. Krüger et al, J. Chem. Phys. 148, 084503 (2018).

DY 30.7 Wed 12:00 H6

Coarsening dynamics of the long-range Ising model — Henrik Christiansen, Suman Majumder, and •Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We report Monte Carlo computer simulations of the nonequilibrium coarsening dynamics of the two-dimensional long-range Ising model. Employing an efficient update scheme, our simulations perform $\sim 10^3$ times faster than the standard approach. We carefully examine previous approaches introducing a cut-off in the long-range potential in order to reduce the computational effort. Special emphasis is put on

a careful analysis of finite-size effects. This enables us to establish agreement with a theoretical prediction for the time dependence of the domain growth, in contrast to previous numerical studies. Our method can easily be generalized to applications in other systems.

[1] H. Christiansen, S. Majumder, and W. Janke, preprint arXiv:1808.10426.

DY 30.8 Wed 12:15 H6

Nonequilibrium monolayer of hard rods: Transient phase transition kinetics and phase boundaries — •Miriam Klopotek and Martin Oettel — Institute for Applied Physics, University of Tübingen, Germany

We perform kinetic Monte Carlo simulations of an idealized lattice model of hard rods with 'sticky' attractions, confined to a monolayer, diffusing under nonequilibrium conditions [1]. The simulations unveil rich (transient) phase transition kinetics including liquid-liquid phase separation, two-step cluster growth, and transient percolation, often enhanced by the strong driving forces: deposition, desorption or heating. In fact, these 'push' the system through its phase diagram, allowing us to map out the boundaries via 'kinks' or 'jumps' in both dynamical and structural observables: it matches the topology of the phase diagram predicted by density functional theory [2]. Our findings may be of direct relevance for experiments of thin film growth with organic molecules such as Pentacene in the first few layers [3], as well as simulations thereof [4,5].

[1] Klopotek *et al.*, *J. Chem. Phys* **146**, 084903 (2017).
[2] Mortazavifar and Oettel, *Phys. Rev. E* **96**, 032608 (2017).
[3] Zhang *et al.*, *Phys. Status Solidi RRL* **12**, 1800230 (2018).
[4] Roscioni *et al.*, *J Phys. Chem. Lett.* **9**, 6900 (2018).
[5] Clancy, *Chem. Mater.* **23**, 522 (2011).

DY 30.9 Wed 12:30 H6

Response of active Brownian particles to shear flow — •Kiryl Asheichyk[1,2], Alexandre Solon[3], Christian Rohwer[1,2], and Matthias Krüger[4] — [1]4th Institute for Theoretical Physics, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max Planck Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [3]Sorbonne University, CNRS, LPTMC, F-75005 Paris, France — [4]Institute for Theoretical Physics, University of Göttingen, 37073 Göttingen, Germany

We study the linear response of interacting active Brownian particles to simple shear flow. Using the path integral approach, we derive the linear response of any state observable after starting shear in terms of correlation functions evaluated for the unperturbed system. For systems and observables which are symmetric under exchange of x and y coordinates, the response formula can be drastically simplified to a form containing only state variables in the corresponding correlation functions (compared to the generic formula containing also time derivatives). The shear couples to the particles by both translational and rotational advection. In the mentioned case of symmetry, we also show that only translational advection is relevant in the linear regime. We apply the obtained formulas analytically and numerically to specific model setups. In particular, we investigate the morphology of a cluster of confined active interacting particles in shear flow, where we show that the activity increases the response.

DY 31: Nonlinear Dynamics, Synchronization and Chaos

Time: Wednesday 10:00–13:15 Location: H20

DY 31.1 Wed 10:00 H20

Scale-dependent Error Growth in Multi-hierarchical Systems — •Jonathan Brisch and Holger Kantz — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Deutschland

Scale-dependent error growth rates can been found, e.g., in two-dimensional turbulence and global weather forecasting models. Both models mentioned admit turbulence and exhibit dynamics on different time and length scales. In this talk I will show that the latter fact is crucial to generate scale-dependent error growth. Thereby we gain insights into the dynamical mechanisms which might be responsible for the fact that real weather forecasts posses an intrinsic limit on forecast time, irrespective of the accuracy of input observations. For this, I introduce a toy-model with a hierarchical coupling between chaotic systems with different time and length scales. I will furthermore discuss the theoretical case of infinite hierarchies in the limit of vanishing perturbations in order to show that these systems have a finite range of predictability independent of the magnitude of the initial perturbation.

DY 31.2 Wed 10:15 H20

Separation of scales in a hierarchical heteroclinic network — •Maximilian Voit and Hildegard Meyer-Ortmanns — Jacobs University Bremen, Bremen, Germany

In the context of winnerless competition we consider a heteroclinic network with a structural hierarchy.[1] It contains two levels of cyclic competition. The lower level is realized by simple heteroclinic cycles between saddle equilibria. The higher level, on the other hand, consists of a heteroclinic cycle whose saddles are the lower level heteroclinic cycles. As a consequence, two different time scales emerge in this system. By a Poincaré map method we derive an analytic description of this dynamics. We thereby show how to predict the ratio between time scales depending on parameters and initial conditions.

[1] M. Voit and H. Meyer-Ortmanns (2018) to be pub. in EPJ ST

DY 31.3 Wed 10:30 H20

Memory induced slow-fast chaotic dynamics in a Chua circuit — •Tom Birkoben[1], Moritz Drangmeister[2], Finn Zahari[1], Serhiy Yanchuk[3], Philipp Hövel[4], and Hermann Kohlstedt[1] — [1]Nanoelektronik, Faculty of Engineering, Kiel University, Kiel, Germany — [2]Institute of Theoretical Physics, TU Berlin, Berlin, Germany — [3]Institute of Mathematics, TU Berlin, Berlin, Germany — [4]School of Mathematical Sciences, University College Cork, Cork, Ireland

Chaotic signatures have been observed in a wide range of different nonlinear systems. Besides the famous Lorenz-equations, which resemble atmospheric convections, the Chua circuit is another prominent representative of chaotic systems. This nonlinear electrical circuit consists of three energy-storing passive elements and a locally active resistor. The circuit allows the experimental study of chaotic phenomena within a mathematically well-described and dynamically rich environment. Here we present experimental and theoretical results on the Chua circuit compromising a memristive double barrier device. The device consists of Nb/Al/Al2O3/NbxOy/Au layers, is forming free and has a typical Roff/Ron ratio of about 100 at 0.7 V. The memory element changes the dynamics of the original system and induces transient suppressions of the intrinsic chaotic oscillations. The analysis of the extended system reveals overall slow-fast oscillations and their cause in the varying memristance.

DY 31.4 Wed 10:45 H20

Application of Machine Learning Methods to Problems in Transition State Theory — •Tobias Mielich and Jörg Main — Institut für Theoretische Physik 1, Universität Stuttgart, Germany

Machine learning algorithms are getting increasingly more popular across various fields of science. Their usage in solving physics problems has already shown them to be an effective tool to assist classical algorithms and solutions [1]. This talk aims to show different approaches of using artificial neural networks to aid in rate calculations of chemical reactions in driven systems in the realm of transition state theory. The networks can be used to approximate functions like the time-dependent dividing surface, the times when trajectories cross that surface, or even the potential parameter dependent reaction rate itself. It is important to use the correct approach during training to get optimal results. Techniques like cyclic learning rates and network ensemble predictions shall be discussed.

[1] P. Schraft et al., Phys. Rev. E 97, 042309 (2018)

DY 31.5 Wed 11:00 H20

Harmonic Oscillator Interacting with Random Ising Spins — •Paul Zech and Günter Radons — Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Hysteresis phenomena can be found in very different research fields, such as magnetic materials, porous materials, shape memory alloys,

etc. One of the most prominent model of hysteresis is the zero-temperature Random Field Ising Model (RFIM). While the hysteretic behavior of the RFIM has been investigated in detail, not much is known about scenarios which arise if the RFIM is coupled dynamically to its environment, especially as the number of spins goes to infinity (thermodynamic limit). In this talk, we want to investigate the dynamical properties of a harmonic oscillator coupled to Ising spins in quenched random local fields. By applying established methods of dynamical systems and piecewise-smooth system theory to this hybrid system we show, how chaos emerges for two different spin set-ups. We first treat independent spins and secondly we introduce hysteretic behavior by a pairwise coupling of the spins, which results in an ensemble of spin dimers. We will show, that the approach to the thermodynamic limit results in an asymptotic nonlinearity in form of a error function and a hysteretic play operator, respectively. For an increasing number of spins we will also demonstrate, that the fractal dimensions of the chaotic attractors of the piecewise-smooth system approach those of the system in the thermodynamic limit and that both fractal dimensions are self-averaging quantities, in contrast to the time-averaged magnetization.

DY 31.6 Wed 11:15 H20

Resonant Doppler effect from delayed feedback leads to multistability and generalized laminar chaos — •Andreas Otto, David Müller, and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Delayed feedback or aftereffects can be found in many dynamical systems ranging, for example, from population dynamics to metal cutting. We show that the effect of a delay variation in such time delay systems is similar to the Doppler effect with self-feedback. We distinguish between the non-resonant and the resonant Doppler effect corresponding to the known dichotomy between conservative and dissipative delays [1]. The non-resonant Doppler effect leads to a quasiperiodic frequency modulation of the signal but the qualitative properties of the solution are the same as for constant delay systems.

In contrast, for the resonant Doppler effect the solutions are characterized by alternating low and high frequency phases. For large delays these phases are clearly separated, which is equivalent to time-multiplexed dynamics. This allows the design of well-defined multistable solutions or periodic temporal switching between different chaotic and periodic dynamics. We systematically study such kind of dynamics and present the most interesting examples. Finally, we show that the recently found laminar chaos [2] is only the zeroth-order case of a bigger class of chaos, which we call generalized laminar chaos.

[1] Otto, Müller, and Radons, Phys. Rev. Lett. 118, 044104 (2017).
[2] Müller, Otto, and Radons, Phys. Rev. Lett. 120, 084102 (2018).

15 min. break

DY 31.7 Wed 11:45 H20

Temperature dependence of butterfly effect in a classical many-body system — •Thomas Bilitewski[1], Subhro Bhattacharjee[2], and Roderich Moessner[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bengaluru 560089, India

We study the chaotic dynamics in a classical many-body system of interacting spins on the kagome lattice. We characterise many-body chaos via the butterfly effect as captured by an appropriate out-of-time-ordered correlator. Due to the emergence of a spin liquid phase, the chaotic dynamics extends all the way to zero temperature. We thus determine the full temperature dependence of two complementary aspects of the butterfly effect: the Lyapunov exponent, μ, and the butterfly speed, v_b, and study their interrelations with usual measures of spin dynamics such as the spin-diffusion constant, D and spin-autocorrelation time, τ. We find that they all exhibit power law behaviour at low temperature, consistent with scaling of the form $D \sim v_b^2/\mu$ and $\tau \sim T^{-1}$. The vanishing of $\mu \sim T^{0.48}$ is parametrically slower than that of the corresponding quantum bound, $\mu \sim T$, raising interesting questions regarding the semi-classical limit of such spin systems.

DY 31.8 Wed 12:00 H20

Bifurcation scenarios in ensembles of two-dimensional excitatory units with global repulsive coupling — •Robert Ronge and Michael Zaks — Humboldt-Universität zu Berlin

We study systems of identical two-dimensional models of neurons with repulsive all-to-all coupling, focusing on the active rotator model with adaptation and the Morris-Lecar model. Parameters are chosen such that for the decoupled case each neuron is at rest, close to the border of class I excitability. Under the action of sufficiently strong repulsion, the collective equilibrium loses stability and is replaced by different form of oscillations. Two main type are oscillations in clusters and the state in which the neurons spike one-by-one in turn. We investigate transitions between these two regimes.

DY 31.9 Wed 12:15 H20

Synchronization of excitable oscillators by matrix-mediated viscoelastic coupling — •Florian Spreckelsen[1,2], Stefan Luther[1,2,3,4,5], and Ulrich Parlitz[1,2,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]University of Göttingen, Institute for Nonlinear Dynamics, Göttingen, Germany — [3]University Medical Center Göttingen (UMG), Institute of Pharmacology and Toxicology, Göttingen, Germany — [4]DZHK (German Center for Cardiovascular Research), Partner Site Göttingen, Germany — [5]Department of Physics and Department of Bioengineering, Northeastern University, Boston, USA

Individually contracting cardiomyocytes mechanically linked by an extracellular matrix belong to the class of viscoelastically coupled excitable oscillators. They exhibit an interesting range of synchronization patterns due to the interplay of autonomous oscillation and refractory period following an excitation, together with the delay introduced by the viscoelaticity. We study numerically the synchronization patterns occuring in mechanically coupled excitable oscillators depending on the viscoelastic properties of the coupling matrix.

DY 31.10 Wed 12:30 H20

Divergence of predictive model output as indication of phase transitions — •Frank Schäfer and Niels Lörch — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

We introduce a new method to identify phase boundaries in physical systems. It is based on training a predictive model such as a neural network to infer a physical system's parameters from its state. The deviation of the inferred parameters from the underlying correct parameters will be most susceptible and diverge maximally in the vicinity of phase boundaries. Therefore, peaks in the divergence of the model's predictions are used as indication of phase transitions. Our method is applicable for phase diagrams of arbitrary dimension and without prior information about the phases. Application to both the two-dimensional Ising model and the dissipative Kuramoto-Hopf model show promising results.

DY 31.11 Wed 12:45 H20

Correlations and hyperuniformity in the avalanche size of the Oslo model — •Rosalba Garcia-Millan[1], Gunnar Pruessner[1], Luke Pickering[2], and Kim Christensen[2] — [1]Department of Mathematics, Imperial College London - London SW7 2AZ, UK — [2]Department of Physics, Blackett Laboratory, Imperial College London - London SW7 2AZ, UK

Certain random processes display anticorrelations resulting in local Poisson-like disorder and global order, where correlations suppress fluctuations. Such processes are called hyperuniform. Using a map to an interface picture we show via analytic calculations that a sequence of avalanche sizes of the Oslo model is hyperuniform in the temporal domain with the minimal exponent $\lambda = 0$. We identify the conserved quantity in the interface picture that gives rise to the hyperuniformity in the avalanche size. We further discuss the fluctuations of the avalanche size in two variants of the Oslo model. We support our findings with numerical results.

DY 31.12 Wed 13:00 H20

Field-theoretic approach to the universality of branching processes — •Johannes Pausch, Rosalba Garcia-Millan, Benjamin Walter, and Gunnar Pruessner — Department of Mathematics, Imperial College London, UK

Branching processes are widely used to model phenomena from networks to neuronal avalanching. In a large class of continuous-time branching processes, we study the temporal scaling of the moments of the instant population size, the survival probability, expected avalanche duration, the so-called avalanche shape, the n-point correlation function and the probability density function of the total avalanche

size. Previous studies have shown universality in certain observables of branching processes using probabilistic arguments, however, a comprehensive description is lacking. We derive the field theory that describes the process and demonstrate how to use it to calculate the relevant observables and their scaling to leading order in time, revealing the universality of the moments of the population size. Our results explain why the first and second moment of the offspring distribution are sufficient to fully characterise the process in the vicinity of criticality, regardless of the underlying offspring distribution. This finding implies that branching processes are universal. We illustrate our analytical results with computer simulations.

DY 32: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Wednesday 15:00–19:15 Location: H3

Invited Talk DY 32.1 Wed 15:00 H3

Phase-separation in an elastic matrix: from living cells to synthetic materials — •Eric Dufresne — ETHZ

In order to function effectively, living cells need to compartmentalize myriad chemical reactions. In the classic view, distinct functional volumes are separated by thin oily-barriers called membranes. Recently, the spontaneous sorting of cellular components into membraneless liquid-like domains has been appreciated as an alternate route to compartmentalization.

I will review the essential physical concepts underlying these phenomena and outline some of the fundamental questions in soft matter physics that they inspire. Then, I will describe our recent experiments exploring the impact of mechanical stresses on the condensation of droplets. This work spans experiments with living cells and synthetic polymer networks, with an eye toward useful new materials.

DY 32.2 Wed 15:30 H3

Breakup of a particulate suspension jet — •Joris Chateau[1,2] and Henri Lhuissier[1] — [1]CNRS, Aix-Marseille University, Marseille, France — [2]Max Planck Institute, Gottingen, Germany

As viscosity is increased, a liquid capillary jet accelerated by gravity stretches over increasingly large distances before eventually breaking up. This Newtonian behavior is profoundly altered for particulate suspensions. Adding solid particles to a liquid, which increases the effective viscosity, can paradoxically shorten the jet considerably. This apparent contradiction is rationalized by considering finite size effects occurring at the scale of a few particles. A model is presented which captures the breakup length of suspension jets observed experimentally for a broad range of liquid viscosities, particle sizes and extrusion velocities of the jet, and recovers the Newtonian case for vanishing particle sizes. These results can be readily extended to any stretched jet configuration and potentially to other fluid media having a granularity.

DY 32.3 Wed 15:45 H3

Self-assembly and dynamics of mixtures of magnetic and non-magnetic liquid crystals under shear and external magnetic field — •Nima H. Siboni, Gaurav P. Shrivastav, and Sabine H. L . Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36 D-10623 Berlin

Doping liquid crystals with magnetic particles of different shapes enables us to control the properties of this delicate phase of matter via an external magnetic field [1,2]. In this talk, we focus on mixtures where the magnetic particles have the same shape as the liquid crystals. We study the self-assembly and dynamics of the mixture in and out of equilibrium [3]. In particular, we utilize non-equilibrium molecular dynamics simulation of Gay-Berne particles [4] to study (i) the (composition-dependent) effect of an external magnetic field on the isotropic-to-nematic transition of the mixture, and (ii) the interplay between shear-induced order and the magnetic field-induced order on the mechanical response of the mixture to an applied external shear.

References:
[1] I. Dierking, and S. E . San, Appl. Phys. Lett. **87**, 233507 (2005).
[2] G. P. Shrivastav, and S. H. L. Klapp, arXiv:1809.08288.
[3] N. H. Siboni, G. P. Shrivastav, and S. H. L. Klapp, *in preparation.*
[4] J. G. Gay, and B. J. Berne, J. Chem. Phys., **74**, 3316 (1981).

DY 32.4 Wed 16:00 H3

Marangoni flow in thin freely suspended liquid films — •Torsten Trittel[1], Christoph Klopp[1], Kirsten Harth[2], Alexey Eremin[1], and Ralf Stannarius[1] — [1]Institute for Physics, Otto von Guericke University, 39106 Magdeburg — [2]Physics of Fluids and Max Planck Center for Complex Fluid Dynamics, P.O. Box 217, 7500 AE Enschede

Next to their great success in display applications, liquid crystals are enormously attractive in the field of fundamental physics. Free-standing films with unique aspect ratios can serve as an ideal system for the investigation of two-dimensional hydrodynamics. We focus on thermocapillary effects in such films under microgravity. We present results of two suborbital rocket flights and show that thermal gradients within the film plane can cause thermocapillary (Marangoni) effects. The temperature dependence of the surface tension $\sigma(T)$ can induce flow from the hot to the cold film edge. Finally we developed a hydrodynamic model that can describe the experimental observations quantitatively. In contrast to Benard-Marangoni or Rayleigh-Benard convection, the relevant control parameter is the temperature difference, not the temperature gradient across the film.

The study was supported by the German Aerospace Center (DLR) within projects 50WM1430 and 50WM1744.

DY 32.5 Wed 16:15 H3

Shear-waves from cavitation in soft solids — •Julien Rapet[1,2], Yoshiyuki Tagawa[3], and Claus-Dieter Ohl[1,2] — [1]Nanyang Technological University, Singapore — [2]Otto-Von-Guerricke Universität, Magdeburg, Germany — [3]Tokyo University of Agriculture and Technology, Tokyo, Japan

While the fluid mechanics of cavitation is a mature research area, very little is known for bubbles undergoing large and non-spherical volume changes in a soft elastic solid. Here soft solids made from gelatin-water mixtures mimic tissue. Previous studies demonstrated that the collapse of a bubble entrapped in soft solids emits longitudinal waves at the speed of sound. Yet the elasticity of the medium supports also transversal waves propagating at a considerable lower speed. We show how cavitation in elastic solids may lead to the emission of such shear waves, particularly the collapse of bubbles near an air/solid interface. The cavitation bubbles are obtained by focusing a pulsed laser into the tissue mimicking material. The bubble dynamics and shear wave propagation are observed with high-speed imaging and photoelastic imaging, respectively. We show that similar to water the cavity moves during collapse away from the free surface accelerating a jet in the direction of the bubble's center of mass motion. During this process the volume between the air/solid interface and the bubble is sheared. Yet the dynamics is much faster than the shear wave speed and therefore the shear stress remains confined. For sufficiently strong and non-spherical collapses, the gelatin surface deforms and a crack starting from the interface propagating towards the bubble.

DY 32.6 Wed 16:30 H3

Self-organized lattices and coalescence of droplets in freely suspended liquid crystal films — •Christoph Klopp[1], Torsten Trittel[1], Kirsten Harth[2], Alexey Eremin[1], and Ralf Stannarius[1] — [1]Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany — [2]Universiteit Twente, Physics of Fluids and Max Planck Center for Complex Fluid Dynamics, 7500 AE Enschede, The Netherlands

Colloids in freely suspended smectic films are an excellent system to study self-organisation in restricted (2D) dimensionality. The dynamics of the colloids in such films is fully 2D. We demonstrate the formation of two-dimensional hexagonal lattices of isotropic droplets stabilized by repulsive interactions in freely suspended films [1]. The dynamics of single droplets in a six-neighbor cage can be described using the Saffman model for mobility in a 2D fluid. We show that the modified model reproduces the experimental observations, the droplet mobility in the lattice depends only on the ratio of cage and droplet sizes, irrespective of droplet sizes. At higher temperatures, droplets coalesce. Droplets on free-standing films have the shapes of flat lentils and their coalescence dynamics are expected to be intermediate between 2D and 3D cases [3]. We measured the coalescence which is

on a time scale of milliseconds depending on the radii of the involved droplets.

[1] Clark N., et al., 2017. Adv. Space. Res. 60 737

[2] Eremin, A., Baumgarten, S., Harth, K., Stannarius, R., 2011. Pys. Rev. Lett. 107, 268301.

[3] Hopper R., 1984, J. Am. Ceram. Soc. 67, C-262

DY 32.7 Wed 16:45 H3

Re-entrant) Splashing of drops impacting on a heated plate at reduced pressure — •Kirsten Harth, Michiel van Limbeek, Paul Hoefnagels, and Detlef Lohse — Physics of Fluids, Max Planck Center and Universiteit Twente, Enschede, The Netherlands

Splashing drops capture our minds with their fascinating beauty - and splash control is highly relevant in a wide range of applications involving impacting drops. It is thus not surprising that diverse criteria for the splash threshold have been put forward over the last decades, with a recent breakthrough by Riboux and Gordillo (e.g. PRL 113 189901 (2014)). The effect of the surrounding gas is included via the mean free path, thus the theory also captures the disappearance of upon decrease of the ambient pressure. In our present understanding, identical drops remain intact at low impact velocities, while they always splash above a critical velocity.

Drop impact on heated surfaces in reduced pressure, however, bears a counterintuitive surprise: At temperatures below the static Leidenfrost point TL, the transition from deposition to splash is followed by another disappearance of splashing, before it reappears at larger impact velocity in a wide range of parameters. Above TL, splashing occurs at tremendously reduced impact velocity. We analyse this peculiar behaviour using different high speed imaging techniques.

DY 32.8 Wed 17:00 H3

Morphology of liquid-liquid dewetting — •Roghayeh Shiri[1], Ralf Seemann[1], Dirk Peschka[2], and Barbara Wagner[2] — [1]University of Saarland, Saarbrucken, Germany — [2]Weierstrass Institute, Berlin, Germany.

We study the spinodal dewetting of nanometric thin liquid polystyrene (PS) films on liquid polymethyl-methacrylate (PMMA) substrates. The initial stage of dewetting consists of the amplification of thermal fluctuations driven by dispersion forces, eventually leading to the formation of holes with a preferred distance λ. According to theoretical predictions, the PS/air and the PS/PMMA interfaces shall evolve in a coupled way. As the surface tension of the PS/PMMA interface is way smaller than the surface tension of the PS/air interface, the amplitude of the corrugation of the PS/PMMA interface will be much larger than that of the PS/air interface. To determine the morphological evolution of the preferred wavelength λ and of the preferred holes distance, we follow the evolution of PS/air interface in situ by atomic force microscopy (AFM). The evolution of the PS/PMMA interface is explored ex situ by AFM using a lift up technique. By matching the PS/air and the PS/PMMA interfaces we can decide if the coupled corrugations of both interfaces evolve in phase or anti phase. We also explore the dependence of the preferred wavelength as function of PS film thickness and compare the result with theoretical predictions.

15 min. break

DY 32.9 Wed 17:30 H3

Multiparticle Collision Dynamics Modeling of Nematic Liquid Crystal with Variable Order Parameter — •Shubhadeep Mandal[1] and Marco G. Mazza[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Loughborough University, Loughborough, United Kingdom

We have generalized the particle-based multiparticle collision dynamics (MPCD) method to model the hydrodynamics of nematic liquid crystals. Following Qian-Sheng theory [Phys. Rev. E 58, 7475 (1998)] of nematic liquid crystals, the spatial and temporal variations of the nematic director field and the nematic degree of order are described by a tensor order parameter. The principle idea is to assign a tensor quantity to each MPCD particle, whose average resembles the macroscopic tensor order parameter. The applicability of this new method is verified by performing several physical and numerical tests. We have tested: (a) the isotropic-nematic phase transition, (b) the annihilation dynamics of a pair of point defects, (c) the flow alignment of the nematic director in shear and Poiseuille flows, and (d) the velocity profile in shear and Poiseuille flows. We have found excellent agreement with existing literature. Additionally, we study the decay of force-dipole flow field in nematic liquid crystals. The present method can have far-reaching implications not only in modeling of nematic flows, but also to study the motion of colloids and microswimmers immersed in an anisotropic medium.

DY 32.10 Wed 17:45 H3

Kinetic Monte Carlo simulations of thin film growth for pure and mixed films — •Eelco Empting, Miriam Klopotek, and Martin Oettel — Institut für angewandte Physik, Tübingen, Germany

We consider a binary lattice model for growth of demixing thin films, i.e. where two species of particles are deposited onto a substrate and undergo diffusion at and above it. Particle interactions include hard-core repulsion and nearest-neighbor attraction, the strength of which depends on the species of the particles involved. In KMC simulations of this model, we consider quite generally all sorts of single particle moves to neighboring sites, thus allowing for species-dependent diffusion constants, desorption, and formation of cavities.

We studied the influence of the various parameters, most notably diffusion rates and interaction strengths, on the structure and evolution of a growing film. Among other things, this system was used to compare simulations to real-world growth experiments of a C60-CuPC blend film where we can identify the defining parameters leading to characteristic structure in the films.

DY 32.11 Wed 18:00 H3

Classical density functional theory for ferrogels with distinguishable particles — •Segun Goh, Andreas M. Menzel, and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany

Classical density functional theory has been widely studied for liquid-like states of materials which consist of indistinguishable particles interacting via pairwise potentials. Meanwhile, there are materials, among which ferrogels provide one of the important examples, where the particles are fixed in an elastic polymer matrix. As particle neighbors do not change over time due to the fixation, particles are distinguishable by positions in those systems. In this talk, we discuss a density functional approach for such systems with distinguishable particles, considering a two-dimensional bead-spring lattice with magnetic dipoles at every bead as a model for ferrogels. We first introduce a mapping of the harmonic springs representing the elastic matrix onto a pairwise pseudo-interaction between indistinguishable particles. The mapping is justified by Monte-Carlo simulations of both the bead-spring model and the frozen states of corresponding pseudo-interaction systems in combination with the density functional theory. We then formulate density functional theory for the dipole-spring model and investigate magnetostriction and compression moduli of ferrogels under magnetic interactions. We expect that our density functional approach may provide a route towards an understanding of a broad range of materials with particle inclusions.

DY 32.12 Wed 18:15 H3

Crystallization of spheres with static and dynamic size dispersity — •Praveen Kumar Bommineni, Nydia Roxana Varela Rosales, Marco Klement, and Michael Engel — Institute for Multiscale Simulation, Friedrich-Alexander University Erlangen-Nürnberg, Nägelsbachstrasse 49b, 91052 Erlangen, Germany

Colloids are rarely uniform but follow a distribution of sizes, shapes, and charges. This dispersity can be inherent (static) or develop and change over time (dynamic). Despite a long history of research, the conditions under which non-uniform particles crystallize and which crystal forms is still not well understood. Here, we demonstrate that hard spheres with Gaussian radius distribution and dispersity up to 19% always crystallize if compressed slow enough, and they do so in surprisingly complex ways [1]. This result is obtained by accelerating event-driven simulations with particle swap moves for static dispersity and particle resize moves for dynamic dispersity. Above 6% dispersity, AB_2 Laves, AB_{13}, and a region of complex Frank-Kasper phases are found. The Frank-Kasper region includes a quasicrystal approximant with Pearson symbol oS276. Our findings are relevant for ordering phenomena in soft matter and alloys.

[1] P.K. Bommineni et al., arXiv:1811.00061.

DY 32.13 Wed 18:30 H3

Elastic turbulence at low Reynolds numbers and its control — •Reinier van Buel, Christian Schaaf, and Holger Stark —

Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The properties of viscoelastic solutions are exceptionally applicable on the micron scale. For example, in microfluidic devices mixing and heat transfer are strongly enhanced. This is due to elastic turbulence [1], which bears similar qualities as inertial turbulence. The relevant dimensionless number characterizing viscoelastic fluids is the Weissenberg number, which compares the polymer relaxation time to the characteristic time of the flow dynamics.

Numerical solutions of the Oldroyd-B model in a two-dimensional Taylor-Couette geometry display a supercritical transition from the laminar Taylor-Couette to the occurence of a secondary flow [2]. The secondary flow is turbulent and caused by an elastic instability beyond a critical Weissenberg number. The order parameter, the time average of the secondary-flow strength, follows the scaling law $\Phi \propto (\mathrm{Wi}-\mathrm{Wi}_c)^\gamma$ with $\mathrm{Wi}_c = 10$ and $\gamma = 0.45$ and the power spectrum of the velocity fluctuations shows a power-law decay with a characteristic exponent. Finally, we present first results on controlling the elastic instability through an oscillating rotation of the outer cylinder of the Taylor-Couette cell, with a frequency close to the characteristic relaxation time of the dissolved polymers.

[1] A. Groisman and V. Steinberg, Nature **405**, 53 (2000).
[2] R. Buel, C. Schaaf, H. Stark, Europhys. Lett. **124**, 14001 (2018).

DY 32.14 Wed 18:45 H3

Gold nanoclusters at room temperature: are they soft matter? — •Luca M. Ghiringhelli, Bryan Goldsmith, Diego Guedes-Sobrinho, Jacob Florian, Jin-Xun Liu, Weiqi Wang, Juarez Da Silva, Ian Hamilton, and Matthias Scheffler — Fritz-Haber- Institut der Max-Planck-Gesellschaft, Berlin, Germany

Soft matter encompasses systems for which the predominant physical behaviors occur at an energy scale comparable with room-temperature (T=300 K) thermal energy. Here, we present a study of free-energy landscapes of neutral gold nanoclusters in the size ranges 10–13 (arXiv:1811.08062) and 25–40 (arXiv:1811.04438) atoms. Gold nanoclusters are interesting for their possible applications in gas sensing, pollution reduction, and catalysis. Our studies are based on extensive Born-Oppenheimer density-functional-theory replica-exchange molecular-dynamics sampling over a wide range of temperatures. We find that the long-standing question "At which *size* (neutral) gold clusters start favoring 3D vs 2D structures?" should be recast, at least in the size range between 10 and 13 atoms, into the question (here answered): "At which *temperatures* are 3D structures favored?". At T=300 K, we find that the typical activation barrier of Au–Au bonds is indeed comparable with the thermal energy, resulting in a continuous reshuffling of bonds and, in the size range 25–40 atoms, in low free-energy structures that significantly differ from the T=0 K structures. In these examples, gold nanoclusters seem indeed to match the definition of soft matter. This might have important implications for the characterization of the chemical reactivity of these systems.

DY 32.15 Wed 19:00 H3

MIEZE spectroscopy of sub-picosecond collective dynamics in bulk liquid water — Olaf Soltwedel[1,2], •Leonie Spitz[3], Johanna K Jochum[3,4], Andreas Wendl[1], Christian Pfleiderer[1], and Christian Franz[3] — [1]Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — [2]Technische Universität Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany — [3]Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [4]Bayerisches Geoinstitut, Universität Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany

The anomalously large dielectric constant of water is intimately connected with a Debye relaxation peak in low frequency dielectric spectra. Despite intense research, a link between the molecular dynamics and the Debye relaxation peak, are still under heavy debate. Proposed mechanisms include translational and/or rotational motions, movement of free water molecules, collective relaxation of a cluster or hopping of defects in the hydrogen bond network. We used MIEZE (Modulation IntEnsity with Zero Effort) neutron spin echo spectroscopy, a high resolution time of flight technique, to measure the dynamic structure factor (S(q,t)) of water over an exceptional dynamical range (0.01 up to 1000ps). Consistent with the literature, we find the bulk transverse diffusion on length scales from 0.1/Å up to 0.4/Å. As our main result, reveals at least two more processes on sub-picosecond time-scales. This provides direct evidence of a vibration and/or delocalization of hydrogen larger than the intermolecular distance as proposed [1].

[1] A. Arbe et al. PRL 117, 185501 (2016)

DY 33: Statistical physics of biological systems I (joint session BP/DY)

Time: Wednesday 15:00–17:30 Location: H4

DY 33.1 Wed 15:00 H4

Active noise fuels the heterogeneous anomalous diffusion of inert nanoparticles in the cytoplasm — •Adal Sabri[1], Xinran Xu[2], Diego Krapf[2], and Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth, Germany — [2]School of Biomedical Engineering, Colorado State University, CO, USA

Diffusive motion of inert particles in the cytoplasm of living cells is generally assumed to be driven by thermal noise. This assumption appears particularly justified for the frequently observed sublinear growth of the particles' mean square displacement ('subdiffusion').

In order to probe quantitatively to which extent also active noise contributes to (sub)diffusional motion in living matter, we have introduced inert quantum dots into the cytoplasm of living cells and performed extensive single-particle tracking experiments in untreated cells and after disrupting the cytoskeleton. In all cases a pronounced subdiffusive motion of the particles with a distinct anti-correlation of successive steps was observed. Yet, the degree of the diffusion anomaly and the generalized diffusion coefficients showed marked changes when the integrity of the cytoskeleton was compromised, i.e. particles moved less vivid when cytoskeleton-associated active transport was erased. This observation highlights that cytoplasmic subdiffusion is partially fueled by active noise. In line with this notion, several measures of the trajectories, e.g. the gaussianity, highlight a strongly heterogeneous random walk with a temporally and/or spatially varying noisy driving.

DY 33.2 Wed 15:15 H4

Self-organised segregation of bacterial chromosomal origins — •Sean Murray — Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

In spite of much effort, many aspects of chromosome segregation in bacteria remain unclear. Like many other bacteria, the chromosomal origin of replication in Escherichia coli is dynamically positioned throughout the cell cycle. Initially maintained at mid-cell, where replication occurs, origins are subsequently partitioned to opposite quarter positions. However the mechanism underlying this is unknown. Here, we provide an explanation based on the self-organisation of the Structural Maintenance of Chromosomes complex, MukBEF. We propose that a non-trivial feedback between the self-organising MukBEF gradient and the origins leads to accurate positioning and partitioning as an emergent property. We find excellent agreement with quantitative experimental measurements and confirm key predictions. In particular, we show that origins exhibit biased motion towards MukBEF, rather than mid-cell, consistent with the model. Overall, our findings suggest that MukBEF and origins act together as a self-organising system for chromosome segregation and introduces protein self-organisation as an important consideration for future studies of chromosome dynamics.

DY 33.3 Wed 15:30 H4

Perfect anomalous transport of subdiffusive cargos by molecular motors in viscoelastic cytosol — •Igor Goychuk — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany

Multiple experiments show that various submicron particles such as magnetosomes, RNA messengers, viruses, and even much smaller nanoparticles such as globular proteins diffuse anomalously slow in the viscoelastic cytosol of living cells. Hence, their sufficiently fast directional transport by molecular motors such as kinesins is crucial for the cell operation. It has been shown recently that the traditional flashing Brownian ratchet models of molecular motors are capable to describe both normal and anomalous transport of such subdiffusing

cargos by molecular motors with a very high efficiency. This work elucidates further an important role of mechanochemical coupling in such an anomalous transport. It shows a natural emergence of a perfect subdiffusive ratchet regime due to allosteric effects, where the random rotations of a "catalytic wheel" at the heart of the motor operation become perfectly synchronized with the random stepping of a heavily loaded motor, so that only one ATP molecule is consumed on average at each motor step along microtubule. However, the number of rotations made by the catalytic engine and the traveling distance both scale sublinearly in time. Nevertheless, this anomalous transport can be very fast in absolute terms.

[1] I. Goychuk, Biosystems, in press, arXiv:1809.08032 [physics.bio-ph]

Invited Talk DY 33.4 Wed 15:45 H4

Chaos in self-propelled droplets — •Annette Zippelius and Reiner Kree — Georg-August-Universität Göttingen, Institut für Theoretische Physik, Friedrich-Hund Platz 1, 37077 Göttingen

Intracellular flow can be generated by a variety of active mechanisms, such as motors transporting cargo. The actively generated flow has at least two effects: it can drive cell locomotion and simultaneously play a central role for intracellular transport. We develop increasingly more complex, but analytically solvable models, starting from a simple fluid droplet or a biphasic droplet, consisting of a fluid and a rigid gel. Active forces or stresses, which are co-localised on the gel, generate internal flow. The trajectories of tracer particles which are advected by the internal flow, are shown to display the full richness of dynamical systems, ranging from closed orbits to quasiperiodic motion and chaotic trajectories in general. We discuss the mixing properties of the internal flow as well as its significance in comparison to diffusive transport. Despite chaos inside the droplet, locomotion of the droplet as a whole remains simple and regular, e.g. motion on a straight line or a spiral.

DY 33.5 Wed 16:15 H4

Three-dimensional membrane confinement and geometry dictate excitable signaling dynamics in Dictyostelium cells. — •Marcel Hörning[1,2,3] and Tatsuo Shibata[2] — [1]Institute of Biomaterials and Biomolecular Systems, University of Stuttgart, 70569 Stuttgart, Germany — [2]Laboratory for Physical Biology, RIKEN Center for Biosystems Dynamics Research, Kobe 650-0047, Japan — [3]Institute for Integrated Cell-Material Sciences, Kyoto University, 606-8501, Kyoto, Japan

Propagating waves on the plasma membrane mediate the membrane protrusive activities in Dictyostelium and mammalian cells. Most studies focus on the dynamics extracted from single focal planes only. Thus, the relation between the dynamics and three-dimensional cell shape remains elusive, due to the lack of signaling information about the unobserved part of the membrane.

We show that PtdInsP3 wave dynamics are directly regulated by the three-dimensional geometry - size and shape - of the plasma membrane. By introducing an analysis method that extracts the three-dimensional spatiotemporal activities on the entire cell membrane, we show that PtdInsP3 oscillatory waves self-regulate their dynamics within the confined membrane area. This leads to changes in speed, orientation and pattern evolution, following the underlying excitability of the signal transduction system. This findings emphasize the role of the plasma membrane topology in reaction-diffusion driven biological systems and indicate its importance in other mammalian systems.

DY 33.6 Wed 16:30 H4

Non-equilibrium spatial scaling reveals intrinsic features of the active driving — •Federica Mura, Grzegorz Gradziuk, and Chase Broedersz — Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München

Recent experiments indicate non-equilibrium activity in a host of biological systems, including chromosomes, cell membranes, and the cytoplasm. Measuring and quantifying non-equilibrium dynamics in such systems is a major challenge in biophysics, due to their many-body nature and the limited number of variables accessible in an experiment. We investigate what information concerning the system's non-equilibrium state can be extracted by non-invasively tracking a subset of degrees of freedom. To this end, we develop a general, yet simple stochastic model of soft elastic networks with spatially-varying internal driving, representing internal enzymatic force generation. With this model, we determine the scaling behavior of non-equilibrium dynamics from the phase space currents of tracer particles with varying spatial separations in the system. Finally, we will discuss how the non-equilibrium dynamics measured on different length scales can reflect the intrinsic microscopic features of the internal active driving.

DY 33.7 Wed 16:45 H4

Dynamical states of a living network — •Philipp Fleig, Mirna Kramar, Michael Wilczek, and Karen Alim — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany

Understanding the emergence of behaviour in living systems from underlying physical mechanisms is a major goal of biophysics. Even very simple, non-neural organisms like the slime mould *Physarum polycephalum* show remarkably complex behaviour including growth, adaptation of the network morphology and foraging for food - despite only being a single, giant, network-shaped cell.

Behavioural dynamics, here, emerge directly from living matter, namely the coordinated contractions of the cell's tubular shaped actomyosin cortex undergoing rhythmic contraction every 100 seconds. We decompose this spatiotemporal dynamics into principal components and identify a reduced set of characteristic large-scale contraction patterns spanning the network. Based on this dictionary of patterns we are able to determine the typical sequence of the network's response patterns to a controlled stimulus, mimicking a natural response scenario. We also find spontaneously occurring breaking of coherent contraction dynamics into decoherent patterns over short time-scales. Finally, we note a power law distribution of the relative amplitudes of the principal components. This may be key in explaining the observed dynamical features from the underlying biomechanics. Our findings connect behaviour with characteristic states of living matter.

DY 33.8 Wed 17:00 H4

Active droplets can center internal particles — •David Zwicker[1,2], Anthony Hyman[3], and Frank Jülicher[2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]Max Planck Institute for the Physics of Complex Systems, Dresden — [3]Max Planck Institute of Cell Biological and Genetics, Dresden

Active droplets are non-equilibrium systems where chemical reactions drive fluxes of the droplet material. These fluxes can control the droplet nucleation as well as the droplet size and thereby stabilize many droplets against the typical coarsening observed in passive systems. Here, we study how the non-equilibrium fluxes affect solid particles inside such active droplets. We find that particles get centered when the droplet is maintained externally, while particles are expelled in the opposite case of autocatalytic droplets. In this case, only catalytically active particles can be centered. An example of such a situation are centrosomes in biological cells. Our theory thus accounts for the observed central positioning of centrioles and it generally provides a mechanism for controlling the morphology of active droplets.

DY 33.9 Wed 17:15 H4

Mesoscopic roughness analysis of propagating cell fronts: physical statistics as an in-vitro phenotype probe — •Guillaume Rapin[1], Audrey Rawleigh[2], Aziza Merzouki[3], Ermano Moriggi[2], Bastien Chopard[3], Thierry Giamarchi[1], Steven A. Brown[2], and Patrycja Paruch[1] — [1]DQMP, University of Geneva, Switzerland — [2]IST, Universtiy of Zurich, Switzerland — [3]CSD, University of Geneva, Switzerland

The competition between elasticity and disorder governs the geometry and dynamics of interfaces in many systems, from ferroic domain walls to bacterial colonies. In the latter case, it has been used as a framework to explore cell front evolution, with local mapping of displacements and forces, and the origin of the cell front roughness.

Here, we report on the geometry and dynamics of propagating rat epithelial cell fronts in artificial wound healing assays over 72 hours, studied over 5 orders of magnitude in length scale ranging from $1\mu m$ to $2cm$. Under standard conditions, they present 3 distinct regimes: power law growth of the roughness with characteristic roughness exponent values of $\zeta = 0.55$ at sub-cell length scales, and of $\zeta \approx 0.3$ at few-cell length scales, reaching a scale-independent maximum beyond $400\mu m$. Exposure to a selection of chemical inhibitors targeting cell division rates, mobility, or intercellular communications changes this roughening behaviour, as well as the initial and steady-state dynamics of the cell front. Our results suggest that collective motion on the order of 4-10 cells plays a key role in the roughness evolution of the front. These experimental results will be compared to numerical simulations.

DY 34: Dynamics of Multilayer Networks II (Focus Session SOE/DY/BP) (joint session SOE/DY/BP)

Time: Wednesday 15:00–16:45 Location: H17

Topical Talk DY 34.1 Wed 15:00 H17

Delay controls chimera relay synchronization in multiplex networks — •Eckehard Schöll, Jakub Sawicki, Iryna Omelchenko, and Anna Zakharova — Institut für Theoretische Physik, Technische Universität Berlin, Germany

We study remote (or relay) synchronization in multilayer networks between parts of one layer and their counterparts in a second layer, where these two layers are not directly connected. A simple realization of such a system is a triplex network where a relay layer in the middle, which is generally not synchronized, acts as a transmitter between two outer layers; an example is provided by the hippocampus connecting distant parts of the brain. We find various partial synchronization patterns, in particular chimera states, i.e., complex patterns of coexisting coherent and incoherent domains, and establish time delay in the interlayer coupling as a powerful tool of control [1]. We demonstrate that the three-layer structure of the network allows for synchronization of the coherent domains of chimera states in the first layer with their counterparts in the third layer, whereas the incoherent domains either remain desynchronized or synchronized. As model dynamics we use the paradigmatic FitzHugh-Nagumo system.

[1] J. Sawicki, I. Omelchenko, A. Zakharova, and E. Schöll, arXiv:1807.11223v2 (2018).

DY 34.2 Wed 15:30 H17

Spiral wave patterns and their synchronization in lattices of nonlocally coupled discrete-time systems — Andrei Bukh, Galina Strelkova, and •Vadim Anishchenko — Saratov State University, Saratov, Russia

We investigate numerically the spatio-temporal dynamics of a 2D lattice of coupled discrete-time systems with nonlocal interaction. The individual map is given by a universal discrete system (the Nekorkin map) proposed for modeling the neural activity. The network behavior is studied for periodic and open boundary conditions. It is shown that for certain values of the nonlinear coupling parameters, rotating spiral waves and spiral wave chimeras can be observed in the considered lattice. We analyze and compare statistical and dynamical characteristics of the local oscillators from coherence and incoherence clusters of a spiral wave chimera. We also explore the effects of partial and complete synchronization of spiral wave chimeras in two coupled lattices of discrete maps with varying the intercoupling between the networks.

DY 34.3 Wed 15:45 H17

Synchronization of spiral wave patterns in coupled 2D lattices of discrete maps — •Andrei Bukh[1], Eckehard Schöll[2], and Vadim Anishchenko[1] — [1]Saratov State University, Saratov, Russia — [2]Technical University, Berlin, Germany

We study numerically the dynamics of two symmetrically and unidirectionally coupled lattices of nonlocally coupled two-dimensional Nekorkin maps. The phenomena of external and mutual synchronization of spiral wave patterns including chimera states are explored. The partial and complete synchronization is analyzed by calculating the number of synchronous elements in the coupled lattices depending on the coupling strength between them. Synchronous regimes are quanitified by using mutual correlation coefficients between the relevant elements in the lattices.

DY 34.4 Wed 16:00 H17

Transmission and synchronization of chimeras in a multilayer network of nonlocally coupled chaotic maps — •Galina Strelkova and Tatiana Vadivasova — Saratov State University, Saratov, Russia

We explore numerically transmission and external synchronization of chimera states in a multilayer network of unidirectionally coupled rings of nonlocally coupled logistic maps. We consider two cases: when all M coupled layers are identical (homogeneous) and when (M-1) identical layers differ from the first driving layer in their nonlocal coupling parameters. It is shown that the master chimera state in the first layer can be retranslating along the network with small distortions which are defined by a parameter mismatch. The synchronization effect is evaluated by calculating the mean-square deviation of the structure in the layers when varying the nonlocal coupling parameters.

DY 34.5 Wed 16:15 H17

Synchronization of chimera states in multilayer heterogeneous network of nonlocally coupled maps — •Elena Rybalova[1], Galina Strelkova[1], Tatiana Vadivasova[1], and Anna Zakharova[2] — [1]Saratov State University, Saratov, Russia — [2]Technical University, Berlin, Germany

We present numerical results on the study of a complex network composed of many asymmetrically coupled heterogeneous layers of nonlocally coupled logistic maps. Transmission and synchronization of chimera states realized in the first (master) layer is considered for mutual and unidirectional inter-coupling between the layers. It is shown that there is a threshold of the forced synchronization, which is different for various chimeras (phase and amplitude) in the master layer. It is established that the presence of feedback (backward) inter-coupling is a significant obstacle for global synchronization across the network. We also analyze and compare the role of heterogeneity in control and coupling parameters on the degree of forced synchronization.

15 min. break

DY 35: Modeling and Simulation of Soft Matter I (joint session CPP/DY)

Time: Wednesday 15:00–17:00 Location: H18

DY 35.1 Wed 15:00 H18

Thermodyanmics of Supramolecular Polymers with Hydrogen Bonding Ends — •Eunsang Lee and Wolfgang Paul — Institut für Physik, Marin-Luther-Universität Halle-Wittenberg, 06108 Halle, Germany

Rheological properties of supramolecular polymers (SMPs) depend on their equilibrium structure including the size, the number, and the topology of aggregates. In this work we investigate the thermodynamics of SMPs with H-bonding ends in a wide range of densities. Replica exchange stochastic approximation Monte Carlo simulations with coarse-grained models for polyethylene and polybuthylene glycols are used. Our heterocomplementary SMP system includes the same concentration of two different molecules, each of which is functionalized by different H-bonding stickers at both ends. Due to the chemical structure of sticker association, the functionality of the sticker varies depending on temperature, which is described by our H-bond potential and optimized parameters. Our simulation shows that SMPs have three transition lines with increasing temperature, a micelle (or gel)-ring transition, a ring-linear transition, and a linear-free chain transition. Because of the temperature-dependent functionality of the sticker, we can see the micelle (or gel)-ring transition at very low temperature which has not been observed in other associating polymers with fixed functionality. Below this transition line, the polymers in dilute concentration form flower-like micelles but polymers in semi-dilute concentration form a gel.

DY 35.2 Wed 15:15 H18

Simulation of a large polymer with untruncated interaction near the collapse — •Stefan Schnabel and Wolfhard Janke — Universität, Leipzig

Off-lattice polymer models usually incorporate monomer-monomer interactions that act – at least in principle – at any distance. In consequence, calculating the energy and in particular the change in energy during a Monte Carlo move is typically an operation of computational complexity $\mathcal{O}(N^2)$, where N is the number of monomers. Since this complexity is inherited by the individual Monte Carlo move, only small

polymers can be simulated without truncating the interaction potentials. We show how this can be avoided at temperatures near or above the collapse transition by using a Metropolis algorithm that tolerates inaccurate estimates of ΔE and present results for a polymer with Lennard-Jones interactions and $N \leq 65536$.

DY 35.3 Wed 15:30 H18

Is there a universal equation of state for flexible polymers beyond the semi-dilute regime? — •Jaroslaw Paturej[1,2], Jens-Uwe Sommer[1], and Torsten Kreer[1] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]University of Szczecin, Szczecin, Poland

We reconsider the isothermal equation of state (EoS) for linear homopolymers in good solvents, $p = p(c, T)$, which relates the osmotic pressure, p, of polymers with the bulk concentration, c, and the temperature, T. The classical scaling theory predicts the EoS in dilute and semi-dilute regimes. We suggest a generalized EoS which extends the universal behavior of polymer solutions up to the highly concentrated state and confirmed it by molecular dynamics simulations and using available experimental data. Our conjecture implies that properties of polymer chains dominate the EoS in the presence of many-body interactions. Our theoretical approach is based on a viral expansion in terms of concentration blobs leading to a superposition of two power laws in the regime of concentrated solutions.

DY 35.4 Wed 15:45 H18

Comparison of strain-induced transitions from liquid to solid of poly(ethylene oxide) and polyamide chains in water — •Sergii Donets[1], Olga Guskova[1], Gary Dunderdale[3], Oleksandr Mykhaylyk[3], and Jens-Uwe Sommer[1,2] — [1]Institute Theory of Polymers, Leibniz-Institute of Polymer Research, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — [3]Department of Chemistry, University of Sheffield, Sheffield, S3 7HF, UK

Aqueous solutions of poly(ethylene oxide) (PEO) and polyamide oligomers are capable of undergoing a phase transition as a result of loss of the hydrated structure. Our simulations using an atomistic model clearly indicate that an elongating force dipole acting on both chain ends of oligomer chains initiates interchain aggregation with the formation of highly oriented fibrillar nanostructures [1]. The strain-induced demixing transition from liquid to solid occurs primarily due to the favorable hydrophobic interactions in case of PEO chains and, in addition, due to the intermolecular hydrogen boding in case of polyamide chains. A tensile stress introduced into the aqueous solution changes the solvent quality from good to poor as a function of conformational state of the chains and, if there are other oligomer chains present in the simulation box, leads to a phase separation from water. The strain-induced demixing of the extended chains provides the possibility to obtain polymer fibers with low energy costs.

[1] J. Phys. Chem. B, 2018, 122 (1), 392-397

DY 35.5 Wed 16:00 H18

Soft deformable colloids: self-assembly and structure through computer simulations — •Mihir Khadilkar and Arash Nikoubashman — Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

Colloids represent a rich class of soft materials that are important not only as model systems to study physical processes at nanoscale, but also as versatile building blocks towards a variety of technological applications. While hard-core models of colloids (with solely excluded volume interaction) have had great success in studying ordering, structure and dynamics in the past, most experimental systems exhibit varying degrees of softness that could potentially drastically alter their static and dynamic properties. Using molecular dynamics (MD) simulations of mesh models, we study the self-assembly of soft spherical and spheroidal colloids as a function of their elasticity and packing density. We quantify their arrangement and deformation using various order parameters. Further, we asses the dependence of eventual thermodynamic properties on the asphericity and softness of the colloids. For instance, we find that soft prolate ellipsoidal colloids (with aspect ratio 2) undergo a convex-to-concave transition at high pressures. The crystal structure also gets distorted, accompanied by an asymmetric deformation of principal directors. Addressing the structure-property relationship between softness arising from microstructure and the macroscopic properties could provide new routes towards designing and fabricating novel materials with tailored structural properties.

DY 35.6 Wed 16:15 H18

Self-assembly of triblock terpolymers system using dissipative particle dynamic simulations — •Deepika Deepika and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany

Self-assembly of triblock polymers into ordered structures has emerged as a promising technique for generating morphologies with nanometer range periodicity. The self-assembled structures dictated by the volume fraction of each block and interactions between them. In this work we are interested in the self-assembly behavior of polystyrene-polybutadiene-polymethyl-methacrylate (SBM) triblock copolymers in melt and in solution. The ternary phase diagram of SBM melt includes complex morphologies like spheres in lamellae cylinders in lamellae, cylinders in cylinder and many other. Equally intriguing is the solution phase behavior of SBM; recent experiments conducted by Groeschel et al. suggested ellipsoid aggregates of SBM in which layers of SBM are stacked in an ABCBA pattern. We conducted extensive DPD simulations to elucidate the effect of the process parameters, such as the volume fraction of each block and the Flory-Huggins interaction parameters, on the self-assembled structures. Our simulations give microscopic insights into the self-assembly behavior and provide useful design guidelines for fabricating structured nanoparticles in experiments.

DY 35.7 Wed 16:30 H18

Construction of core-double-shell nanostructures via adsorption of mixed star polymers — •Qiyun Tang and Marcus Mueller — Institut für Theoretische Physik, Universität Göttingen

The adsorption of two kinds of star polymers with strongly adsorbing arm ends but distinct arm lengths onto one big gold nanoparticle results in the formation of a core-double-shell nanostructure. This radial-organized nanostructure finds potential applications in plasmonic and biomedical disciplines. Here we use theory and simulation to systematically study the formation process of this advanced nanostructure. Theoretical calculations predict that this structure does not reach equilibrium, but strongly depends on the formation kinetics. Simulation results show that the adsorption of short star polymers are chiefly dictated by diffusion whereas the adsorption of the end of a long star polymer implicates a high free-energy barrier generated by other chains, resulting in a protracted adsorption. The fabrication of the core-double-shell nanostructure is a combination of the diffusion-limited and the reaction-limited processes of short and long polymers, respectively, which is confirmed by experimental findings.

DY 35.8 Wed 16:45 H18

Mixtures of Dendrimers and Linear Polymers — •Martin Wengenmayr[1,2], Ron Dockhorn[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]TU Dresden, Germany

One of the largely unsolved problems in polymer science is the effect of polymer architecture on the thermodynamics and functional properties of a polymer system. In particular, there is no commonly accepted explanation for the conformation properties of branched polymers immersed in a melt of chemically identical linear polymers. Based on Monte Carlo simulations of dendrimers with various generations and spacer lengths immersed in a solution of polymer chains of different degree of polymerization and concentrations we show that flexible dendrimers do not collapse into a compact globule as the concentration of linear chains is increased. Instead, we observe a crowded state distinct from athermal or theta solvent state. Beside the nontrivial conformational changes of the dendrimer the mixing of polymers of the same chemical composition but different branching induces secondary interactions between the species. Our work addresses the question of the strength of the secondary interactions in terms of intermolecular interactions and depletion attraction.

DY 36: Condensed-matter simulations augmented by advanced statistical methodologies (joint session DY/CPP)

Time: Wednesday 15:00–18:45 Location: H20

Invited Talk DY 36.1 Wed 15:00 H20

Quantum Machine Learning — •Anatole von Lilienfeld — Institute of Physical Chemistry, University of Basel

Many of the most relevant chemical properties of matter depend explicitly on atomistic and electronic details, rendering a first principles approach to chemistry mandatory. Alas, even when using high-performance computers, brute force high-throughput screening of compounds is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of chemical space, i.e. all compositional, constitutional, and conformational isomers. Consequently, efficient exploration algorithms need to exploit all implicit redundancies present in chemical space. I will discuss recently developed statistical learning approaches for interpolating quantum mechanical observables in compositional and constitutional space. Results for our models indicate remarkable performance in terms of accuracy, speed, universality, and size scalability.

DY 36.2 Wed 15:30 H20

Quantum Monte Carlo method for Vibrational Frequencies — •Yu Yang Liu and Gareth Conduit — University of Cambridge, UK

Quantum Monte Carlo methods have become a leading contender for high accuracy calculations for the electronic structure. Calculating energy derivatives such as atomic forces and the matrix of force constants is important in relaxing structures, calculating vibrational properties, and performing molecular dynamics simulations. We develop a quantum mechanical expectation value to evaluate the matrix of force constants directly in Quantum Monte Carlo. The approach allows the full modeling of correlation effects such as Van der Waals force, opening new applications to molecules and solids in condensed matter.

DY 36.3 Wed 15:45 H20

Localized Basis Functions for Variationally Enhanced Sampling — •Benjamin Pampel, Kurt Kremer, and Omar Valsson — Max Planck Institute for Polymer Research, Mainz, Germany

Variationally Enhanced Sampling (VES) is a recently developed method for molecular dynamics simulations. It enhances sampling by introducing a bias potential along certain collective variables that is constructed via minimisation of a convex functional.

This bias potential is usually represented by a linear expansion in some basis set, with delocalised functions such as plane waves or Chebyshev/Legendre polynomials as common choices. However, it is an open question if localised functions perform better. In particular, the wavelet family of Daubechies might be a good choice. These functions offer the favourable property of forming an orthonormal basis with a tunable number of vanishing moments. Furthermore, their intrinsic principle of multiresolution allows increasing the precision of the bias representation at specific points of interest.

We have implemented Daubechies wavelets into the VES code and have tested their performance in various systems. As a direct comparison of the different basis sets is difficult, we have developed a new measure of the error of free energy calculations. The Daubechies wavelets are observed to perform better than both Chebyshev/Legendre polynomials and Gaussian basis functions, resulting in faster convergence and yielding more accurate free energy surfaces without increases in computational cost.

DY 36.4 Wed 16:00 H20

Representing molecules and materials for accurate interpolation of quantum-mechanical calculations — •Marcel Langer, Alex Goessmann, and Matthias Rupp — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The search for novel materials, the exploration of phase diagrams and other high-throughput applications require numerical simulations of molecules and materials from first principles, but are limited by their high computational cost. By interpolating between reference calculations, machine learning can act as a fast accurate surrogate for these calculations, greatly increasing the number of accessible systems. [1] This requires a *representation* of molecules and materials suitable for interpolation. We show how the state-of-the-art representations can be understood in a unified framework [2] based on local descriptions of atomic environments via k-body functions, group averaging and tensor products, and discuss implications. We benchmark predictive accuracy of selected representations by carefully controlling for all other factors, including data distribution, regression method and optimization of free parameters. For the latter, we employ a consistent and fully automatic procedure to optimize both numerical and categorical free parameters, such as the choice of k-body functions, using sequential model-based optimization with tree-structured Parzen estimators. [3]

References: [1] a) Rupp et al, Phys Rev Lett **108**, 058301, 2012. b) Rupp, Int J Quant Chem **115**, 1058, 2015. [2] Willatt et al, Phys Chem Chem Phys, accepted, 2018. [3] a) Bergstra et al, NIPS **24**, 2546, 2011; b) Bergstra etal, ICML **30**, I-115, 2013.

DY 36.5 Wed 16:15 H20

Machine Learning of Free Energies — •Clemens Rauer and Tristan Bereau — Max Planck Institute for Polymer Science, Ackermannweg 10, 55128 Mainz, Germany

Free energies are important molecular properties which can provide an insight into the thermodynamic state of the respective system. Accurate calculations of free energies are an important tool for many biophysical applications, ranging from protein-ligand binding[1] to the insertion of small molecules into a lipid[2]. However, computationally expensive high level simulations are necessary in order to obtain accurate free energy estimates, and therefore, only a small subset of chemical space can be accurately covered. We overcome this problem by building a Δ-machine learning[3] model. Using this approach we can use a "cheap" low level method to predict free energies and learn the correction to a higher level method or experimental value. Then, we can predict high level free energies for significantly larger compound sets than was used in the training of the model. We show that by using only limited high level data, highly accurate free energies can be calculated using this method. As a first system we apply this approach to the prediction of hydration free energies.

[1] Mobley, D.L. & Gilson, M.K. *Annu. Rev. Biophys.* **2017**, 46:531-58

[2] Menichetti, R. et al. *J. Chem. Phys.* **2017**, 147, 125101

[3] Ramakrishnan et al. *J. Chem. Theory Comput.* **2015**, 11, 2087-2096

DY 36.6 Wed 16:30 H20

Deep Learning for Multiscale Simulations of Soft Matter Systems — •Marc Stieffenhofer[1], Tristan Bereau[1], and Michael Wand[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz — [2]Institute of Computer Science, Johannes Gutenberg University Mainz

The great success of Deep Neural Networks (DNNs) is based on their ability to learn and extract descriptive features directly from training data and to build a hierarchical, abstract representation of the input that takes multiple length scales into account. Such multiscale representations can also be found in soft matter systems where many physical phenomena and properties are governed by a large range of different length- and timescales.

In this work, we explore links between multiscale representations of DNNs and multiscale simulations of soft matter systems. The main focus is to investigate if DNNs can be used to link distribution functions generated at different resolutions. We have applied DNNs to the backmapping of coarse-grained molecular configurations to higher-resolution representations. This requires to reproduce the fine-grained statistics that match the coarse-grained representation.

Our model relies on 3D convolutional neural networks that are trained to generate molecular equilibrium structures. The training of the model is based on the generative adversarial approach and results are discussed for a system of octane molecules.

DY 36.7 Wed 16:45 H20

Unsupervised machine learning of chemical compound space for hierarchical screening and coarse-graining applications — •Kiran Kanekal, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Recently, the number and type of chemical fingerprints used for super-

vised learning of molecular properties has increased significantly, as the importance of properly encoding the 3D structure of a molecule to greatly increase accuracy has been recognized. Some of the most successful of these fingerprints encode a great deal of physical information, including coefficients for potential energy functions commonly used in classical atomistic molecular dynamics simulations [1]. In this work, we incorporate these fingerprints into an unsupervised machine learning (clustering) scheme to define subspaces in the chemical compound space, for which we use the Generated DataBase [2] (GDB) as a proxy. We show that the use of different molecular fingerprints leads to significant differences in the clustering observed, as each fingerprint will highlight specific molecular properties. Therefore, unsupervised learning, when coupled with these fingerprints, naturally enables hierarchical screening approaches for materials design. Furthermore, the presence of strong correlations between clusters identified using different fingerprints implies that a lowering of resolution (i.e. coarse-graining) is viable for that specific region of chemical compound space.

1. B. Huang and O. A. von Lilienfeld, J. Chem. Phys. 2016, 145, 161102. 2. T. Fink and Jean-Louis Reymond, J. Chem. Inf. Model. 2007, 47, 342.

15 min. break

DY 36.8 Wed 17:15 H20

Understanding three-body contributions to coarse-grained force fields — •Christoph Scherer, Rene Scheid, Tristan Bereau, and Denis Andrienko — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Coarse-graining (CG) is a systematic reduction of the number of degrees of freedom (DOF) used to describe a system of interest. CG can be thought of as a projection on the CG DOF and is therefore dependent on the number and type of CG basis functions. We present an extension of the two-body basis set with three-body basis functions [1]. The CG scheme is implemented in the VOTCA-CSG toolkit [2]. We show that naive extensions of the CG force field can result in substantial changes of the two-body interactions making them much more attractive. This is related to the three-body basis functions of the Stillinger-Weber type having a significant two-body component. This interference can be alleviated by CG the two-and three-body contributions separately. Furthermore, we employ Kernel-based Machine learning (ML) [3] overcoming the restrictions of a fixed basis set. The approach is illustrated on liquid water where three-body interactions are essential to reproduce the structural properties, and liquid methanol where two-body interactions are sufficient to reproduce the main features of the atomistic system. [1] Scherer, Andrienko, PCCP, 20, 22387 (2018); [2] Rühle, Junghans, Lukyanov, Kremer, Andrienko, JCTC, 5, 3211 (2009); [3] Glielmo, Sollich, De Vita, PRB, 95, 214302 (2017)

DY 36.9 Wed 17:30 H20

Reweighting Dynamics of Nonequilibrium Steady States — •Marius Bause, Timon Wittenstein, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

Markov State Models(MSM) are a discrete representation of the kinetics of a given system constructed by coarse-graining microtrajectories. While frequently applied to equilibrium systems, a protocol for non-equilibrium steady state systems (NESS) has not been developed due to loss of dynamic properties like detailed balance. We propose to apply the principle of Maximum Caliber by Jayne's, postulating that the distribution of paths is given by the maximal path entropy. The markovian assumption alleviates the combinatorial explosion of microtrajetories. The entropy production between states is chosen for a physical constraint and defines the NESS ensemble. By choosing a reference system for a prior, reweighting between ensembles becomes possible. The entropy productions become the defining elements of the ensemble. The method is tested on a minimal model under non-conservative forces.

DY 36.10 Wed 17:45 H20

Free Energy Landscape of Phase Transitions Investigated by Enhanced Sampling over Degenerate Collective Variables — •Bin Song, Kurt Kremer, and Omar Valsson — Max Planck Institute for Polymer Research, Mainz, Germany

Phase transition events such as nucleation of atomic or molecular crystals, self-assembly of micelles etc. have been intriguing scientists not only for their underlying physical principles, but also for their potential applications. Molecular dynamic simulations are increasingly called upon to either provide the detailed mechanistic insights and to prognosticate such events that may be too expensive or slow to examine with experiments. As potential energy surface of such events are often complex and difficult to sample, free energy surface (FES) are preferred. However, FES presents its own challenge to sample when the height of barriers are higher than or comparable to the thermal energy. Enhanced sampling methods biasing on properly chosen collective variables (CVs) can help overcome these barriers. Sometimes globally defined CVs are not sufficient, and more than a few of locally defined ones are needed. The increased dimensionality of the bias potential could be another source of frustration for achieving properly sampled FES, which we would like to alleviate with our new development of Variational Enhanced Sampling (VES) in cases where the local CVs are permutationally invariant. We demonstrate the capability of the new development by sampling the phase transitions in systems of increased complexity, including Lennard-Jones clusters and liquid-solid transition in materials.

DY 36.11 Wed 18:00 H20

Efficient Equilibration of Hard Particles with Collective Moves – A Comparison of Computational Methods — •Marco Klement and Michael Engel — Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen, Germany

Particle simulations are an important method to study the phase behavior of fluids and solids. A common task is structure prediction via thermal equilibration. Examples are crystallization or melting and the aging of glasses. Near the liquid-solid phase transition of hard spheres event driven molecular dynamics is known as most efficient. Monte Carlo simulations are boosted by event-chain in the same region. It is neither clear how equilibration does benefit from Newtonian motion nor how the efficiency of an algorithm should be quantified; and several ways are in use. Here we present further improvement of event-chain Monte Carlo by bringing the chain closer to natural movement with particle reflection events and quantify the improvement using different approaches from literature.

DY 36.12 Wed 18:15 H20

The temperature dependence of the mechanical unfolding of a supramolecular complex studied by molecular simulations — Takashi Kato, Ken Schäfer, Stefan Jaschonek, and •Gregor Diezemann — Institu für Physikalische Chemie, Universität Mainz

The conformational dynamics of supramolecular complexes can be studied on a single molecule level using the techniques of dynamic force spectroscopy and important kinetic information can be extracted. Using models for the free energy landscape of the system as a function of the molecular extension it is possible to obtain parameters like the bare unfolding rate, the activation free energy in the force-free case and also the distance between the folded configuration and the transition state. In the present work we performed molecular simulations of the mechanical unfolding of a model molecular complex, a pair of interlocked calixarene catenanes. From rupture force distributions the kinetic rates for the opening transition were extacted for varying parameters of the pulling device. In order to be able to perform a model-free analysis we performed simulations over a broad range of temperatures and found Arrhenius behavior for the kinetic rates. This allows to determine the activation free energy and the bare rate independently as a function of the force without using specific models for the shape of the energy landscape. We discuss our findings in light of the models that are usually used in the analysis of force dependent kinetic rates obtained from experimental or simulation data.

DY 36.13 Wed 18:30 H20

An efficient anharmonic free energy method applied to vacancies in ZrC — •Thomas Mellan[1], Andrew Duff[2], Blazej Grabowski[3], and Michael Finnis[1] — [1]Imperial College, London, UK — [2]Hartree Centre, Daresbury, UK — [3]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

We have developed a thermodynamic integration approach to calculate the anharmonic contribution to the volume and temperature dependent free energy of a crystal. The method provides an effective balance between accuracy and computational efficiency, giving a factor of 15 speed-up on comparable free energy approaches with average errors less than 1 meV/atom. The method is demonstrated with new predictions on the thermodynamics of substoichiometric ZrC, including vacancy concentration and heat capacity.

DY 37: Quantum Chaos

Time: Wednesday 15:30–17:00 Location: H6

DY 37.1 Wed 15:30 H6

Resonance eigenfunctions in systems with partial escape — •Konstantin Clauss[1], Eduardo Altmann[2], Arnd Bäcker[1,3], and Roland Ketzmerick[1,3] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]School of Mathematics and Statistics, University of Sydney — [3]MPI für Physik komplexer Systeme, Dresden

The phase-space distribution of chaotic resonance eigenfunctions corresponds to conditionally invariant measures of the classical system. This is well-understood if particles completely leave the system from a leaky phase-space region [1]. However, in many situations there occurs a partial escape of intensity, e.g., in optical microcavities. For such systems a similar understanding of resonance eigenfunctions is still missing and a completely new approach is required. For this we (i) find conditionally invariant measures for a given decay rate γ, and (ii) define a meaningful quantitative distance measure between phase-space densities to evaluate quantum-classical correspondence. We apply these methods to investigate the semiclassical limit and the limit of full escape.

[1] K. Clauß, M. J. Körber, A. Bäcker, and R. Ketzmerick, Phys. Rev. Lett. **121** (2018), 074101.

DY 37.2 Wed 15:45 H6

Towards universal Hong-Ou-Mandel correlations in topological insulators — •Andreas Bereczuk, Juan Diego Urbina, Cosimo Gorini, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

The indistinguishable-distinguishable transition for the transmission probability for two fermions propagating through a quantum point contact is a known manifestation of the celebrated Hong-Ou-Mandel (HOM) effect [1] in electron quantum optics [2]. As shown in [3], universal HOM correlations are expected by substituting the quantum point contact by a chaotic cavity in a mesoscopic regime [3] where universal correlations of the scattering matrix entries at different energies predicted by Random Matrix Theory (RMT) [4] and semiclassical analysis enter. Here we present an analytical and numerical study of these correlations and propose a HOM setup with cavities as complex beam splitters and edge states instead of waveguides to observe universal HOM correlations in a topological insulators (TI). In this new setup where both TIs and normal metal scattering take place, the issue of the appropriate symmetry of the universality class requires further analysis.

[1] C. K. Hong, Z. Y. Ou and L. Mandel, Phys. Rev. Lett. 59, 2044 (1987)
[2] E. Bocquillon et al., Annalen der Physik 526, 1 (2014)
[3] J. D. Urbina et al., Phys. Rev. Lett. 116, 100401 (2016)
[4] M. Novaes, J. Math. Phys. 57, 122105 (2016)

DY 37.3 Wed 16:00 H6

Transport timescales in mixed phase space systems — •George Datseris[1,2], Lukas Hupe[1,2], Theo Geisel[1,2], and Ragnar Fleischmann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization — [2]Faculty of Physics, Georg-August-Universität Göttingen

In Hamiltonian systems with mixed phase space, nonlinear resonances form islands of regular motion in a chaotic sea of irregular motion. It is a well known that chaotic trajectories can get trapped near nonlinear resonances leading to long time tails in the correlation decay. We recently found, however, that due to the link between transit times and phase space volume ratios (as manifested by Kac's lemma), nonlinear resonances may influence correlation decays on fast time scales as well, simply by the phase space volume they occupy. This can explain puzzling experimental observations in magneto-transport in electronic nanodevices.

We extend on this finding studying billiards models with mixed phase space, like the mushroom billiard, and explore the relation between the resonance phase space fractions and the Lyapunov exponent.

DY 37.4 Wed 16:15 H6

Analytical Fresnel laws at convex and concave non-planar interfaces from a transfer matrix approach — •Sebastian Luhn and Martina Hentschel — Institute for Physics, Group for Theoretical Physics II / Computational Physics, Technische Universität Ilmenau Weimarer Str. 25, 98693 Ilmenau, Germany

Fresnel laws, the quantitative information of the amount of light reflected from a plane wave in dependence on its angle of incidence, are at the core of ray optics at planar interfaces. However, these formulae do not hold at curved interfaces and deviations are appreciable when wavelength and radius of curvature are of similar order. This is of particular importance for optical microcavities that play an important role in many modern research fields. Their convexely curved interfaces modify Fresnel's law in a characteristic manner. Most notably, the onset of total internal reflection is shifted to angles larger than critical incidence. Here, we fill the missing bit and derive exact Fresnel laws for concavely curved refractive index boundaries, enabling the exact description of light in complex mesoscopic optical structures that will be important in future nano- and microphotonic applications.

DY 37.5 Wed 16:30 H6

Resonance–Assisted Tunneling in Deformed Optical Microdisks with a Mixed Phase Space — •Felix Fritzsch[1], Roland Ketzmerick[1,2], and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

In optical microcavities dynamical tunneling leads to finite lifetimes of whispering gallery modes, which are classically confined by total internal reflection. The lifetimes of such modes may drastically decrease by resonance–assisted tunneling due to the presence of classical nonlinear resonances in the ray dynamics. We extend the description of resonance–assisted tunneling from near integrable systems to systems with a mixed phase space showing regular as well as chaotic dynamics. In particular, we present a qualitative semiclassical description based on ray dynamics. This provides an intuitive picture depending only on classical properties. For the case of a quadrupol cavity we combine these methods with a perturbative approach resulting in an accurate quantitative prediction of lifetimes and quality factors.

DY 37.6 Wed 16:45 H6

Motional narrowing in microwave graphs — •Tobias Hofmann[1], Aimaiti Rehemanjiang[1], Ulrich Kuhl[1,2], and Hans-Jürgen Stöckmann[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]InPhyNi, Université Côte d'Azur, 06100 Nice, France

Motional narrowing is a well-known phenomenon in nuclear magnetic resonance (NMR) spectroscopy and is caused by rapidly moving atoms in an inhomogeneous magnetic environment [1]. If there are just two sites involved, realized e. g. by a molecular flip between two geometries or configurational changes in a glassy network, an analytical solution is known [2]. Also in superconducting qubits with two stochastically fluctuating energies an analogue of the effect could be seen [3].

To simulate the effects of motional averaging and motional narrowing in microwave graphs stochastic switching has to be employed. This means to flip a resonance frequency of the graph between two values stochastically. The flip frequency is thereby comparable to or greater than the energy difference of the two resonance frequencies involved. By using a special diode circuit this frequency regime of typically some 10 MHz becomes accessible and the effects of motional averaging and motional narrowing can be observed in microwave graphs. The setup and experimental results will be presented.

[1] A. Abragam, Principles of Nuclear Magnetism, University Press Oxford 1961
[2] P. W. Anderson, J. Phys. Soc. Jpn. **9**, 316 (1954)
[3] J. Li et al., Nat. Comm. **4**, 1420 (2013)

DY 38: Microswimmers (joint session DY/CPP)

Time: Wednesday 15:30–18:00 Location: H19

DY 38.1 Wed 15:30 H19

Orientational ordering and collective motion in (semi-)dilute suspensions of active microswimmers — Christian Hoell, Giorgio Pessot, Hartmut Löwen, and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Polar orientational ordering in crowds of self-propelled particles is connected to the emergence of collective motion. We study orientational ordering in suspensions of active microswimmers. These objects propel by setting the surrounding fluid into motion. Since we focus on (semi-) dilute suspensions, such hydrodynamic effects dominate the swimmer interactions. For simplicity, we concentrate on planar arrangements of so-called pushers and pullers, which induce different flow fields.

In such a situation, our simulations indicated polar orientational ordering for puller microswimmers, in contrast to pushers [1]. Thus, we analyzed the behavior of binary pusher–puller mixtures. Interestingly, we found that smaller amounts of pusher microswimmers can show a larger degree of orientational order than surrounding puller microswimmers in an ordered suspension of mainly pullers [1]. Increasing the amount of pushers makes the orientational order break down.

To further quantify these phenomena, we performed a linear stability analysis of a corresponding dynamical density functional theory for pusher and puller suspensions [2]. Indeed, we found homogeneous polar orientational order to arise from a linear instability of disordered suspensions of strong pullers, in contrast to pushers.

[1] G. Pessot et al., *Mol. Phys.* **116**, 3401 (2018).
[2] C. Hoell et al., *J. Chem. Phys.* **149**, 144902 (2018).

DY 38.2 Wed 15:45 H19

Maximum in density heterogeneities of active swimmers — •Fabian Jan Schwarzendahl[1] and Marco G. Mazza[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]Interdisciplinary Centre for Mathematical Modelling and Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire LE11 3TU, United Kingdom

Suspensions of unicellular microswimmers such as flagellated bacteria or motile algae can exhibit spontaneous density heterogeneities at large enough concentrations. We introduce a novel model for biological microswimmers that creates the flow field of the corresponding microswimmers, and takes into account the shape anisotropy of the swimmer's body and stroke-averaged flagella. By employing multiparticle collision dynamics, we directly couple the swimmer's dynamics to the fluid's. We characterize the nonequilibrium phase diagram, as the filling fraction and Péclet number are varied, and find density heterogeneities in the distribution of both pullers and pushers, due to hydrodynamic instabilities. We find a maximum degree of clustering at intermediate filling fractions and at large Péclet numbers resulting from the competition of hydrodynamic and steric interactions between swimmers. We develop an analytical theory that supports these results. This maximum might represent an optimum for the microorganisms' colonization of their environment.

DY 38.3 Wed 16:00 H19

Stabilization of a square vortex lattice in microswimmer suspensions by periodic arrays of obstacles — •Henning Reinken[1], Sebastian Heidenreich[2], Igor S. Aranson[3], Markus Bär[2], and Sabine H.L. Klapp[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [3]Pennsylvania State University, University Park, PA 16802, USA

Bacterial suspensions, a paradigmatic example of an active fluid, are known to exhibit a state denoted as mesoscale turbulence which is characterized by chaotic dynamics of vortices of a characteristic size. In a recent experiment, these vortices have been stabilized into a square lattice with antiferromagnetic order by geometrically constraining the bacterial suspension using periodic arrays of obstacles with a spacing in the range of the unconstrained vortex size [1]. Interestingly, the vortices are consistently located in the gaps between the obstacles rather than forming around them [1]. We aim to reproduce the patterns observed in the experiment using a recently derived fourth-order field theory for a vectorial order parameter representing an effective microswimmer velocity [2]. In this continuum theoretical framework, we numerically explore different implementations of the constraints: Obstacles that favor negatively charged topological defects straightforwardly reproduce the observed vortex lattice configuration. For topologically neutral defects, higher order nonlinear effects are required to break the topological symmetry and stabilize a certain configuration.

[1] D. Nishiguchi et al., Nat Commun. **9**, 4486 (2018).
[2] H. Reinken et al., Phys. Rev. E **97**, 022613 (2018).

DY 38.4 Wed 16:15 H19

Complex dynamic response of magnetocapillary swimmers — •Alexander Sukhov[1], Sebastian Ziegler[2], Ana-Suncana Smith[2], and Jens Harting[1,3] — [1]Helmholtz Institute Erlangen-Nuernberg for Renewable Energy (IEK-11), Forschungszentrum Juelich GmbH, 90429 Nuernberg, Germany — [2]Institute for Theoretical Physics, Friedrich-Alexander University Erlangen-Nuernberg, 91054 Erlangen, Germany — [3]Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, NL-5600MB Eindhoven, The Netherlands

Using the lattice Boltzmann method and the Shan-Chen model for multiple fluid components we simulate an interface with several rigid magnetic particles floating on it. The stability of the system is reached when the attractive capillary forces resulting from the weights of the particles are balanced by the repulsive magnetic forces induced by an external static magnetic field applied perpendicularly to the interface. The particles can propel themself at the interface when a smaller oscillating magnetic field of the right frequency is applied in the plane of the interface. We aim at understanding the contributions of interparticle and hydrodynamic interactions as well as that of the interface to the dynamic response of the swimmer when simulating a single, two and three particles at the interface separately.

DY 38.5 Wed 16:30 H19

Microswimmers in an axisymmetric vortex flow: from Hamiltonian dynamics to clustering — •José-Agustín Arguedas-Leiva and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Microswimmers appear in a wide variety of settings, ranging from phytoplankton in the ocean to bacteria in laboratory flows, and are known to give rise to many physically interesting phenomena. One such phenomenon is the clustering of otherwise neutrally buoyant particles. Its occurrence, and in particular the importance of physical parameters such as particle shape and swimming velocity, are currently not fully understood.

Here, we study the the distribution and clustering of swimmers in a two-dimensional axisymmetric vortex flow. Due to its simplicity, this system allows for a number of insights: We find that spherical swimmers follow phase-space preserving Hamiltonian dynamics, excluding the possibility for clustering. Interestingly, changing the particles' shape breaks the Hamiltonian structure of the dynamics, and clustering can occur. Based on this observation we identify a single control parameter: an effective swimming velocity, which takes into account both the particles' shape and velocity. By characterizing the topology of the underlying phase space our results help to clarify the role of motility and shape-dependent hydrodynamic interactions.

15 min. break

DY 38.6 Wed 17:00 H19

Oscillatory dynamics of swimming E. coli bacteria in wall-bounded Poiseuille flow — •Andreas Zöttl[1,2], Arnold Mathijssen[1,3], Nuris Figueroa-Morales[2], Gaspard Junot[2], Éric Clément[2], and Anke Lindner[2] — [1]University of Oxford, UK — [2]ESPCI Paris, France — [3]Stanford University, USA

Swimming microorganisms respond to flows in highly diverse and complex environments, at scales ranging from open oceans to narrow capillaries. The combined effects of fluid flow and boundaries lead to preferred swimmer orientation breaking the up/down-stream and left/right symmetry. To date, this so-called bacterial surface rheotaxis has been quantified by measuring instantaneous orientation distributions or average transport velocities, but a complete picture is still missing.

We investigate the time-resolved orientation dynamics of E.coli bacteria, theoretically and experimentally, as a function of applied shear

close to walls. With increasing flow, we identify four regimes separated by critical shear rates: (I) circular swimming with a bias along the direction of vorticity; (II) upstream swimming without oscillations; (III) oscillatory motion, increasingly more to the left; (IV) coexistence of swimming to the left and to the right, with dynamical switching between these states. By modeling bacterial rheotaxis comprehensively - accounting for their chiral nature, hydrodynamic and steric interactions, elongation, fore-aft asymmetry and activity - we assess the relative importance of these contributions throughout a trajectory, and explain the full dynamics.

DY 38.7 Wed 17:15 H19

Polarization of Brownian swimmers with spatially heterogeneous activity — •Sven Auschra[1], Nicola Söker[2], Paul Cervenak[1], Viktor Holubec[1], Klaus Kroy[1], and Frank Cichos[2] — [1]Institute for Theoretical Physics, University of Leipzig, 04103 Leipzig, Germany — [2]Peter Debye Institute for Soft Matter Physics, University of Leipzig Leipzig, 04103 Leipzig, Germany

Janus particles fuelled by laser heating are paradigmatic autophoretic microswimmers. Their dynamics under constant driving has been well characterized [1-3]. We consider situations in which the particles' propulsion strength fluctuates in space and time, due to a variable fuel supply. Specifically, we analyze their spatial and orientational distribution experimentally, realizing prescribed spatial and temporal activity variations via the laser heating. We find depletion in regions of higher activity and polarization in activity gradients. Using Brownian dynamics simulations and a powerful numerical solver for Fokker-Planck equations [4], we can reproduce the experimental observations. A simple run-and-tumble process captures the observed features, qualitatively, and provides some analytical insights.

[1] A. Bregulla and F. Cichos: Faraday Discuss. 184, 381-391 (2015)
[2] H. Jiang, N. Yoshinaga, and M. Sano: PRL 105, 268302 (2010)
[3] A. Würger: Rep. Prog. Phys. 73, 126601 (2010)
[4] V. Holubec, K. Kroy and S. Steffenoni: arXiv:1804.01285v2 (2018).

DY 38.8 Wed 17:30 H19

Efficiency limits of the three-sphere swimmer in viscous fluids — •Babak Nasouri[1], Andrej Vilfan[1,2], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany — [2]J. Stefan Institute, Ljubljana, Slovenia — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom

We consider a swimmer consisting of a collinear assembly of three spheres connected by two slender rods. This swimmer, as first shown by Najafi and Golestanian (Phys. Rev. E 69, 062901 2004), can propel itself forward by varying the lengths of the rods in a way that is not invariant under time reversal. Although any non-reciprocal strokes of the arms can lead to a net displacement, the energetic efficiency of the swimmer is strongly dependent on the details and sequences of these strokes. We define the efficiency of the swimmer using Lighthill's criterion, i.e., the power that is needed to pull the swimmer by an external force at a certain speed, divided by the power needed for active swimming with the same average speed. Here, we determine numerically the optimal stroke sequences while limiting the maximum extension of the rods. Our calculation takes into account both far-field and near-field hydrodynamic interactions. We specifically show that the swimming efficiency initially rises by increasing the maximum allowable extension of the rods, and then converges to a maximum value.

DY 38.9 Wed 17:45 H19

Actuation of particles in modulated Poiseuille flow — •Winfried Schmidt[1,2], Matthias Laumann[1], Eva Kanso[2], and Walter Zimmermann[1] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, USA

What is the dynamical behavior of micro-particles in Poiseuille flow with oscillating flow direction at low Reynolds number? We investigate the overdamped motion of bead-spring models, e.g., capsules and red blood cells. We predict net motion of the particles, despite vanishing mean flow. This effect is generic as it does not depend on the model and is explained by a broken symmetry. The mean actuation velocity of passive particles is caused by their varying shape in both half periods. Since the net velocity depends also on the size and the elasticity of the particles, this novel actuation mechanism is appropriate for particle sorting. The system is also explored for active particles.

DY 39: Quantum matter: Chaos, correlation

Time: Wednesday 17:15–18:30 Location: H6

DY 39.1 Wed 17:15 H6

Quantum signatures of a classical dynamical transition — •Remy Dubertrand[1], Mathias Steinhuber[1], Juan-Diego Urbina[1], Denis Ullmo[2], Peter Schlagheck[3], Klaus Richter[1], and Steve Tomsovic[4] — [1]Institut für Theoretische Physik Universität Regensburg Universitätsstraße 31 D-93053 Regensburg — [2]LPTMS, CNRS, Univ. Paris-Sud, Universite Paris-Saclay, 91405 Orsay, France — [3]CESAM research unit, University of Liege, 4000 Liege, Belgium — [4]Department of Physics and Astronomy, Washington State University, Pullman, WA 99164-2814, USA

We consider the quantum dynamics of a coherent density wave under Bose-Hubbard model. It was recently shown [1] that the corresponding classical density undergoes a dynamical transition between an ergodic and a nonergodic regime. This is due to a dramatic change of the stability of the associated classical trajectories, when changing the ratio between hopping and onsite interaction energy. We claim in [2] that this dynamical transition can be very clearly seen through purely quantum observables. This provides with a generalisation of the seminal self-trapping transition [3] to higher dimension. A possible way to observe it in a cold-atom experiment is also discussed.

[1] S. Tomsovic, Phys. Rev. E 98, 023301 (2018)
[2] R. Dubertrand, M. Steinhuber, J.-D. Urbina, D. Ullmo, P. Schlagheck, K. Richter, S. Tomsovic, in preparation
[3] J. C. Eilbeck, P. S. Lombdahl, A. C. Scott, Physica D 16, 318 (1985)

DY 39.2 Wed 17:30 H6

Effect of hopping correlations on localization — Pavel Nosov[1,2,3], •Ivan Khaymovich[3], and Vladimir Kravtsov[4] — [1]Department of Physics, St. Petersburg State University, St. Petersburg 198504, Russia — [2]NRC Kurchatov Institute, Petersburg Nuclear Physics Institute, Gatchina 188300, Russia — [3]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187-Dresden, Germany — [4]Abdus Salam International Center for Theoretical Physics - Strada Costiera 11, 34151 Trieste, Italy

The standard picture of the 3d Anderson localization is known to be restored in low-dimensional systems by adding either the correlations in the diagonal disorder or long-range hopping terms.

Recently, the Anderson's picture has been argued by providing counterintuitive examples of long-ranged systems with almost all localized states even in a nominally ergodic regime. These "new" models demonstrate either critical or localized wavefunction behavior with a "mysterious" duality of decay rates [1]. These systems belong to a new universality class where the localization properties are governed by hopping correlations.

In my talk I provide general localization-delocalization principles [2] needed for such models to find a full phase diagram and uncover the role of correlations and the origin of the duality [1]. I present a new class of random Hamiltonians with translation-invariant hopping terms demonstrating the duality in the momentum and coordinate space.

[1] X. Deng et al., PRL 120, 110602 (2018). [2] P. A. Nosov, I. M. Khaymovich, and V. E. Kravtsov, arXiv:1810.01492 (2018).

DY 39.3 Wed 17:45 H6

Logarithmic spreading of out-of-time-ordered correlators without many-body localization — •Adam Smith[1], Johannes Knolle[1,2], Roderich Moessner[3], and Dmitry Kovrizhin[4,5] — [1]T.C.M. group, Cavendish Laboratory, Cambridge, UK — [2]Blackett Laboratory, Imperial College London, London, UK — [3]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [4]Rudolf Peierls Centre for Theoretical Physics, Oxford, UK — [5]NRC Kurchatov institute, Moscow, Russia

Out-of-time-ordered correlators (OTOCs) have received renewed attention in the studies of non-equilibrium quantum many-body dynamics. They describe information scrambling under unitary time evolution and provide a useful probe of the emergence of quantum chaos. Here we calculate OTOCs for a model of disorder-free localization whose exact mapping to free fermions allows us to study long-time behaviour in large systems. Remarkably, we observe logarithmic spreading of correlations, which is markedly different to that of both thermalizing and Anderson localized systems. While this behaviour is a signature of many-body localization, our findings are for an essentially non-interacting model. We provide an explanation for this unusual behaviour and suggest a novel Loschmidt echo protocol as a probe of correlation spreading.

DY 39.4 Wed 18:00 H6

Information dynamics in chaotic electron systems — •Markus Klug[1] and Sergey Syzranov[2] — [1]Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]University of California, Santa Cruz, USA

Chaotic systems are by definition exponentially sensitive to initial conditions. The chaotic dynamics of quantum systems are characterized by Lyapunov exponents λ_L, the rates of growth of the so-called out-of-time order correlators, quantities of the form $\langle[P(t), P(0)]^2\rangle \propto \exp(\lambda_L t)$, where P is an observable, e.g. the total momentum of the electrons in a quantum dot. In this work, we compute λ_L for electrons in the presence of neutral excitations, such as plasmons or phonons, in a weakly disordered metal. We demonstrate that the rate of exponential growth matches the rate of change of information associated with the uncertainty in the system's total momentum. Our work establishes for the first time explicit connection between quantum chaos characteristics and the rate of change of information stored in a system's observable and thus presents a way to measure λ_L in experiments.

DY 39.5 Wed 18:15 H6

Bloch-like oscillations in periodically driven Dirac systems — •Vanessa Junk[1], Phillipp Reck[2], Cosimo Gorini[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Germany — [2]CEA, Paris-Saclay, France

Since the discovery of Floquet topological insulators [1] the scientific interest in periodically driven systems has been growing rapidly. However, there are still a lot of open questions concerning the dynamics of particles in the Floquet quasi-band structure and analogies to undriven Bloch bands.

We show that Bloch-like oscillations can be observed in a continuous Dirac system when periodically opening a mass gap. By applying an additional static electric field, a particle is driven through the resulting Floquet quasi-band structure. As this band structure is oscillatory in k-space, the position- and velocity expectation value of the particle are oscillating as well and resemble those of conventional Bloch oscillations [2]. Additionally, the characteristic features of the Floquet quasi-bands are displayed in the movement of the particle. Hence, these Floquet-Bloch oscillations could also provide a way to directly measure the quasi-band structure. On top of that, we find features of Zitterbewegung in the particle velocity caused by the Dirac character of our system.

[1] N. H. Lindner, G. Refael, and V. Galitski, Nature Physics **7**, 13368 (2016)

[2] K. Leo, P. Haring Bolivar, F. Brüggemann, R. Schwedler, and K. Köhler, Solid State Comm. **84**, 943 (1992)

DY 40: Talk R. Metzler

Time: Thursday 9:30–10:00 Location: H3

Invited Talk DY 40.1 Thu 9:30 H3

Non-Brownian diffusion: from disorder to physical insights — •Ralf Metzler — Institute of Physics & Astronomy, University of Potsdam, 14476 Potsdam

More than a hundred years ago Einstein, Smoluchowski, and Langevin formulated the laws of diffusion, and Perrin presented his systematic experiments tracking single, microscopic diffusing particles. Following several technological revolutions such as superresolution microscopy, experimentalists now measure the passive and active motion of submicron tracers and single molecules in complex systems such as living biological cells at unprecedented precision. Quite typically the measured motion significantly deviates from the laws of normal Brownian motion. Instead, anomalous diffusion is observed, in the form of non-Gaussian, long-range correlated, non-ergodic, or ageing dynamics. Based on state-of-the-art data from single particle tracking experiments and in silico systems this talk will elucidate the precise features unveiled in the data and established new theoretical approaches needed to understand the physical mechanisms behind the measured dynamics.

DY 41: Modeling and Simulation of Soft Matter II (joint session CPP/DY)

Time: Thursday 9:30–12:00 Location: H13

Invited Talk DY 41.1 Thu 9:30 H13

Systematic Dynamic Coarse-Graining with Memory — Gerhard Jung, Martin Hanke, and •Friederike Schmid — Johannes Gutenberg Universität Mainz, Germany

In soft matter, systematic coarse-graining (CG) approaches often face the problem that the separation of time scales is incomplete, and memory effects become important. One challenge is to extract the CG dynamical equations, namely the memory kernel, from equilibrium all-atom simulations. Another challenge is to devise an algorithm that efficiently deals with pair-memory contributions to the dynamical equations. Such pair-memory interactions may become important, e.g., in dispersions of nanocolloids when the frequency dependence of hydrodynamic interactions cannot be neglected.

The talk will address these two problems. We propose a "generalized Langevin Dynamics" model, which has the form of a generalized Langevin equation with distance-dependent two-particle contributions to the self- and pair-memory kernels. A simulation algorithm is developed that scales linearly with the number of coarse-grained particles. Furthermore, we present a robust iterative method for the accurate reconstruction of memory kernels from dynamic correlation functions.

We apply the method to a suspension of nanocolloids with frequency-dependent hydrodynamic interactions. The GLD simulations perfectly reproduce the dynamics of the underlying fine-grained system and accelerate the simulation by a factor of roughly 10.000.

DY 41.2 Thu 10:00 H13

Accurate structure-based coarse-graining leads to consistent barrier-crossing dynamics — •Tristan Bereau and Joseph F. Rudzinski — MPI for Polymer Research, Mainz

Structure-based coarse-graining of molecular systems offers a systematic route to reproduce the many-body potential of mean force. Unfortunately, common strategies are inherently limited by the molecular-mechanics force field employed. Here we extend the concept of multi-surface dynamics, initially developed to describe electronic transitions in chemical reactions, to accurately sample the conformational ensemble of a classical system in equilibrium. In analogy to describing different electronic configurations, a surface-hopping scheme couples distinct conformational basins beyond the additivity of the Hamiltonian. The incorporation of more surfaces leads systematically toward improved cross-correlations. The resulting models naturally achieve consistent long-time dynamics for systems governed by barrier-crossing events. [Bereau and Rudzinski, arXiv:1808.05644]

DY 41.3 Thu 10:15 H13

Mapping multiple timescales in heterogeneous melts with

predictive and adaptive subdomains — •Horacio V Guzman[1] and Hideki Kobayashi[2] — [1]Max Planck Institute For Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Theory Research Interest Group, University of Cambridge Lensfield Road Cambridge

Heterogeneous molecular systems can be modeled by means of advanced simulations methods, as it is done with multiscale concurrent representations and non-equilibrium simulations. Interestingly, the heterogeneity of the mentioned systems has a huge potential to map and span time and length scales beyond fully atomistic simulations, since in most cases a subdomain of the simulation box can be tackled with slowly diffusive regime, while other remains in a faster diffusive regime. From this description, a crucial question arises on how to map those heterogeneous time scales without losing the theoretical speedup planned from the method development perspective. Here, we introduce the heterogeneous time-spatial domain decomposition approach which is a combination of an heterogeneity sensitive spatial domain decomposition with a time evolution average of particles' diffusion domainwise estimated. Within this approach, we present the theoretically modeled and results in scaling-laws for the force calculation time, while timewise the subdomains with different diffusivity are adapted by means of the number of neighboring shells to a unique frequency of neighbour list updates. We explore the new approach capabilities, by comparing it with the state-of-the-art spatial domain decomposition techniques.

DY 41.4 Thu 10:30 H13

Automated detection of many-particle solvation states for accurate characterizations of diffusion kinetics — •Joseph Rudzinski, Marc Radu, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Markov state models are powerful tools for reducing the complexity of molecular dynamics trajectories, but require configuration-space representations that accurately characterize the relevant dynamics. Well-established, low-dimensional order parameters for constructing this representation have led to widespread applications to study conformational dynamics of biomolecules. On the contrary, applications to characterize single-molecule diffusion have been scarce and typically employ system-specific, higher-dimensional order parameters to characterize local solvation states. In this work, we propose an automated method for generating a coarse configuration-space representation, using the coordination numbers about each particle. To overcome the noisy behavior of these low-dimensional observables, we treat the features as indicators of a latent Markov process. The resulting hidden Markov models filter the trajectories of each feature into the most likely latent solvation state at each time step. The filtered trajectories are then used to construct a configuration-space discretization, which accurately describes the diffusion kinetics. The method is validated on a standard model for glassy liquids, where particle jumps between local cages determine the diffusion properties. The resulting models provide quantitatively accurate characterizations of the diffusion constant and also reveal a mechanistic description of diffusive jumps.

DY 41.5 Thu 10:45 H13

Simulating liquid alkanes from first principles with machine learning potentials — •Max Veit — École Polytechnique Fédérale de Lausanne, 1015 Lausanne, CH — Department of Engineering, University of Cambridge, Cambridge CB2 1PZ, UK

The reliable prediction of the macroscopic properties of molecular liquids requires potential energy surface (PES) models that are not only accurate, but computationally efficient enough to handle large systems and reach long time scales typically inaccessible to explicit quantum-mechanical methods. This work introduces a new approach to the systematic approximation of the first-principles PES of a molecular liquid using the GAP machine learning method [A. Bartók, M. Payne, R. Kondor, and G. Csányi, Phys. Rev. Lett. 104, 136403 (2010)]. By applying machine learning to separately approximate each physical component of the interaction energy in a full many-body framework and with high and controllable accuracy, we can simulate the liquid accurately across a wide range of temperatures and pressures (with the inclusion of quantum nuclear effects) while gaining physical insight into the inner workings of the fluid. Following the recent success of this approach on predicting the equation of state of compressed fluid methane [M. Veit, S. K. Jain, S. Bonakala, I. Rudra, D. Hohl, and G. Csányi, arXiv:1810.10475], I will discuss how this approach can be extended to other molecular liquids with the help of emerging techniques in machine learning potential development, and how these ideas can be applied to other important molecular materials.

DY 41.6 Thu 11:00 H13

Effective interaction between fillers and their effect on phase separation of polymer blends. — •Alexander Chervanyov — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, DE

Effective interactions between fillers immersed in polymer blends are shown to arise from the interplay between the conventional compressibility mechanism and the mechanism relying on the polymer compositional variations in the vicinity of fillers. By developing and making use of the liquid state theory, we calculate the potentials of the effective interactions acting between fillers having different affinities for polymer species comprising the blend. Further, we study the effect of interacting fillers on phase separation in polymer blends. The calculated shift of the spinodal point and critical temperature are shown to significantly depend on the interactions between fillers and polymers.

Financial support of Deutsche Forschungsgemeinschaft (DFG) through Grant No. CH 845/2-1, is gratefully acknowledged.

15 min. break

DY 41.7 Thu 11:30 H13

Relative resolution: A multipole approximation at appropriate distances — •Aviel Chaimovich[1], Kurt Kremer[2], and Christine Peter[3] — [1]Max Planck Institute of Colloids and Interfaces, 14476 Potsdam — [2]Max Planck Institute for Polymer Research, 55128 Mainz — [3]University of Konstanz, 78464 Konstanz

Recently, we introduced Relative Resolution as a hybrid formalism for fluid mixtures [1]. The essence of this approach is that molecular resolution switches in terms or relative separation: While near neighbors are characterized by a detailed fine-grained model, far neighbors are characterized by a simplified coarse-grained model. In this presentation, we notably show the comprehensive mathematics of our multiscale algorithm: We cast our Hamiltonian in terms of a multipole approximation at appropriate distances, which allows us for an analytical parameterization between the fine-grained and coarse-grained models. We consequently test the ability of Relative Resolution in describing various nonpolar liquids, in turn, capturing correctly and efficiently the statics and dynamics of many structural correlations and thermal properties across state space. Furthermore, we show that our multiscale approach works best if we switch between the fine-grained and coarse-grained potentials between the primary and secondary coordination shells: At this location, all orientations become negligible in the Hamiltonian. We conclude by discussing how Relative Resolution is the inherent variant, for molecular simulations, of the famous "cell-multipole" approach.

[1] A. Chaimovich, C. Peter, and K. Kremer (JCP, 2015).

DY 41.8 Thu 11:45 H13

Cononsolvency of thermoresponsive polymers: theory and simulation — •Nico van der Vegt, Swaminath Bharadwaj, Cahit Dalgicdir, and Divya Nayar — Technische Universität Darmstadt, Germany

Cononsolvency of thermoresponsive polymers is an intriguing phenomenon whose molecular-scale mechanism remains elusive ever since it was first reported in the late 1980s. I will present theoretical results and computer simulations which provide a new angle on this question. Significantly, direct cosolvent binding to the polymer is shown to be an entropy-driven process, which leads to polymer dehydration resulting in coil-globule collapse and phase separation in poly(N-isopropyl acrylamide)/water/methanol solutions. Specific cosolvent interactions with the polymer play no role in this mechanism. Instead of that, cosolvent enrichment around hydrophobic groups frustrates hydration of the amide group and induces phase separation. Theoretical arguments and simulation results are furthermore presented which illustrate that direct cosolvent binding is not a necessary requirement for cononsolvency.

D. Nayar, N.F.A. van der Vegt, J. Phys. Chem. B 122, 3587-3595 (2018) N.F.A. van der Vegt, D. Nayar, J. Phys. Chem. B 121, 9986-9998 (2017) C. Dalgicdir, F. Rodriguez-Ropero, N.F.A. van der Vegt, J. Phys. Chem. B 121, 7741-7748 (2017)

DY 42: Focus: Many-Body Quantum Chaos

The inter-relation between the complex time evolution of interacting many-body quantum systems and the corresponding often classically chaotic, high-dimensional dynamics of their classical counterparts has received increasing interest in various fields in the recent past, ranging from quantum statistical mechanics and quantum chaos via atomic and condensed quantum matter to high energy physics. This Focus Session will comprise recent developments and different perspectives in this emerging research area.

Andreas Buchleitner, Thomas Guhr, Klaus Richter

Time: Thursday 9:30–13:00 Location: H20

Invited Talk DY 42.1 Thu 9:30 H20

Quantum dynamics in strongly correlated one-dimensional Bose gases — •Hanns-Christoph Nägerl — Institut für Experimentalphysik, Universität Innsbruck, A-6020 Innsbruck

We have experimentally studied the dynamics of strongly correlated bosonic quantum gases confined to a one-dimensional (1D) geometry, with focus on two different model systems. We have realized 1D Hubbard chains and have studied correlated tunneling dynamics when the many-body system is suddenly exposed to a strong force. This has allowed us to observe how interacting quantum particles prepared in the Mott-insulating phase tunnel through multiple wells of the lattice potential in a situation where a single particle cannot move at all [1]. Our studies further comprise the coherent evolution of an interacting superfluid that exhibits Bloch-oscillations modulated by interaction-driven collapse and revival dynamics [2]. In a certain parameter regime, the transition to quantum chaotic behavior can be observed. The second system of interest constitutes a uniform Luttinger liquid with highly tunable interactions. We have probed the dynamics of a strongly coupled impurity atom injected into the liquid and have found an intriguing Bloch-oscillation type motion induced in the correlated system in the absence of an imprinted lattice structure [3].

[1] F. Meinert et al., Science 344, 1259 (2014). [2] F. Meinert et al., Phys. Rev. Lett. 112, 193003 (2014). [3] F. Meinert et al., Science 356, 945 (2017).

Invited Talk DY 42.2 Thu 10:00 H20

Extreme Decoherence and Quantum Chaos — Zhenyu Xu[1,2], Aurélia Chenu[3,4], Luis Pedro García-Pintos[2], Javier Molina-Vilaplana[5], and •Adolfo Del Campo[3,4] — [1]School of Physical Science and Technology, Soochow University, Suzhou 215006, China — [2]Department of Physics, University of Massachusetts, Boston, MA 02125, USA — [3]Donostia International Physics Center, E-20018 San Sebastián, Spain — [4]IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao, Spain — [5]Technical University of Cartagena, UPCT, 30202, Cartagena, Spain

We study the ultimate limits to the decoherence rate associated with dephasing processes. Fluctuating chaotic quantum systems are shown to exhibit extreme decoherence, with a rate that scales exponentially with the particle number, thus exceeding the polynomial dependence of systems with fluctuating k-body interactions. Our findings suggest the use of quantum chaotic systems as a natural test-bed for spontaneous wave function collapse models. We further discuss the implications on the decoherence of AdS/CFT black holes resulting from the unitarity loss associated with energy dephasing [1]. To conclude, we shall elucidate the connection between quantum work statistics, Loschmidt echo dynamics and information scrambling in chaotic quantum systems [2].

Bibliography:

[1] Zhenyu Xu, Luis Pedro García-Pintos, Aurélia Chenu, Adolfo del Campo, Phys. Rev. Lett. 122, 014103 (2019).

[2] Aurélia Chenu, Javier Molina-Vilaplana, Adolfo del Campo, arXiv:1804.09188 (2018).

DY 42.3 Thu 10:30 H20

Many-Body Quantum Interference and the Saturation of Out-of-Time-Order Correlators — •Josef Rammensee, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

Out-of-time-ordered correlators $\langle[\hat{V},\hat{W}(t)]^\dagger[\hat{V},\hat{W}(t)]\rangle$ have been found to be highly suitable tools to identify the onset of chaos in many-body quantum systems[1]. Contrary to already known indicators, the unusual time ordering of the operators is able to directly capture the local hyperbolic nature of the classical counterpart as one expects an exponential increase at short times with a rate related to classical Lyapunov exponents. Numerical studies in chaotic systems[2] further indicate a saturation after the time scale for the classical-to-quantum-crossover, known as Ehrenfest or scrambling time. We provide insight into the physical origin of the exponential growth and the saturation by using semiclassical methods based on the Van-Vleck-propagator for single- and many-body systems[3]. We show[4] that the notion of interfering classical trajectories is well suited to provide a quantitative picture and we explicitly discuss the emergence of the Lyapunov exponent, and the relevant time scales.

[1] Maldacena, Shenker, and Stanford, JHEP 2016:106 (2016)
[2] Rozenbaum, Ganeshan, Galitski, PRL **118**, 086801 (2017)
[3] Engl, Dujardin, Argüelles, Schlagheck, Richter, J. D. Urbina, PRL **112**, 140403 (2014)
[4] Rammensee, Urbina, Richter, PRL **121**, 124101 (2018)

DY 42.4 Thu 10:45 H20

Many-body Multifractality in Fock space for Interacting Bosons — Jakob Lindinger, Andreas Buchleitner, and •Alberto Rodríguez — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany

We analyse the many-body multifractality of the Bose-Hubbard Hamiltonian's eigenstates in Fock space, for arbitrary values of the interparticle interaction. For the ground state, generalized fractal dimensions unambiguously signal, even for small system sizes, the emergence of a Mott insulator. We show that the scaling of the derivative of any generalised fractal dimension with respect to the interaction strength encodes the critical point of the superfluid to Mott insulator transition, and we establish that the transition can be quantitatively characterized by one single wavefunction amplitude from the exponentially large Fock space [1]. Furthermore, multifractality of the excited eigenstates is investigated and the possible existence of localization in Fock space is thoroughly studied.

[1] J. Lindinger, A. Buchleitner, A. Rodríguez, arXiv:1810.06369

DY 42.5 Thu 11:00 H20

Particle-Evolution Operator in Spin Chains with Spin 1/2 — •Daniel Waltner[1], Maram Akila[1], Boris Gutkin[2], and Thomas Guhr[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg — [2]Department of Applied Mathematics, Holon Institute of Technology, 58102 Holon, Israel

A major difficulty in describing interacting many-body systems is the enormous size of the Hilbert space: usually it grows exponentially with the number of particles. In order to overcome this difficulty I will introduce in my talk an evolution in *particle* instead of *time* direction. The dimension of the particle-evolution operator grows exponentially with *time* making it especially appropriate to describe the short-time dynamics of the system. I will consider a chain of spin 1/2 particles with nearest neighbor Ising interaction and on-site magnetic field. I will discuss the properties of this particle-evolution operator and the spectral form factor that is used to analyze the correlation properties of the eigenvalues of the underlying quantum system.

DY 42.6 Thu 11:15 H20

Scrambling and quantum butterfly effect in critical systems: instability vs. chaos — •Benjamin Geiger, Quirin Hummel, Juan Diego Urbina, and Klaus Richter — Universität Regensburg

The investigation of scrambling of information in interacting quantum systems has recently attracted a lot of attention as a manifestation of many-body quantum chaos. However, it has been demonstrated that

certain integrable systems that are subject to quantum phase transitions allow for fast information scrambling if they are tuned close to their critical point [1]. To investigate the origin of this quasi-chaotic behavior we studied a momentum-truncated model of an attractive one-dimensional Bose gas using established semiclassical methods. We find that the quantum critical behavior has its origin in the appearance of a separatrix in the classcial phase space that renders the classical dynamics locally unstable. This leads to quasichaotic features the underlying quantum system, i.e., a fast growth of multiparticle entanglement and exponential growth of certain out-of-time ordered correlators, in counter-intuitive coexistence with asymptotic periodicity of the respective quantities.

[1] Dvali et al. Phys. Rev. D **88**, 124041 (2013)

15min. break

DY 42.7 Thu 11:45 H20

Hamiltonian Matrix Elements of the Stadium Billiard — •Jaewon Kim[1,2], Martina Hentschel[1], and Chil-Min Kim[2] — [1]Institute for Physics, Theoretical Physics II/Computational Physics Group, Technische Universität Ilmenau, Weimarer Straße 25, 98693 Ilmenau, Germany — [2]Department of Emerging Materials Science, DGIST,

We study the Hamiltonian matrix elements of the stadium billiard using a method of coordinate transformation. We apply special coordinate transformation which gives a remarkable simple form of the Hamiltonian. The spectrum from the Hamiltonian matrix shows good agreement with the fully numerical result from the BEM. Also, the simple Hamiltonian implies theoretically interesting points. With proper extensions, the Hamiltonian matrix elements calculated from the first principle provide a new way of studying quantum billiard system, especially for chirality and exceptional points.

DY 42.8 Thu 12:00 H20

Spin Diffusion Triggered by the Onset of Quantum Chaos in Surrounding Spin Bath — •Walter Hahn and Viatcheslav Dobrovitski — QuTech, Delft University of Technology, The Netherlands

We theoretically investigate spin diffusion driven by a finite quantum spin bath for a realistic solid-state NMR experiment. The total system consists of a disordered spin system which is acted upon by a surrounding spin bath via dipolar coupling. The bath consists of strongly coupled groups which are weakly interacting among each other. By means of numerical simulations, we show that the common expectation that only bath spins contributing to local noise are relevant is violated. In fact, nearby and farther bath spins can be equally important. While nearby bath spins govern the driving noise, the farther bath spins provide ergodicity within the bath by breaking integrability and, thereby, drastically change the spin diffusion dynamics. Specifically, we consider polycrystalline L-alanine in a realistic solid-state NMR setting including all experimental details. Spin diffusion occurs within the disordered carbon-spin subsystem and the spin bath is given by the surrounding proton spins. To modify the properties of the bath, we also consider deuterated alanine with protons replaced by deuterons having a smaller nuclear magnetic dipole moment. For deuterated L-alanine, we show that the driving noise is insufficient to allow for spin diffusion. Instead, spin diffusion is governed by the spin-lattice relaxation of deuteron spins on much larger time scales.

DY 42.9 Thu 12:15 H20

Spectral structure of systems of partially distinguishable bosons — •Gabriel Dufour[1,2], Tobias Brünner[1], Alberto Rodríguez[1], and Andreas Buchleitner[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg — [2]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität Freiburg

We consider bosons whose single-particle "external" Hilbert space is augmented by an "internal" degree of freedom, which allows to tune their mutual distinguishability and switch many-particle interference effects on or off. The resulting many-particle Hilbert space decomposes as a direct sum of irreducible representations of the external unitary group. Hamiltonians which do not act on the internal degree of freedom can be accordingly block-diagonalised. We discuss the consequences for the spectra of non-interacting and interacting systems as the distinguishability of the particles is varied [1]. In particular, we show how the transition between regular and chaotic spectra is affected by the distinguishability of the bosons.

[1] T. Brünner, Signatures of partial distinguishability in the dynamics of interacting bosons, PhD thesis, Albert-Ludwigs-Universität Freiburg (2018)

Invited Talk DY 42.10 Thu 12:30 H20

Semiclassical approach in Bose-Hubbard models: from universal spectral statistics to far-out-of-equilibrium dynamics — •Remy Dubertrand — Institut für Theoretische Physik Universität Regensburg Universitätsstraße 31 D-93053 Regensburg

Semiclassical techniques from quantum chaos have been recently generalised to describe many-body interacting bosonic systems written as second quantised models. To understand the emergence of new phenomena due to many-body coherent effects I will first motivate how to build a quantum/classical correspondence, and how to follow the semiclassical program from there. This will be used first to state when universal spectral and eigenstate statistics appear in Bose-Hubbard models. This involves more precisely the connection with Random Matrix Theory and Berry's ansatz of random superpositions of Fock states respectively. A second, more recent application aims at studying the far-out-of-equilibrium dynamics of interacting cold atom systems, where the semiclassical perspective enables one to identify a dramatic change of the dynamical regime using both classical probes (well beyond the truncated Wigner range of validity) and quantum signatures.

DY 43: Anomalous diffusion / Brownian motion

Time: Thursday 10:00–13:15 Location: H3

DY 43.1 Thu 10:00 H3

Fractional electron transfer kinetics and a quantum breaking of ergodicity — •Igor Goychuk — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany

The dissipative curve-crossing problem provides a paradigm for electron-transfer (ET) processes in condensed media. It is studied both analytically and numerically for subdiffusive or sub-Ohmic dynamics of the reaction coordinate in the contact approximation, both from the ensemble and single-trajectory perspectives [1]. Depending on the electron coupling strength, the transfer occurs either in non-adiabatic or in a solvent-controlled adiabatic regime. It is shown that the relaxation of electronic populations has universally a power law tail even in a deeply non-adiabatic regime. For a sufficiently strong tunnel coupling, it is described by a Mittag-Leffler function. The statistics of electron transitions is, however, very different from both the ensemble and single-trajectory perspective. For large sojourn times, it is featured by a stretched exponential Weibull distribution and not by a power law dependence. Moreover, a profound difference occurs for the distribution of residence times in the electronic states on the ensemble level and on the level of single trajectories. Ergodicity is broken dynamically even in a more spectacular way than in the memoryless case [2].

[1] I. Goychuk, arXiv:1811.03838 [cond-mat.stat-mech] (2018).
[2] I. Goychuk, Phys. Chem. Chem. Phys. **19**, 3056 (2017).

DY 43.2 Thu 10:15 H3

Dynamics of ellipsoidal particles in random light fields — Rene Hermann[1], Christoph Zunke[1], •Florian Platten[1], Arjun G. Yodh[2], and Stefan U. Egelhaaf[1] — [1]Heinrich Heine University Duesseldorf — [2]University of Pennsylvania, Philadelphia, USA

Ellipsoidal polystyrene particles are exposed to a random light field applying different laser power, and the particle motions are tracked by video microscopy. From the particle trajectories, mean-squared (angular) displacements are analyzed. Initial and long-time diffusion, as well as transient intermediate sub-diffusive behavior, are observed for the center-of-mass and angular displacements.

DY 43.3 Thu 10:30 H3

Ideal circle microswimmers in crowded media — •Oleksandr Chepizhko and Thomas Franosch — University of Innsbruck, Innsbruck, Austria

Microswimmers in nature move in crowded environments and their transport properties depend in a subtle way on the interaction with obstacles. Here, we study a model for a single ideal circle swimmer exploring a two-dimensional disordered array of impenetrable obstacles. The microswimmer moves on ideal circular orbits in the freely accessible space and follows the surface of an obstacle for a certain time upon collision. Depending on the obstacle density and the radius of the circular orbits, the microswimmer displays either long-range transport or is localized in a finite region. We show that there are transitions from two localized states to a diffusive state each driven by an underlying static percolation transition. We determine the non-equilibrium state diagram and calculate the mean-square displacements and diffusivities by computer simulations. Close to the transition lines transport becomes subdiffusive which is rationalized as a dynamic critical phenomenon. Additionally, we discuss the influence of inclusion of a stochastic noise term into the equation of orbital motion.

DY 43.4 Thu 10:45 H3

Anomalous transport in the soft Lorentz model of crowded media — •Charlotte Petersen and Thomas Franosch — Institute for Theoretical Physics, University of Innsbruck, Austria

Transport in heterogeneous crowded environments occurs in many situations, including inside of cells, in catalysts, and in porous rock during oil recovery. Both experimentally, and in simple models, the transport in complex crowded media can be subdiffusive. The origin of this anomalous diffusion has been explained theoretically for the paradigmatic Lorentz model. Here, a single particle moves with Newtonian dynamics through a random array of identical fixed obstacles. The moving particle has specular collisions with the obstacles. At the percolating density of the obstacles, the mean square displacement grows subdiffusively. We extend the Lorentz model towards realistic systems by relaxing the hard-exclusion interaction assumption, and find that they system exhibits a percolation transition dependent on the energy of the probe particle, and the dynamics remain anomalous at the percolation point.

DY 43.5 Thu 11:00 H3

First passage statistics for Brownian yet non-Gaussian diffusion. — •Vittoria Sposini[1,2], Aleksei V. Chechkin[1,3], and Ralf Metzler[1] — [1]Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany — [2]Basque Center for Applied Mathematics, 48009 Bilbao, Spain — [3]Akhiezer Institute for Theoretical Physics, 61108 Kharkov, Ukraine

A rapidly increasing number of systems is identified in which the stochastic motion of tracer particles follows the Brownian law $\langle \mathbf{r}^2(t)\rangle \simeq Dt$ yet the distribution of particle displacements is strongly non-Gaussian. A central approach to describe this effect is the diffusing diffusivity (DD) model in which the diffusion coefficient itself is a stochastic quantity, mimicking heterogeneities of the environment encountered by the tracer particle on its path. In this talk I will discuss how to quantify, in terms of analytical and numerical approaches, the first passage behaviour of the DD model. We observe significant modifications compared to Brownian-Gaussian diffusion, in particular that the DD model may have a more efficient first passage dynamics. Moreover we find a universal crossover point of the survival probability independent of the initial condition.

[1] Chechkin A V, Seno F, Metzler R & Sokolov I 2017 Brownian Yet Non-Gaussian Diffusion: From Superstatistics to Subordination of Diffusing Diffusivities *Phys. Rev. X* **7** 021002.

[2] Sposini V, Chechkin A V & Metzler R 2018 First passage statistics for diffusing diffusivity *arXiv:1809.09186 [cond-mat.stat-mech]*.

DY 43.6 Thu 11:15 H3

Bayesian statistics for models of diffusion: theory and applications — •Samudrajit Thapa[1], Michael A. Lomholt[2], Jens Krog[2], Andrey G. Cherstvy[1], and Ralf Metzler[1] — [1]Institute for Physics & Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany — [2]MEMPHYS, Department of Physics, Chemistry & Pharmacy, University of Southern Denmark, 5230 Odense M, Denmark

Particle diffusion in heterogeneous systems poses the following question: Can a single model describe the entire dynamics of a particle in complex biological, soft matter systems? Indeed, often several different physical mechanisms are at work and it is more insightful to rank them based on the likelihood of them explaining the dynamics. This talk will discuss—within the Bayesian framework—,(a) how maximum-likelihood model selection can be done by assigning probabilities to each feasible model and (b) how to estimate the parameters of each model. In particular, the implementation of this powerful statistical tool using the Nested Sampling algorithm to compare—at the single trajectory level-models of Brownian motion, viscoelastic anomalous diffusion and normal yet non-Gaussian diffusion will be discussed. Finally, the application of this method to experimental data of tracer diffusion in polymer-based hydrogels (Mucin) will be presented.

[1] S. Thapa, M. A. Lomholt, J. Krog, A. G. Cherstvy, & R. Metzler, *Bayesian analysis of single-particle tracking data using the nested-sampling algorithm: maximum-likelihood model selection applied to stochastic-diffusivity data*,Phys. Chem. Chem. Phys., **20** 29018 (2018).

15 min. break

DY 43.7 Thu 11:45 H3

Flat-to-curved transition during clathrin-mediated endocytosis — •Felix Frey[1], Delia Bucher[2], Kem A. Sochacki[3], Susann Kummer[2], Jan-Philip Bergeest[4], William J. Godinez[4], Hans-Georg Kräusslich[2], Karl Rohr[4], Justin W. Taraska[3], Steeve Boulant[2], and Ulrich S. Schwarz[1] — [1]ITP, Heidelberg University — [2]Department of Virology, University Hospital Heidelberg — [3]NHLBI, NIH, Bethesda, U.S.A. — [4]IPMB, Heidelberg University

Biological cells constantly transport material and information across their plasma membrane. The most important pathway for the uptake of nutrients and receptors is clathrin-mediated endocytosis (CME). Although CME has been studied for decades, the exact sequence of molecular and structural events remains elusive. Two basic models have been suggested for the way CME proceeds, namely the constant curvature and the constant area models [1]. Here, we combine correlative electron and light microscopy, super-resolution microscopy, single particle tracking and simple mathematical grow laws to estimate the temporal sequence of ultrastructural rearrangements of the clathrin coat. Our quantitative analysis shows that neither model is correct and that clathrin-coated structures initially grow flat but start to acquire curvature when on average 70% of the final clathrin content is reached [2].

[1] Haucke, Volker, and Michael M. Kozlov. "Membrane remodeling in clathrin-mediated endocytosis." J. Cell Sci. (2018), 131(17):jcs216812.
[2] Bucher, Delia, et al. "Clathrin-adaptor ratio and membrane tension regulate the flat-to-curved transition of the clathrin coat during endocytosis." Nat. Commun. (2018), 9(1):1109.

DY 43.8 Thu 12:00 H3

Long-time tails of correlation functions of Brownian particles — Suvendu Mandal[1], •Lukas Schrack[2], Hartmut Löwen[1], Matthias Sperl[3], and Thomas Franosch[2] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany — [2]Institut für Theoretische Physik, Leopold-Franzens-Universität, Technikerstraße 21A, 6020 Innsbruck, Austria — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, 51147 Köln, Germany

The dynamics of Brownian particles of a hard-sphere fluid can be described by generalized Langevin equations. Starting with the microscopic motion of the colloids we use the Zwanzig-Mori projection operator formalism to derive equations of motion for correlation functions. To close the equations, suitable mode-coupling approximations (slowing down of the dynamics due to the caging by neighboring particles) are used. Introducing a logarithmically spaced wavevector grid we investigate the long-wavelength behavior of the system. The velocity autocorrelation function of a tagged particle decays algebraically as $\propto t^{-5/2}$ rather than exponentially due to repeated interactions. Comparing the collective dynamics with the self-dynamics for different packing fractions near the glass transition we find that contrary to the self-dynamics the collective dynamics do not slow down.

DY 43.9 Thu 12:15 H3

Controlled dispersion in periodic microchannels and regular obstacle parks — •Matthieu Mangeat[1,2], Thomas Guérin[1], and David S. Dean[1] — [1]Univ. Bordeaux and CNRS, LOMA, Talence, France — [2]Universität des Saarlandes, Saarbrücken, Germany

The dispersion of Brownian particles in heterogeneous media is a widely studied problem which appears in many contexts (chemical reactions, biological systems, zeolites, porous media, pollutant spreading, ...). A cloud of particles disperses over time without reaching the Boltzmann equilibrium distribution and its spreading is then characterized by an effective long-time diffusivity D_e lower than the microscopic diffusivity. The analytical expression of D_e is given by an exact Kubo-type formula [Phys. Rev E **92**, 062103 (2015)] for periodic systems. The dispersion in periodic microchannels is controlled by the confinement geometry via an entropic trapping. Three different dispersion regimes are then identified for continuous and discontinuous channels [EPL **118**, 40004 (2017)]. The expression of D_e is thus well-described by the Fick-Jacobs' approximation, narrow escape problems or the diffusion problem in comb-like geometries in each regime. This analysis can be extended to the dispersion in regular obstacle parks. The presence of short-range attractive potential on the surface of obstacles enhance the dispersion of Brownian particles. The optimal value of D_e is then analytically characterized in the dilute limit of obstacles.

DY 43.10 Thu 12:30 H3

Orientational and directional locking of colloidal clusters driving across periodic surfaces — •Xin Cao[1], Emanuele Panizon[2], Andrea Vanossi[2,3], Nicola Manini[4], and Clemens Bechinger[1] — [1]Fachbereich Physik, University Konstanz, 78464 Konstanz, Germany — [2]International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy — [3]CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy — [4]Dipartimento di Fisica, Universita degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy

When isolated particles are driven over atomically corrugated crystalline surfaces, their trajectories do not necessarily follow the applied force but become locked to directions imposed by the substrate symmetry. Such directional locking is relevant for the manipulation and steering of nano-objects on surfaces. Contrary to previous studies which have been performed for single particles, here we study the motion of extended crystalline clusters composed of colloidal particles on a periodic surface. We observe that both their orientational and their center-of-mass motion become locked in the presence of a driving force. Contrary to single particles, the locking directions do not coincide with the substrate symmetry, but are determined by the geometrical moiré superstructure of the cluster-substrate contact. For certain incommensurabilities, competing locking directions exist and a cluster may spontaneously switch from one direction to another depending on its size. Our research provides insights to the transport of crystalline islands on top of crystalline surfaces.

DY 43.11 Thu 12:45 H3

The cage effect in systems of hard spheres — •Hans Joachim Schöpe[1] and William van Megen[2] — [1]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10,72076 Tübingen, Germany — [2]Department of Applied Physics, Royal Melbourne Institute of Technology, Melbourne, Victoria 3000, Australia

The cage effect is generally invoked when discussing the delay in the decay of time correlation functions of dense fluids. In an attempt to examine the role of caging more closely we consider the temporal evolution of the displacement distributions of Brownian particles. In an equilibrium fluid these distributions are necessarily biased by the presence of neighbouring particles. Accommodation of this bias by those neighbours conserves the displacement distribution locally and it presents a collective mechanism for exploring configuration space that is more efficient than the intrinsic Brownian motion. In contrast caging of some particles incurs a delayed, non-local collective transport process due to the fact that of the displacement distribution must be conserved globally. Both collective mechanisms incur delay or stretching of time correlation functions, in particular the particle number and flux densities [1]. We identify and distinguish these mechanisms in existing data from experiments [2,3] and computer simulations [4] on systems of particles with hard sphere interactions.

[1] J. Chem. Phys. 146, 104503 (2017) [2] Phys. Rev. Lett. 103 (25) (2009) [3] 4th International Symposium on Slow Dynamics in Complex Systems: Tohoku Univ, edited by M. Tokuyama and I. Oppenheim (2013), Vol. 1518, pp. 214-221 [4] Nature Comm. 5 (2014)

DY 43.12 Thu 13:00 H3

Memory-induced acceleration and slowdown of barrier crossing — •Julian Kappler[1,2], Jan O. Daldrop[1], Florian N. Brünig[1], Moritz D. Boehle[1], and Roland R. Netz[1] — [1]Freie Universität Berlin, 14195 Berlin, Germany — [2]Cambridge University, Cambridge CB3 0WA, United Kingdom

We study the mean first-passage time τ_{MFP} for the barrier crossing of a single massive particle with non-Markovian memory by Langevin simulations in one dimension. Compared to the Markovian case, we find barrier crossing to be accelerated for intermediate memory time, while for long memory time, barrier crossing is slowed down and τ_{MFP} increases with τ_Γ as a power law $\tau_{\mathrm{MFP}} \sim \tau_\Gamma^2$. A simple and globally accurate heuristic formula for τ_{MFP} in terms of all relevant time scales of the system is presented and used to establish a scaling diagram featuring the Markovian overdamped and the Markovian inertial regimes, as well as the non-Markovian intermediate memory time regime where barrier crossing is accelerated and the non-Markovian long memory time regime where barrier crossing is slowed down.

DY 44: Active Matter C (joint session DY/CPP)

Time: Thursday 10:00–12:45 Location: H19

DY 44.1 Thu 10:00 H19

Self-propelled Janus particles in evaporating droplets — Maziyar Jalaal[1,2], Borge Ten Hagen[1], Hai Le The[3], Christian Diddens[1], Detlef Lohse[1,2], and •Alvaro Marin[1] — [1]Physics of Fluids, University of Twente, The Netherlands — [2]Max-Planck Center for Complex Fluid Dynamics, University of Twente, The Netherlands — [3]BIOS-Lab on a Chip, University of Twente, The Netherlands

According the kids britannica encyclopedia: "Living things have the ability to move in some way without outside help.". Following this precise definition, artificial self-propelled particles are not alive, but they almost are since they move taking advantage of chemical/physical reactions or more complex interactions with their environment. Such active particles have been developed and thoroughly characterized in recent years *in vitro*: in either quiescent liquid media or stationary flow fields. However, in most situations *living things* encounter unsteady flows and interfaces of different types. To approach more realistic situations, we choose to study the dynamics of self-propelling Janus particles in evaporating droplets. Our system consists on polysterene-platinum Janus colloids immersed in a sessile droplet containing an hydrogen peroxide solution. The system is analyzed using three-dimensional particle tracking measurements and numerical simulations of the nontrivial fluid flow within the evaporating droplet. To our surprise, the dynamics of the active particles turns to be extremely rich due to several mechanisms as the proximity to interfaces, concentration gradients and evaporation-driven flows.

DY 44.2 Thu 10:15 H19

Tuning propulsion modes in active emulsions — •Corinna C. Maass, Babak Vajdi Hokmabad, and Kyle A. Baldwin — Max-Planck-Institut für Dynamik und Selbstorganisation

Single cell organisms show a variety of swimming behaviours: e.g. persistent, helical, run-and-tumble or switch-and-flick, all dependent on intricate biophysical machinery and serving various strategies of navigation, e.g. persistence against external flow, efficiency of gradient sensing or expanding their range of exploration. Their locomotion has to adapt to low Reynolds numbers, highly viscous or non-Newtonian environments. An important aspect to the construction of biomimetic model swimmers is to mimic as many of those strategies as possible, based on simple principles of non equilibrium physics without requiring intricate biochemical machinery. Here, we investigate the dynamics of active droplets dependent on the viscosity of the bulk phase. We can tune their propulsion from almost ballistic persistence over a quite diffusive "run-and-spiral" mode to a "stop-and-go" behaviour that is noisy on short, but persistent on long time scales, simply by changing the composition of the bulk phase with a varying fraction of glycerol. Such unsteady swimming is caused by a dynamic instability in the chemical and hydrodynamic fields around the droplets which we have mapped simultaneously via multichannel fluorescent video microscopy.

DY 44.3 Thu 10:30 H19

Swimming droplet in confined geometries — •Charlotte de Blois, Mathilde Reyssat, and Olivier Dauchot — Gulliver Laboratory, UMR CNRS 7083, ESPCI Paris, PSL University

Micro-swimmers rarely evolve in a 3D infinite and unbounded medium. Instead, they are confined by external geometries which strongly modify their behavior. There is however no exact theoretical knowledge of the flow fields in this context and experimental data are scarce. Here we consider a swimming water droplet [1], denser than the continuous phase, in confined geometries from 2D motion parallel to a bottom wall to 1D motion in capillaries. [1] Izri et al. PRL 113, 248302 (2014).

DY 44.4 Thu 10:45 H19

Active liquid crystal shells: stability and dynamics — •Babak Vajdi Hokmabad, Kyle A. Baldwin, Carsten Krüger, Christian Bahr, and Corinna C. Maass — Max Planck Institute for Dynamics and Self-organization

Production of controllable, active microcapsules is of great interest in synthetic biology and microchemistry. Inactive microcapsules, also known as double emulsions or droplet shells, are already widely used as artificial cells, micro-reactors, and in food and drug applications. However, combining activity, stability, and control remains a significant challenge. Using established concepts of active emulsions we have developed a new approach to the problem of encapsulation by using nematic active double emulsions, where a solubilization mechanism induces activity and the molecular nematicity provides stability. We show that using a nematic liquid crystal as the shell material and imposing homeotropic anchoring at both interfaces will result in a nematoelastic force on the internal droplet and act as a topological barrier against the coalescence of the core droplet with the outer phase. We further present a peculiar self-propulsion mode where the interplay of spontaneous symmetry breaking and autochemotaxis results in a "shark-fin meandering" motion of the shell in a 2D-confined geometry and a helical swimming in 3D. This behavior can be controlled or switched off by introducing chemical gradients, topographical guidance or through shell topology variation.

DY 44.5 Thu 11:00 H19

Flow of active granular particles through a bottleneck — •Tina Hanselka and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

We use screws performing a self-propelled motion on a vibrated plate as a simple model to analyze the collective behavior of active matter systems passing through a constriction. For this we employ a slight tilt of the plate to simulate an effective gravity and to give the particles a preferred direction towards the bottleneck, and we examine the characteristics of flow and clogging as a function of geometrical and driving parameters.

15 min. break

DY 44.6 Thu 11:30 H19

Autonomous engines driven by active matter: Energetics and design principles — •Patrick Pietzonka[1], Etienne Fodor[1], Christoph Lohrmann[2], Michael E. Cates[1], and Udo Seifert[2] — [1]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK — [2]II. Institut für Theoretische Physik, Universität Stuttgart, Germany

We explore how active matter in a non-equilibrium steady state can autonomously deliver mechanical work against a constant mechanical force or torque. For this purpose, we consider systems that contain one or several active components and a single passive component that is asymmetric in its geometrical shape or its interactions. Generally, one expects that such an asymmetry leads to a persistent, directed current in the passive component, which can be used for the extraction of work. We show which two-dimensional shapes of the passive particle are best suited for the extraction of work. Approximating their effect on the dynamics of the particles leads to analytical results for the power and efficiency. A mean field approach reveals that the interaction with the passive particle can mediate cooperativity between otherwise non-interacting active particles, leading to an enhanced efficiency.

DY 44.7 Thu 11:45 H19

Pair-distribution function of active Brownian particles in three spatial dimensions* — •Stephan Bröker, Jens Bickmann, and Raphael Wittkowski — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

The pair-distribution function is a key quantity for analyzing many-particle systems. It characterizes the particle configuration and is often required when describing such systems via field theories. While for passive particles this correlation function has been extensively studied and analytical approaches exist for it, little is known about the pair-distribution function for active particles.
Therefore, based on Brownian dynamics simulations, we have determined the full pair-distribution function of a homogeneous system of spherical active Brownian particles in three spatial dimensions. The full pair-distribution function takes not only the positions, but also the orientations of the particles into account and depends additionally on the speed and mean concentration of the particles. We discuss the structure of this function and present an analytical expression that represents the function with good accuracy. In addition, we present a new field theory for active Brownian particles that uses this expression. Our results will be beneficial for future research that aims at describing the collective dynamics of active Brownian particles or at developing methods for predicting the pair-distribution function in nonequilibrium many-particle systems.
**Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

DY 44.8 Thu 12:00 H19

Locomotion of self-acoustophoretic colloidal particles — •Johannes Voss and Raphael Wittkowski — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

During the last two decades, a large number of different realizations of artificial self-propelled colloidal particles has been developed. A particularly advantageous realization is given by self-acoustophoretic colloidal particles, which exhibit self-propulsion when they are exposed to ultrasound. Compared to other types of artificial self-propelled particles, they have a biocompatible propulsion mechanism and can move in various liquids and soft materials. Furthermore, they can permanently be supplied with energy and, via the ultrasound intensity, it is even possible to adjust their speed. This makes self-acoustophoretic particles relevant for potential applications in, for example, medicine and materials science. Up to now, however, these particles have not been investigated in depth. Even the details of their propulsion mechanism are still unclear.

Therefore, based on direct computational fluid dynamics simulations, we have extensively studied the locomotion of self-acoustophoretic colloidal particles. We present results that explain the self-propulsion mechanism of these particles and how their locomotion depends on the shape and other properties of the particles. Our results are helpful especially for future experimental work further investigating or applying self-acoustophoretic colloidal particles.

DY 44.9 Thu 12:15 H19

Pairing, waltzing and scattering of chemotactic active colloids — •Supriya Saha[1], Sriram Ramaswamy[2], Ramin Golestanian[1], and Ramin Golestanian[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17 37077 Göttingen — [2]Indian Institute of Science, Bangalore, India

Two chemotactic active colloids, which can rotate their polar axis to align with an imposed chemical gradient, form bound states by cancellation of velocities. Their interactions are dynamical in origin, with contributions from self-propulsion and phoretic response to chemical field generated by each other, are thus non-central and non-reciprocal. Two swimmers remain bound at long times when the chemotactic response of at least one of the swimmers is positive, i.e. it rotates its polar axis to point up a linear gradient. These bound states fall in two broad categories *(i) active dimers, separation fixed and polar axes orient along a line (ii) periodic orbits, relative inclination of the polar axes fixed, while the centre of mass executes cyclic motion. Chemotactic swimmers unbind and scatter away depending on initial conditions or with an increase of self-propulsion; while mutually anti-chemotactic swimmers always scatter away. These findings are summarized in state diagrams and representative trajectories are calculated to illustrate the rich dynamics. For the special case of a swimmer moving in a localised source of fuel, the fixed points underlying the bound states and the bifurcations that lead to transition between from one type of f inal state to another are classified.

DY 44.10 Thu 12:30 H19

Diffusion of active particles in a complex environment: role

of surface scattering — •Theresa Jakuszeit, Ottavio A. Croze, and Samuel Bell — Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, U.K

Microfluidic experiments have shown that self-propelled particles can slide along the surface of a circular obstacle without becoming trapped over long times for obstacles below a critical radius. Using simulations and theory, we study the impact of different boundary conditions on the diffusive transport of active particles in a lattice of such obstacles. We find that particle dynamics with sliding boundary conditions can result in large diffusivities even at high obstacle density, unlike classical specular reflection as in the Lorentz gas. These dynamics are very well described by a model based on Run-and-Tumble particles with microscopically derived tumbling frequencies and reorientation functions arising from obstacle-induced tumbles. This model, however, fails to describe fine structure in the diffusivity at high obstacle density predicted by simulations. Using a simple deterministic model, we show that this structure results from particles being guided by the lattice.

DY 45: The Physics of Power grids (joint session DY/SOE)

Time: Thursday 10:30–11:15 Location: H6

DY 45.1 Thu 10:30 H6

Comparison of coupled nonlinear oscillator models for the transient response of power generating stations connected to low inertia systems — Marios Zarifakis[1], William Coffey[2], Yuri Kalmykov[3], Serguey Titov[4], •Declan Byrne[2], and William Dowling[2] — [1]Electricity Supply Board, Dublin, Ireland — [2]Department of Electronic and Electrical Engineering, Trinity College, Dublin 2, Ireland — [3]Laboratoire de Mathematiques et Physique (EA 4217), Universite de Perpignan Via Domitia, F-66860, Perpignan, France — [4]Kotel'nikov Institute of Radio Engineering and Electronics of the Russian Academy of Sciences, Vvedenskii Square 1, Fryazino, Moscow Region 141120, Russia

Coupled nonlinear oscillators, e.g., Kuramoto models, are commonly used to analyze electrical power systems. Recently the cage model from the statistical mechanics of liquids has also been used for the modelling of the dynamics of synchronously connected generation stations. It appears that while the Kuramoto model is good for describing high inertia grid systems, the cage model allows both high and low inertia grids to be modelled. This is demonstrated by comparing both the synchronization time and relaxation towards synchronization of each model of power generating stations by treating the model equations of motion via a common framework rooted in the dynamics of many coupled phase oscillators. A solution of these equations via matrix continued fractions is implemented rendering the characteristic relaxation times of a grid-generator system over a wide range of inertia and damping.

DY 45.2 Thu 10:45 H6

Enhancing power grid synchronization and stability through time delayed feedback control — •Halgurd Taher[1,2], Simona Olmi[2,3], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Inria Sophia Antipolis Méditerranée Research Centre, 2004 Route des Lucioles, 06902 Valbonne, France — [3]CNR - Consiglio Nazionale delle Ricerche - Istituto dei Sistemi Complessi, 50019, Sesto Fiorentino, Italy

The increasing inclusion of renewable energy sources into the power grid brings new challenges for its stable operation, due to the presence of various forms of perturbations which may possibly harm stability and synchronization. In this talk asynchrony of single nodes in power grids is investigated using real data of the sparsely connected German high-voltage transmission grid. Based on time-delayed feedback control, diffferent control strategies are proposed and compared. The strategies not only take into account solitary states, but also the Lyapunov vector corresponding to the largest (positive) Lyapunov exponent. Starting from an unstable state out of synchrony, we are able to frequency-synchronize and stabilize power grids by just controlling a small set of nodes. The numerical calculation of the Lyapunov spectrum allows us to explore the mechanism behind the control-induced resynchronization transition.

DY 45.3 Thu 11:00 H6

Control of synchronization in two-layer power grids — •Carl H. Totz[1], Simona Olmi[2], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, D-10623 Berlin — [2]INRIA Sophia Antipolis Méditerranée, 2004 Route des Lucioles, 06902 Valbonne, France

The dynamics of a two-layer network modeling the Italian high voltage power grid is investigated: the first layer represents the generators and consumers, while the second layer represents a dynamic communication network between generators that serves as controller of the first layer. The dynamics of the power grid is modeled by the Kuramoto model with inertia, while the second layer provides a control signal P_i^c for each generator to improve frequency synchronization within the power grid.

We investigate different realizations of the communication layer topology and different control methods. The two-layer system is tested for different perturbation scenarios (disconnecting some generators, increasing demand of consumers, generators with stochastic output) and, irrespectively of the applied perturbation, we find that the control scheme aimed to synchronize the frequency of the generators with the consumers is very efficient against almost all perturbation scenarios.

DY 46: Energy Networks (joint SOE/DY) (joint session SOE/DY)

Time: Thursday 11:30–12:30 Location: H17

DY 46.1 Thu 11:30 H17

Principal flow patterns across renewable electricity networks — •Mirko Schäfer[1], Fabian Hofmann[2], Johannes Kruse[3], Tom Brown[4,2], Jonas Hörsch[4,2], Stefan Schramm[2], and Martin Greiner[3] — [1]Department of Sustainable Systems Engineering (INATECH), Albert-Ludwigs-Universität Freiburg — [2]Frankfurt Institute for Advanced Studies — [3]Department of Engineering, Aarhus University, Denmark — [4]Institute for Automation and Applied Informatics, Karlsruhe Institute of Technology

Using Principal Component Analysis (PCA), the nodal injection and line flow patterns in a network model of a future highly renewable European electricity system are investigated. Remarkably, the application of PCA to the transmission line power flow statistics shows that irrespectively of the spatial scale of the system representation a very low number of only 8 principal flow patterns is sufficient to capture 95% of the corresponding spatio-temporal variance. This result can be theoretically explained by a particular alignment of some principal injection patterns with topological patterns inherent to the network structure of the European transmission system. By connecting these insights to a spectral clustering method it is shown how through topological changes the flow patterns on the network can be controlled.

DY 46.2 Thu 11:45 H17

Flow Redistribution after Link Failures in Linear Flow Networks — •Franz Kaiser[1,2], Julius Strake[1,2], Henrik Ronellenfitsch[3], and Dirk Witthaut[1,2] — [1]Forschungszentrum Jülich, Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE) — [2]University of Cologne, Institute for Theoretical Physics — [3]Department of Mathematics, Massachusetts Institute of Technology

Failing links can degrade the operation of a supply network up to the point of complete collapse. Yet, the interplay between network topology and locality of the response to such damage is poorly understood. Here, we study the role of topology for the redistribution of flow after the failure of links in linear flow networks with a special focus on power

grids. In particular, we analyze the decay of flow changes with distance after a link failure and examine the interplay of multiple lines failing at the same time. In addition to that, we introduce a rerouting distance to predict this decay for real-world networks and use this tool for describing the interaction of multiple outages. Our results show that it is possible to forecast flow rerouting after link failures to a large extent based on purely topological measures and that these effects generally decay with distance from the failing link.

DY 46.3 Thu 12:00 H17

Understanding power-grid-frequency dynamics with stochastic modelling: The influence of the electricity market — •Leonardo Rydin Gorjão[1,2], Mehrnaz Anvari[3], Holger Kantz[3], Marc Timme[4,5], Benjamin Schäfer[4,5], and Dirk Witthaut[1,2] — [1]Forschungszentrum Jülich, Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE), 52428 Jülich, Germany — [2]Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany — [3]Max–Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Chair for Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute for Theoretical Physics, Technical University of Dresden, 01062 Dresden, Germany — [5]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

The ongoing energy transition transforms the power system by introducing additional fluctuations via intermittent renewable energy generation To evaluate the various proposed strategies of implementation of renewable energy generation and the impact of market design on the power grid's stability, a solid understanding of the power grid dynamics, specifically its frequency, is necessary. A pure empirical study on existing power grids is limited due to their small number, limited available data and high costs of implementing control and market schemes in real grids. Our model allows predictions of the frequency statistics for diverse power grids and ultimately enables us to quantify the impact of control proposals and market designs.

DY 46.4 Thu 12:15 H17

Effects of time delay on the control of synchronous electricity grids — •Philipp C. Böttcher[1], Andreas Otto[2], and Stefan Kettemann[3] — [1]DLR-Institut für Vernetzte Energiesysteme, Oldenburg — [2]Institute of Physics, TU Chemnitz, Chemnitz — [3]Department of Physics and Earth Sciences, Jacobs University, Bremen

In the course of the 'Energiewende', highly volatile energy sources (i.e. wind and photovoltaics) will be introduced to a system built with conventional energy sources in mind. Removing conventional energy sources and replacing them with fluctuating renewable generation that does not provide inertia could make the system vulnerable to disturbances. Control mechanisms can only be employed by accurately measuring the system state (i.e. frequencies and load flows) and correctly communicating theses values. The delay associated with the measurement, communication and deployment of control might play an increasingly important role in a system that relies on strongly fluctuating feed-in.
The control mechanisms used at the moment are integrated into a model of coupled oscillators which resembles the second order Kuramoto model. This model is used to investigate the behavior of the interconnected electricity grid. To identify regions in parameter space that make stable grid operation possible, the linearized system is analyzed to create the system's stability chart. The influence of the control parameters, the underlying network topology and the delay on the grid frequency is of special interest.

DY 47: Statistical physics of biological systems II (joint session BP/DY)

Time: Thursday 15:00–17:30 Location: H11

DY 47.1 Thu 15:00 H11

Experimental evidence of symmetry breaking of transition-path times — •Jannes Gladrow[1], Marco Ribezzi-Crivellari[2,3], Felix Ritort[3,4], and Ulrich F. Keyser[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [2]Laboratoire de Biochimie (LBC), ESPCI Paris, PSL Research University, CNRS UMR8231 Chimie Biologie Innovation, Paris, France — [3]Condensed Matter Physics Department, University of Barcelona, 08028 Barcelona, Spain — [4]CIBER-BBN de Bioingenieria, Biomateriales y Nanomedicina, 28029 Madrid, Spain

While thermal rates of state transitions in classical systems have been studied for almost a century, associated transition-path times have only recently received attention. Uphill and downhill transition paths between states at different free energies should be statistically indistinguishable. Here, we systematically investigate transition-path-time symmetry and report evidence of its breakdown on the molecular- and meso-scale out of equilibrium. In automated Brownian dynamics experiments, we establish first-passage-time symmetries of colloids driven by femtoNewton forces in holographically-created optical landscapes confined within microchannels. Conversely, we show that transitions which couple in a path-dependent manner to fluctuating forces exhibit asymmetry. We reproduce this asymmetry in folding transitions of DNA-hairpins driven out of equilibrium and suggest a topological mechanism of symmetry breakdown. Our results are relevant to electrophysiology and single-molecule fluorescence experiments.

DY 47.2 Thu 15:15 H11

Unveiling lineage decisions in zebrafish neurogenesis — Emmanuel Than-Trong[1,2], •Bahareh Kiani[3], Alessandro Alunni[1,2], Benjamin D. Simons[4,5,6], Laure Bally-Cuif[1,2], and Steffen Rulands[3] — [1]Institut Pasteur, Unit Zebrafish Neurogenetics, Department of Developmental & Stem Cell Biology, 25 rue du Dr Roux, 75015 Paris, France — [2]CNRS, UMR3738, 25 rue du Dr Roux, 75015 Paris, France — [3]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Deutschland — [4]Cavendish Laboratory, Department of Physics, University of Cambridge, Cambridge CB3 0HE, UK — [5]The Wellcome Trust/Cancer Research UK Gurdon Institute, University of Cambridge, Cambridge CB2 1QN, UK — [6]The Wellcome Trust/Medical Research Council Stem Cell Institute, University of Cambridge, Cambridge CB2 1QN, UK

Zebrafish neural tissue hosts specialised precursor cells which fuel the ongoing production of neurons into discrete brain regions. To understand how neural maintenance is achieved in this system, we performed a quantitative clonal analysis of the fate of precursor cells. Lineage tracing in growing tissues is complicated by the fact that labelled clones fragment into disconnected clusters, rendering the retrospective analysis of cell fate highly ambiguous. Combining statistical inference with biophysical modelling we reconstructed the clonal origin of labelled cells, revealing that progenitor containing clones persist over the lifetime of the animal. Using stochastic modelling, we unveiled lineage relationships and proliferation kinetics in the adult zebrafish pallium.

DY 47.3 Thu 15:30 H11

Revealing chromosome organization from Hi-C data using a maximum entropy approach — •Joris Messelink[1], Jacqueline Janssen[2], and Chase Broedersz[1] — [1]Arnold Sommerfeld Centre for Theoretical Physics, LMU Munich — [2]Max Planck Institute for the Physics of Complex Systems, Dresden

The bacterial DNA outsizes the cell by roughly a factor of a thousand. The DNA must not only be highly condensed to fit inside the cell, but this condensed DNA must be organized inside the cell to facilitate functional processes of the chromosome. Thus, understanding the three-dimensional spatial organization of the bacterial chromosome is important to understand how the core biological processes are regulated inside of the cell. Recent chromosome conformation capture experiments provide genome-wide data on chromosome folding. In particular, the Hi-C method provides contact frequency maps of the chromosome, revealing its highly organized structure. We develop a maximum entropy approach to extract the three-dimensional structure of the bacterial chromosome from such data. The aim of our method is to develop a coarse-grained model for the statistical mechanics of the folding of the whole bacterial chromosome. From this model, we obtain the full distribution of chromosome configurations in the cell.

DY 47.4 Thu 15:45 H11

Control of droplet coarsening in active emulsions — •Christoph Weber[1], Marta Tena-Solsona[2], Jacqueline

Janssen[1], Caren Wanzke[2], Fabian Schnitter[2], and Job Boekhoven[2] — [1]MPIPKS, Dresden — [2]TUM, Munich

Spatial-temporal regulation of liquid phase separation is crucial inside living cells. While spatial control can be achieved through concentration gradients, temporal control is often limited by the slow coarsening processes of droplet fusion and Ostwald ripening. Here we present a new class of active emulsions where the rate of coarsening can be dramatically accelerated in a controlled manner. This class of active emulsions involves a fuel that drives a chemical reaction from thermodynamically stable precursor molecules to metastable building blocks. At large enough concentrations of building blocks liquid droplets can form. We show by experimental studies of various active emulsions and a theory which quantitively coincides with the experimental measurements, how the metastable building blocks actually accelerate the coarsening kinetics in this novel class of phase separated systems. This class of active emulsions indicates novel possibilities to control sizes of assemblies in chemical engineering and may also rely on a mechanism used for the size regulation of membrane-less organelles in living cells.

DY 47.5 Thu 16:00 H11

Immune Repertoire Dynamics out of Steady State — •Mario Udo Gaimann[1], Jonathan Desponds[2], and Andreas Mayer[3] — [1]Ludwig-Maximilians-Universität München, Faculty of Physics, Munich, Germany — [2]University of California San Diego, Department of Physics, La Jolla, CA, USA — [3]Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ, USA

Over the last ten years high-throughput sequencing of lymphocyte receptor repertoires has provided an increasingly precise view of how immune defenses are organized. A highly reproducible finding of these sequencing efforts has been that the clone sizes of lymphocytes which share the same receptor are heavy-tail distributed. Here, we present a simple neutral birth-death model kept out of steady-state by the arrival of new clones in which competition between cells for a global resource couples the birth rate to the total size of the immune repertoire. We show that this model produces transient, but long-lived power-law scaling of clone sizes through a rich-get-richer mechanism resembling preferential attachment. Our model predicts an onset of power-law scaling early in life, which should persist throughout the human lifespan in the biologically relevant parameter regime. We verify both predictions by reanalyzing previously published T cell receptor sequencing data from a human aging study. Furthermore, we demonstrate that our mechanism is robust to relaxations of the model assumptions including when competition is based on the lymphocyte receptor specificity. Overall, our work suggests that early life has a strong influence on the long-term structure of the immune repertoire.

DY 47.6 Thu 16:15 H11

Topological dynamics of small degree networks: percolation, rate equation, and stochastic network growth — •Adrian Fessel and Hans-Günther Döbereiner — Universität Bremen, Bremen, Deutschland

In self-organizing networks, topology and dynamic processes interact in a unique way: the network adapts its structure based on local activity, enabling the emergence of global dynamic properties on an optimized topology.
Working with *Physarum polycephalum* as an experimentally accessible model for an adaptive transportation system, we seek to formalize topological development into a sequence of discrete events intended to serve as basis for studying the interaction of flow and topology. We focus on reorganization of *P. polycephalum* networks after fragmentation, a process occurring in a prominent percolation transition in a system where system size is not fixed.
The theoretical description follows a master equation with parameters obtained from statistical analysis of experimental data. Computational investigation of the model recreates the dynamics of the topological phase transition and enables characterization of finite size effects and critical exponents. Comparing the influences of system growth and fusion within the system reveals a significant shift of the transition when system growth dominates.

Invited Talk DY 47.7 Thu 16:30 H11

Spontaneous buckling of active matter — •Karsten Kruse — NCCR Chemical Biology, Departments of Biochemistry and Theoretical Physics, University of Geneva, 1211 Geneva, Switzerland

Active matter in living systems is often organized in the form of quasi two-dimensional sheets. Examples are the actin cortex of animal cells or epithelial cell monolayers in organisms. In many processes, these sheets fold, for instance, during cell division or gastrulation, which is the developmental process of inward folding of a single-cell layered sphere in early embryogenesis. The molecular players and signaling cascades involved in these processes have been studied in detail. In contrast, the underlying mechanics remains poorly characterized. This is in large part due to technical difficulties in measuring the material properties of these systems as well as the forces acting on them. Theoretical analysis can shed light on the mechanics governing the spontaneous buckling of active matter as I will illustrate by two model systems: One system consists of an initially homogenous actomyosin sheet reconstituted *in vitro* that can buckle spontaneously into states of positive and negative Gaussian curvature upon contraction. The other example is provided by a cell monolayer growing on the inside of an elastic sphere. It buckles spontaneously as cells continue to proliferate beyond the state when the whole inner surface of the sphere is covered with cells. In both cases, theoretical analysis allows to extract mechanical properties of the active materials that are difficult to assess otherwise.

DY 47.8 Thu 17:00 H11

Phase separation in the ensemble of fixed pH — •Omar Adame-Arana[1], Christoph A. Weber[1], Vasily Zavurdaev[1,2], Jacques Prost[3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Friedrich-Alexander Universität Erlangen-Nürnberg, Cauerstr. 11, 91058 Erlangen, Germany — [3]Institut Curie, 26 rue d'Ulm, 75248 Paris Cedex 05, France

Recent developments at the interface of biology and physics brought to light the importance of phase separation in explaining biological processes in the cell. It has been shown that some proteins are able to phase separate in solution and form liquid-like droplets in the cytoplasm that carry out a distinct biological function. Particularly, a drop in the cytosolic pH leads to a widespread protein assembly in the cytoplasm, this phenomenon triggered our interest to the mechanism of protein phase separation as a function of pH. In order to study this mechanism, we define a model of a solution composed of macromolecules which can exist in three different charge states and have a tendency to phase separate. The pH dependence is introduced in terms of chemical reactions which control the charge state of the macromolecules. Using conservation laws and chemical equilibrium, we identify the conjugate variables of the system. We then perform a Legendre transform which defines the free energy corresponding to a fixed pH ensemble. We conclude by showing phase diagrams as a function of pH, where we find that under most conditions, phase separation is most pronounced near the isolectric point.

DY 47.9 Thu 17:15 H11

Kleiber's law scaling of the metabolic rate in planarians — Albert Thommen[1,2], Steffen Werner[2,3], Olga Frank[1], Jenny Philipp[4], Oskar Knittelfelder[1], Yihui Quek[2,5], Karim Fahmy[4], Andrej Shevchenko[1], •Benjamin M. Friedrich[2,6], Frank Jülicher[2], and Jochen C. Rink[1] — [1]MPI CBG, Dresden. Germany — [2]MPI PKS, Dresden, Germany — [3]AMOLF, Amsterdam, Netherlands — [4]HZDR, Dresden, Germany — [5]MIT, Cambridge, USA — [6]cfaed, TU Dresden, Germany

Kleiber's law states that the metabolic rate of animals scales with the 3/4 power of their body mass. It is considered one of the few quantitative laws in biology, yet its mechanistic basis remains unknown. Here, we take advantage of the reversible changes in body size by 2 orders of magnitude as function of food abundance in the planarian *Schmidtea mediterranea*. Using microcalometry, we show that Kleiber's law applies to adult organisms of this flatworm species. Intriguingly, the metabolic rate per cell is independent of organism size. Instead, Kleiber's law in planarians results from a size-dependent increase in mass per cell, reflecting a higher proportion of energy stores in large animals. Using a minimal energy balance model, we relate energy currents to growth and degrowth rates, in quantitative agreement with experiment. Our study is a first step to link energy fluxes, metabolism, and pattern formation in living matter.

[1] Thommen et al. BioRxiv; doi: https://doi.org/10.1101/332916 (accepted in eLife)

DY 48: Theory of Stochastic Processes with Applications in Biology (joint session SOE/BP/DY/AKjDPG)

Session initiated and organized by Rosalba Garcia Millan, Johannes Pausch and Ignacio Bordeu Weldt (Imperial College, UK), in cooperation with divisions DY, BP, SOE and the jDPG.

Time: Thursday 15:00–18:45 Location: H17

Invited Talk DY 48.1 Thu 15:00 H17

Ecosystem stability and altruistic advantage — •Nick Jones — Imperial College Mathematics, London, UK

In this talk I consider why many, empirically observed, directed networks might contain a lack of feedback loops. An answer might be network growth mechanisms that favour clear trophic levels and which generate assymetries between the in degrees and out degrees of nodes. This is a partial answer to May's (Complexity-Stability) Paradox. Finally I will outline an, ageing relevant, concrete biological example of spatial demographic stochasticity where altruists can dominate a system even when actively selected against.

DY 48.2 Thu 15:45 H17

Thermodynamics of steady-state switching — •Jacob Cook[1,2] and Robert G. Endres[1,2] — [1]Department of Life Sciences, Imperial College, London, UK — [2]Centre for Integrative Systems Biology and Bioinformatics, Imperial College, London, UK

Entropy production is a hallmark of nonequilibrium processes in stochastic thermodynamics. Multistable nonequilibrium systems are abundant outcomes of nonlinear dynamics with feedback yet relatively little is known about what determines the stability of the steady states and their switching rates in terms of entropy and entropy production. Here, we will link the fluctuation theorem for the entropy production along trajectories and the large-deviation approach of minimum-action-path theory to elucidate the thermodynamics of steady-state switching. Interestingly, we find that the entropy production at steady state plays no explicit role, but the entropy production along switching trajectories is key. Alternative stabilising and destabilising mechanisms such as steady-state entropy and diffusive noise are also investigated.

DY 48.3 Thu 16:00 H17

Dynamical phase transition in assemblies of chemotactic cells — •Charlie Duclut — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We consider a large number of chemotactic cells that diffuse, die, divide and interact at long range via the release of chemicals. We investigate the dynamics at long time and focus on the phase transition that occurs between a dilute and a dense phase using a renormalization group analysis. If we consider only interactions that conserve the particles number, exact scaling exponents can even be obtained; this analysis predicts in particular a superdiffusive behaviour of the cells close to the phase transition.

Invited Talk DY 48.4 Thu 16:15 H17

Topological Hindrance and Jamming Transitions in Multi-Species Transport — •Erwin Frey — Arnold-Sommerfeld-Center for Theoretical Physics, Ludwig-Maximilians-Universität München, München, Germany

Motivated by recent experimental studies that have addressed the stepping behavior of kinesins, we investigate a lattice gas model for simultaneous transport of two species of active particles on a microtubule. The species are distinguished by their different gaits: While the first species moves straight ahead, the second follows a helical path. We show that the collective properties of such systems critically differ from those of one-species transport as described by generalised totally asymmetric exclusion processes. This is most evident in a jamming transition far below full occupation, as well as in nonequilibrium pattern formation. The altered behavior arises because - unlike the case in single-species transport - any given position may be targeted by two particles from different directions at the same time. However, a particle can leave a given position only in one direction. This simple change in connectivity significantly amplifies the impact of steric interactions and thus becomes a key determinant of mixed species transport. We computationally characterize this type of hindrance and develop a comprehensive stochastic theory for collective two-species transport along a cylinder. Our observations show high robustness against model extensions that account for additional biomolecular features which suggests relevance also in a biological context.

15 min. break

Invited Talk DY 48.5 Thu 17:00 H17

Seeing and believing at super-resolution — •Susan Cox — Randall Centre for Cell and Molecular Biophysics, King's College London

Super-resolution microscopy is a powerful tool for imaging structures at a lengthscale of tens of nm, but its utility for live cell imaging is limited by the time it takes to acquire the data needed for an image. For localisation microscopy the acquisition time can be cut by more than two orders of magnitude by using advanced algorithms which can analyse dense data, trading off acquisition and processing time. Information can be traded for resolution: for example, the whole dataset can by modelled as arising from blinking and bleaching fluorophores (Bayesian analysis of Blinking and Bleaching), although at a high computational cost. However, all these approaches will come with a risk of artefacts, which can mean that the image does not resemble the underlying sample. We have recently developed Harr Wavelet Kernel Analysis, a multi-timescale prefiltering technique which enables high density imaging without artefacts. The results of benchmarking with other techniques reveal that at high activation densities many analysis approaches may achieve high apparent precision (very sharp images), but poor accuracy (the images don't look like the sample). I will discuss the relationship between precision, accuracy and information content in super-resolution microscopy images.

DY 48.6 Thu 17:45 H17

Filament flexibility enhances power transduction of F-actin bundles — •Alessia Perilli[1], Carlo Pierleoni[2], Giovanni Ciccotti[1], and Jena-Paul Ryckaert[3] — [1]Dept. of Physics, Sapienza University of Rome, Italy — [2]Dept. of Physical and Chemical Sciences, University of L'Aquila, Italy — [3]Dept. of Physics, Free University of Brussels, Belgium

In different biophysical cellular processes, semiflexible biofilaments like Factin and F-tubulin are known to exploit chemical free energy, associated to their growth by polymerization, to perform mechanical work against an external load. In vitro experiments have recently been set up to measure the force-velocity relationship of an actin bundle or to equilibrate the bundle polymerizing force by an optical trap restoring force. Theoretical interpretation is usually based on multi filament brownian ratchet models assuming perfectly rigid filaments (Mogilner-Oster). In this talk, we will exploit statistical mechanics tools and a coarse grained stochastic dynamic approach based on the discrete Wormlike Chain (WLC) model, to study the influence of filament flexibility on the non-equilibrium velocity-load relationship for a bundle of parallel un-crosslinked actin filaments pressing against a mobile wall. Using a realistic value of the actin persistence length, we show that flexibility enhances the power developed by the polymerizing force against the load in a way which increases with the length of the bundle, as long as the pushing filaments remain in the nonescaping regime.

Topical Talk DY 48.7 Thu 18:00 H17

Reconstructing the topographic landscape of epithelial-mesenchymal plasticity — •Francesc Font-Clos, Stefano Zapperi, and Caterina A. M. La Porta — Center for Complexity and Biosystems, University of Milan, Italy

We construct a topographic map underlying epithelial-mesenchymal plasticity by combining numerical simulations, statistical physics methods and analysis of bulk and single-cell gene expression data. The map reveals a multitude of metastable hybrid phenotypic states, separating stable epithelial and mesenchymal states, and is reminiscent of the free energy measured in glassy materials and disordered solids.

Topography of epithelial-mesenchymal plasticity, Francesc Font-Clos, Stefano Zapperi, Caterina A. M. La Porta, Proceedings of the National Academy of Sciences Jun 2018, 115 (23) 5902-5907; DOI:

10.1073/pnas.1722609115

DY 48.8 Thu 18:30 H17

Beating cancer 'escape room': let's use mathematical modelling to unlock cells! — •Núria Folguera-Blasco — The Francis Crick Institute, London, UK

The inherent capacity of differentiated cells to switch their phenotype in vivo in response to damage stimuli might have a pivotal role in ageing and cancer. However, how the mechanisms of phenotype reprogramming are established remains poorly understood. In order to elucidate such mechanisms, we present a stochastic model of combined epigenetic regulation (ER)-gene regulatory network (GRN) to study the plastic phenotypic behaviours driven by ER heterogeneity. Our analysis of the coupled system reveals the existence of pluripotent stem-like and differentiated steady-states. Crucially, ER heterogeneity is responsible for conferring abnormal robustness to pluripotent stem-like states, which cause the locking of the cells in a stem cell-like state prone to cancer development. By analysing the ER heterogeneity, we formulate epigenetic heterogeneity-based strategies capable of unlocking and facilitating the transit from differentiation-refractory (pluripotent stem-like) to differentiation-primed epistates. Our results suggest that epigenetic heterogeneity regulates the mechanisms and kinetics of phenotypic robustness of cell fate reprogramming. The occurrence of tunable switches capable of modifying the nature of cell fate reprogramming from pathological to physiological might pave the way for new therapeutic strategies to regulate reparative reprogramming in ageing and cancer.

DY 49: Quantum-Critical Phenomena (joint session TT/DY)

Time: Thursday 15:00–18:00 Location: H23

DY 49.1 Thu 15:00 H23

Superconductivity from the Condensation of Topological Defects in a Quantum Spin-Hall Insulator — Yuhai Liu[1], Zhenjiu Wang[2], Toshihiro Sato[2], Martin Hohenadler[2], Chong Wang[3], Wenan Guo[1], and •Fakher F. Assaad[2] — [1]Department of Physics, Beijing Normal University, Beijing 100875, China — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada N2L 2Y5

The discovery that spin-orbit coupling can generate a new state of matter in the form of quantum spin-Hall (QSH) insulators has brought topology to the forefront of condensed matter physics. While QSH states from spin-orbit coupling can be fully understood in terms of band theory, fascinating many-body effects are expected if the state instead results from interaction-generated symmetry breaking. In particular, topological defects of the corresponding order parameter provide a route to exotic quantum phase transitions. Here, we introduce a model in which the condensation of skyrmion defects in an interaction-generated QSH insulator produces a superconducting (SC) phase. Because vortex excitations of the latter carry a spin-1/2 degree of freedom numbers, the SC order may be understood as emerging from a gapless spin liquid normal state. The QSH-SC transition is an example of a deconfined quantum critical point (DQCP), for which we provide an improved model with only a single length scale that is accessible to large-scale quantum Monte Carlo simulations.

DY 49.2 Thu 15:15 H23

Studies of Deconfined Quantum Criticality in a Half-filled Laudau Level — •Zhenjiu Wang[1], Matteo Matteo Ippoliti[2], Roger S. K Mong[3], and Michael P Zaletel[2,4] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, Princeton University, Princeton, NJ 08544, USA — [3]Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA — [4]Department of Physics, University of California, Berkeley, CA 94720, USA

We perform Quantum Monte Carlo studies of deconfined quantum criticality (DQC) based on models of interacting fermions. As opposed to previous studies, this suggests an emergent SO(5) symmetry at criticality, our model has an exact SO(5) symmetry at the Hamiltonian level. This relies on the fact that our model is defined in the continuum. As opposed to lattice regularization, that would break the SO(5) symmetry, we follow a suggestion by [1], where the ultra-violet cutoff is realized by a magnetic field. Our model corresponds to 4 flavors of fermions with Hilbert space restricted to the zeroth Landau level (ZLL) of 8 component Dirac fermions as realized in Graphene, which maps to a nonlinear sigma model containing only bosonic degrees of freedom is studied, with the competition between the stiffness and an SO(5) Wess-Zumino-Witten topological term. AFQMC studies are free of the negative sign problem due to the existence of two anti-unitary particle-hole transformations that leaves the propagator invariant for each MC configuration.
[1] Ippoliti et al., arXiv:1810.00009 (2018)

DY 49.3 Thu 15:30 H23

Deconfined criticality from the QED3-Gross-Neveu model — •Lukas Janssen[1], Bernhard Ihrig[2], Luminita N. Mihaila[3], and Michael M. Scherer[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Germany — [3]Institut für Theoretische Physik, Universität Heidelberg, Germany

The QED$_3$-Gross-Neveu model is a (2+1)-dimensional U(1) gauge field theory involving Dirac fermions and a critical real scalar field. It has been argued that this theory represents a dual description of the deconfined quantum critical point between Néel and valence bond solid orders in frustrated quantum magnets. I will present evidence for a novel scaling relation that implies emergent SO(5) symmetry at criticality.

DY 49.4 Thu 15:45 H23

Deconfined quantum criticality in the two-dimensional Su-Schrieffer-Heeger model — •Stefan Beyl, Martin Hohenadler, Florian Goth, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

The Su-Schrieffer-Heeger model is one of the most basic models for electron-phonon coupling. It captures the effects of fluctuating bond lengths—as described by quantum mechanical bond phonons—on the electronic hopping. While much work has been devoted to the one-dimensional case, systematic results in two dimensions are not available. Here, we present results from sign-free hybrid quantum Monte Carlo simulations at half-filling that support a deconfined quantum critical point between a valence bond solid and an antiferromagnet, as well as remarkable connections to an Ising lattice gauge theory with topologically ordered metallic and insulating phases.

DY 49.5 Thu 16:00 H23

Quantum Criticality near the Mott Transition — •Heike Eisenlohr[1], Seung-Sup B. Lee[2], Andreas Weichselbaum[2], and Matthias Vojta[1,3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 München, Germany — [3]Center for Transport and Devices of Emergent Materials, Technische Universität Dresden, 01062 Dresden, Germany

The Mott metal-insulator transition is known to be a first order transition, with the transition line terminating in a classical critical end point at finite temperature Tc. Recent numerical studies of the half-filled Hubbard model, which employed dynamical mean-field theory and a quantum Monte Carlo impurity solver, and experiments in 2d organic salts have concordantly observed apparent quantum critical scaling of the resistivity in the regime T>Tc [1,2]. Although this conventionally indicates a nearby quantum critical point at T=0, the studied system shows only a classical first order transition at T=0. So far no theoretical explanation was able to identify the degrees of freedom which behave as if they were quantum critical, and why. To understand this unexpected scaling regime, we study the system with dynamical mean-field theory in combination with the numerical renormalization group.

DY 49.6 Thu 16:15 H23

Quantum critical behaviour in 2D Fermi systems with

quadratic band touching — •Shouryya Ray, Matthias Vojta, and Lukas Janssen — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We consider two-dimensional Fermi systems with quadratic band touching and C_3 symmetry, as realizable in Bernal-stacked honeycomb bilayers. Within a renormalization-group analysis, we demonstrate the existence of a quantum critical point at a finite value of the density-density interactions, separating a semimetallic disordered phase at weak coupling from a gapped ordered phase at strong coupling. The latter may be characterized by, for instance, antiferromagnetic, quantum anomalous Hall, or charge density wave order. In the semimetallic phase, each point of quadratic band touching splits into four Dirac cones as a consequence of the nontrivial interaction-induced self-energy correction, which we compute to the two-loop order. We show that the quantum critical point is in the $(2 + 1)$-dimensional Gross-Neveu universality class, characterized by emergent Lorentz invariance and a dynamic critical exponent $z = 1$. At finite temperatures, $T > 0$, we hence conjecture a crossover between $z = 2$ at intermediate T and $z = 1$ at low T, and construct the resulting nontrivial phase diagram as function of coupling strength and temperature.

15 min. break.

DY 49.7 Thu 16:45 H23

Quantum Criticality of an Ising-like Spin-1/2 Antiferromagnetic Chain in a Transverse Magnetic Field — •Zhe Wang[1], Thomas Lorenz[2], Denis Gorbunov[1], Pham Thanh Cong[1], Yoshimitsu Kohama[3], Sandra Niesen[2], Olivier Breunig[2], Johannes Engelmayer[2], Alexander Herman[2], Jianda Wu[4], Koichi Kindo[3], Joachim Wosnitza[1], Sergei Zherlitsyn[1], and Alois Loidl[5] — [1]Helmholtz Zentrum Dresden Rossendorf, Dresden, Germany — [2]University of Cologne, Cologne, Germany — [3]University of Tokyo, Kashiwa, Japan — [4]Tsung-Dao Lee Institute, Shanghai — [5]University of Augsburg, Germany

We report on magnetization, sound velocity, and magnetocaloric-effect measurements of the Ising-like spin-1/2 antiferromagnetic chain system $BaCo_2V_2O_8$ as a function of temperature down to 1.3 K and applied transverse magnetic field up to 60 T [1]. At $B_\perp^c = 40$ T, the $T(B)$ curve shows a broad minimum, accompanied by a broad minimum in the sound velocity and a saturation-like magnetization. These features signal a quantum phase transition which is further characterized by the divergent behavior of the Grüneisen parameter $\Gamma_B \propto (B - B_\perp^c)^{-1}$. By contrast, around the critical field, the Grüneisen parameter converges as temperature decreases, pointing to a quantum critical point of the one-dimensional transverse-field Ising model [2].
[1] Zhe Wang et al., Phys. Rev. Lett. 120, 207205 (2018)
[2] Jianda Wu et al., Phys. Rev. B 97, 245127 (2018)

DY 49.8 Thu 17:00 H23

Phase diagram of SU(N) Dirac fermions on the π-flux lattice with a bond-bond interaction — •Johannes S Hofmann, Martin Hohenadler, and Fakher F Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We use auxiliary-field quantum Monte Carlo simulations to study the phase diagram of SU(N) Dirac fermions with a bond-bond interaction V similar to Ref. [1] and an associated O($2N$) symmetry. In contrast to previous work, we consider a π-flux rather than a honeycomb lattice. The different coordination number is expected to favor antiferromagnetic (AFM) over valence bond solid (VBS) order. Accordingly, whereas AFM order is absent from the N-V phase diagram for $N > 2$ in Ref. [1], we find an AFM phase up to $N = 3$. Our results are consistent with Gross-Neveu semimetal-VBS transitions for $N > 1$ and deconfined VBS-AFM quantum critical points for $N = 2$ and $N = 3$.
[1] Z.-X. Li, Y.-F. Jiang, S.-K. Jian, and H. Yao, Nature Communications 8, 314 (2017)

DY 49.9 Thu 17:15 H23

Quantum criticality on a chiral ladder: a model study — Philipp Schmoll[1,2], •Andreas Haller[1,2], Matteo Rizzi[1], and Román Orús[1,3,4] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany — [3]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [4]Ikerbasque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain

In our work we focus on exotic SU(2) invariant three-spin interactions which are exploited to engineer non-trivial helical phases in quasi one-dimensional ladder setups, also dubbed as wire deconstructionism. Such interactions are typically treated as a perturbation of the famous spin-1/2 Heisenberg model. Here, we extend the existing literature and tackle the non-perturbative low-energy regime by means of exact diagonalization, blockspin renormalization and bosonization. Our Luttinger Liquid (LL) analysis predicts a subtle gapping mechanism between two of the four helical modes in the ladder, which yields a critical model with central charge c=1. We support our analysis by numerical data obtained from an SU(2) symmetric implementation of the infinite Density Matrix Renormalization Group (iDMRG) algorithm.

DY 49.10 Thu 17:30 H23

Quantum criticality on a chiral ladder: an $SU(2)$ iDMRG study — •Philipp Schmoll[1,2], Andreas Haller[1,2], Matteo Rizzi[1], and Román Orús[1,3,4] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany — [3]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [4]Ikerbasque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain

We study the ground state properties of a ladder Hamiltonian with chiral $SU(2)$-invariant three-spin interactions, a possible first step towards the construction of truly two dimensional non-trivial systems with chiral properties starting from quasi-one dimensional ones. Extending our analysis by means of blockspin renormalization and bosonization we use a recent implementation of $SU(2)$ symmetry in the infinite Density Matrix Renormalization Group (iDMRG) algorithm. The numerical findings agree very well with the theoretical prediction of a gapless phase. In particular, the scaling of the entanglement entropy as well as finite-entanglement scaling data show that the ground state properties match those of the universality class of a $c = 1$ conformal field theory (CFT) in $(1 + 1)$ dimensions.

DY 49.11 Thu 17:45 H23

Statistically induced quantum phase-transitions in the extended Anyon-Hubbard model — •Martin Bonkhoff, Kevin Jägering, Shijie Hu, Imke Schneider, Axel Pelster, and Sebastian Eggert — Departement of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Recently it has been shown that one-dimensional abelian anyons can be realized via density dependent Peierls-phases in bosonic models [1]. Furthermore extended interactions as well as a particle number constraint in bosonic Hubbard models can lead to a Symmetry-Protected-Topological (SPT) Haldane insulator phase [2]. We study the fate of SPT-order under statistical transmutation, and additionally observe a new gapped dimerized phase for attractive on-site interaction. By the technique of bosonization, we establish a unified low-energy field theory characterizing phases and relevant quantum phase transitions in the whole parameter region. We analyze the mechanism behind statistically induced phase transitions in combination with large-scale numerical simulations by the density-matrix renormalization group method.
[1] T. Keilmann, S. Lanzmich, I. McCulloch, and M. Roncaglia, Nat. Comm. 2, 361 (2011)
[2] E. Berg, E. G. D. Torre, T. Giamarchi, and E. Altman, Phys. Rev. B 77, 245119 (2008)

DY 50: Poster: Nonlinear Systems, Patterns, Flows ..

Time: Thursday 15:00–18:00 Location: Poster B2

DY 50.1 Thu 15:00 Poster B2

Relaxation of hydrogen bond network in water subject to an E-field — •Andreas Baer[1], David Matthew Smith[2,3], and Ana-Sunčana Smith[1,2] — [1]PULS Group at the Institute for Theoretical Physics, FAU Erlangen-Nürnberg, Germany — [2]Division of Physical Chemistry, Institute Ruđer Bošcović, Zagreb, Croatia — [3]Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Most of the amazing properties of liquid water stem from the fluctuations in the uninterrupted network of hydrogen bonded molecules.[1] One such phenomena is the splitting of transport coefficients in an electric field, which is not yet understood from the microscopic point of view. We address this by investigating the influence of an externally imposed electric field on liquid water at ambient conditions with the use of extensive molecular dynamics and rigorous statistical analysis.[2] The time dependent stress relaxations are related to different individual and cooperative motions of water molecules, identifying a filed-induced relaxation, occurring on the picosecond time scale, which was hitherto not reported in the literature. This process is shown to be primarily responsible for the anisotropic splitting of the shear viscosity in electric fields. It is further associated with cooperative transitions of several hydrogen bonded water molecules between the states of zero torque imposed by the field.[3] [1] Luzar, A.; Chandler, D. Nature 1996 379, 55-57. [2] Milicevic Z., Marrink S. J., Smith A.-S., Smith D. M. J. Mol. Mod. 2014 20, 2359 [3] Baer A., Milicevic Z., Smith D. M., Smith A.-S., submitted

DY 50.2 Thu 15:00 Poster B2

Reduced order model for the velocity gradient dynamics in fully developed turbulence — •Leonhard A. Leppin[1,2] and Michael Wilczek[2] — [1]Georg-August-Universität Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Fully developed homogeneous isotropic turbulence exhibits statistically and geometrically complex small-scale structures. A promising approach to advance the understanding of these structures has been to formulate low-dimensional dynamical systems for the velocity gradient. However, the evolution equation of the velocity gradient tensor along Lagrangian fluid particle trajectories contains non-local terms, e.g. the pressure Hessian, which prohibit a statistically closed description of the dynamics. Here, we formulate a general closure by employing results from the theory of tensor function representation. We find that the conditional pressure Hessian can be expressed in terms of only seven known tensors with unknown coefficients that depend on the tensor invariants. To investigate the influence of the different terms of the closure we numerically integrate an ensemble of stochastic differential equations whose coefficients are dynamically adapted such that the ensemble fulfills a number of physical constraints of homogeneous turbulence. By exploring the general tensorial structure of the unclosed terms and the resulting nonlinear dynamics, our work contributes to an improved understanding of the small-scale motions in turbulence by means of low-dimensional dynamical systems.

DY 50.3 Thu 15:00 Poster B2

Synchronization in optical neurons — •Felix Köster[1], Benjamin Lingnau[1,2], Philipp Hövel[1,3], and Kathy Lüdge[1] — [1]Institute of theoretical Physics, Technische Universität Berlin — [2]Physics Department, University College Cork, College Rd, Irland — [3]School of Mathematical Science, University College Cork, Irland

Recent studies have shown that information processing in neurons could be positively influenced by noise via noise-induced spiking. Inspired by this and the similar behavior of neurons and lasers, a network of quantum dot (QD) lasers is simulated in the steady state (continuous intensity output) close to a saddle-node infinite period (SNIPER) bifurcation. In this setup the QD lasers can be excited through noise into emitting pulses, i.e. spikes. Then the QD laser network can exhibit the counterintuitive effect of coherence resonance on the global network scale. We find that the regularity of noise-induced spiking has a maximum in its correlation at a finite value of the noise strength. We show that this collective coherence resonance effect is connected to the stability of the synchronized manifold and the global SNIPER bifurcations of the network. Additionally a scheme is introduced for identifying the network and parameter configurations where this collective coherence resonance effect can be detected.

DY 50.4 Thu 15:00 Poster B2

Simulation of horizontally rotating compressible convection: Towards the Boussinesq limit — •Kevin Lüdemann and Andreas Tilgner — Institut für Geophysik, Georg-August-Universität Göttingen, Deutschland

The band structure on Jupiter consisting of alternating east and west winds stems from compressible convective motion under the influence of Coriolis force. In order to investigate this structure, a numerical study of an ideal gas is performed in a cuboid geometry with gravitation in vertical direction and rotation around a horizontal axis. This geometry in a 3D case has been investigated before but only with an incompressible fluid in the Boussinesq approximation. Density and temperature scale heights are additional parameters in the compressible equations. Those are varied towards the Boussinesq limit for validation. Furthermore a parameter study of the thermal transport shows a decrease during departure from incompressibility as has also been proposed in prior work. At the same time, plume outbursts loose strength and a crossover from convective rolls to the thermal wind is observed.

DY 50.5 Thu 15:00 Poster B2

Dynamics of magnetic gears — •Stefan Hartung, Simeon Völkel, and Ingo Rehberg — Universität Bayreuth

The coupling of two rotating spherical magnets is investigated experimentally. Those motions where the driven magnet is phase-locked to the driving one are so-called cogging free couplings [1]. We find that configurations not following this condition show a more complex dynamical behavior. The experimental results are compared to a model based on pure dipole-dipole interaction. Technical applications of these kinds of couplings are foreseeable particularly for small machines.

[1] Exploring cogging free magnetic gears; Stefan Borgers, Simeon Völkel, Wolfgang Schöpf, and Ingo Rehberg; American Journal of Physics 86, 460 (2018); https://doi.org/10.1119/1.5029823.

DY 50.6 Thu 15:00 Poster B2

Evolving Transport Networks — •Janosch Brandhorst and Pawel Romanczuk — Institute for Theoretical Biology, Department of Biology, Humboldt Universität zu Berlin, Germany

Ant colonies and slime moulds are known to effectively explore and exploit their environment by setting up a complex transport network. Interestingly, the scales of these networks are much larger than the area a single agent of these colonies can sense. Here, we present an agent-based model of a collective which adapts to explore and exploit arbitrary resource fields. Agents are stationary placed on an randomly generated resource field. In each iteration, an agent can harvest resources from the resource field and collect resources from its neighbours. The efficiency of these processes is dependent on the phenotype of each agent. The phenotype is allowed to evolve during the simulation. The performance of this collective is measured by the amount of resources which is delivered to the centre of the collective. This leads to the self-organized formation of a transport system which effectively assimilates randomly spatial distributed resources in its centre, even though the agents do not have any information about their neighbours, the location of resources nor the location of centre of the collective. Eventually, we are interested in the ability of such collective to adapt to spatio-temporally varying environments.

DY 50.7 Thu 15:00 Poster B2

Work statistics in the classical periodically driven anharmonic oscillator — •Mattes Heerwagen and Andreas Engel — Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

For a small, time-dependent Hamiltonian system starting in thermal equilibrium the probability distribution of work arises due to the interplay between random initial conditions and deterministic dynamics. This distribution has been studied in detail for several examples of integrable systems. When regular and chaotic motion coexist new mechanisms for phase space mixing arise that will leave signatures in the work statistics.

We consider a classical anharmonic oscillator initially at equilibrium. Then the heat bath is removed and a periodic driving with slowly in-

creasing envelope function is switched on. After reaching a maximum the driving is again switched off smoothly such that the final Hamiltonian coincides with the initial one. By the first law of thermodynamics, the work of the external driving equals the energy change of the system during the process. We determine the probability density $P(E_f|E_i)$ for transitions from initial energy E_i to final energy E_f and deduce from it the work statistics for the periodically driven anharmonic oscillator.

DY 50.8 Thu 15:00 Poster B2

Met Mast Array to measure high temporal and spatial resolution wind fields — •Abdulkarim Abdulrazek, Joachim Peinke, and Michael Hölling — ForWind, Institute of Physics, University of Oldenburg, Oldenburg, Germany

Atmospheric wind fields are turbulent, in which the flow frequently changes speed and direction, creating a sudden increase of wind speed and generation of vortices. Such turbulent flows can affect for example wind turbine loads and performance causing damages resulting in expensive downtimes. In order to study these effects, a met mast array consisting of three meteorological masts will be installed between two wind turbines. The mast array will be equipped with up to XX ultrasonic and cup anemometers. The challenge is how to distribute these anemometers in horizontal and vertical direction to achieve high resolution in time and space. On the poster we will present the concept of the layout of the anemometers based on the detailed analysis of already existing atmospheric measurements data. Therefore, we propose an unevenly distributed arrangement of the anemometers in two dimensions. The anemometers will be distributed according to scaling factor of 2.52n on the three masts which should extract an optimal amount of information on a large range of scales as well as capture finer wind variations and vortices of different sizes.

DY 50.9 Thu 15:00 Poster B2

The parameter space of thermohaline stairs — •Axel Rosenthal and Anderas Tilgner — Friedrich-Hund-Platz 1, 37077 Göttingen

Convection and diffusion in water can be observed when a gradient in temperature or in salinity takes effect on density in presence of gravity. Both gradients can force or stabilize the process. We conducted experiments where the salt gradient is the driving force and simultaneously the temperature gradient is stabilizing in opposite direction, observed by particle image velocimetry (PIV). The question is at which gradients, expressed by Rayleigh numbers, does the transport occure in stable so called "thermohaline stairs"? Thermohaline stairs are a sequence of two flow systems, a finger regime and a large scale circulation.

DY 50.10 Thu 15:00 Poster B2

Wasserklangbilder — •Carla Corsi[1], Thomas Grillenbeck[1,2] und Michael Memminger[3] — [1]Ignaz-Günther-Gymnasium Rosenheim — [2]Rosenheim University of Applied Sciences — [3]Magic Aqua Rosenheim

Die Kunst bei der Erzeugung von Wasserklangbildern liegt darin, das aus dem Physikunterricht bekannte Konzept der *stehenden Welle* dafür zu nutzen, ein faszinierendes Bild zu erzeugen, obwohl man im Grunde *einfach nur Wasser fotografiert*. Klangschwingungen werden über ein Gefäß auf das Wasser übertragen, wodurch in diesem und an seiner Oberfläche, durch die sich ständig durchdringenden und überlagernden Wellen eine Vielzahl eindrucksvoller Strukturen entstehen, welche dann durch besondere Lichtreflexion sichtbar gemacht und fotografiert oder gefilmt werden können.

DY 50.11 Thu 15:00 Poster B2

Semi-classical treatment of chaotic systems — •Sebastian Rosmej — Carl-von-Ossietzky Universität Oldenburg

Up to today chaos is a fascinating but complicated topic in physics. So dealing with quantum chaos is extremely difficult but already the classical treatment of chaotic systems is non-trivial. A helpful bridge between classical and quantum chaos might be the semi-classical approach.

Using time-dependent semi-classical methods simple models are considered where regular and chaotic motion are possible. One example is the periodically driven anharmonic oscillator. A currently investigation of this periodically driven anharmonic oscillator is the derivation of probability distributions for work in the quantum case which is of fundamental interest in physics. An important step in this challenge is the semi-classical treatment of such systems.

DY 50.12 Thu 15:00 Poster B2

Controlling soliton molecules: Driven vibrations and separation switching — •Felix Kurtz[1], Claus Ropers[1], and Georg Herink[2] — [1]IV. Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Experimental Physics VIII - Ultrafast Dynamics, University of Bayreuth, Bayreuth, Germany

Solitons, localized excitations balanced by dispersion and nonlinearity, are of particular interest in various nonlinear systems. In analogy to real molecules, they can bind together and form "soliton molecules". Here, we study the behavior of soliton molecules in a mode-locked Ti:Sapph laser oscillator. Previously hidden internal dynamics of soliton molecules can now be accessed by employing the time-stretch dispersive Fourier transform (TS-DFT), which enables us to track the double-pulse separation and relative phase in real-time [1].

In the current work, we actively drive internal vibrations over a range of frequencies and amplitudes by weakly modulating the pump power. We resolve internal resonances of the soliton molecule, and detect higher harmonic and subharmonic responses. These observations are related to simulations in the framework of the complex Ginzburg-Landau equation. Beyond perturbative excitations, we apply stronger stimuli, which leads to a reversible switching between discrete pulse separations.

[1] G. Herink, F. Kurtz, B. Jalali, D.R. Solli, C. Ropers, *Science* **356**, 50-54 (2017)

DY 50.13 Thu 15:00 Poster B2

Minkowski Tensors: Robust and Versatile Shape Descriptors — •Fabian Schaller[1,2], Michael Klatt[3], and Sebastian Kapfer[1] — [1]Theoretical Physics, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Institute of Stochastics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]Department of Physics, Princeton University, Princeton, NJ 08544, USA

Minkowski scalars and tensors are a versatile, sensitive and robust way to quantify shape. Minkowski tensors are explicitly sensitive to anisotropy, relevant for example for elastic moduli or permeability of microstructured materials. Here, we present exemplary applications to real world data and to mathematical models. As examples, we analyze Voronoi and Delaunay tessellations of jammed disk packings and different point patterns. Furthermore we use the Minkowski tensors to analyze objects in gray-scale images. You can explore the possibilities of these shape measures online in our morphometer, an interactive sandbox which will be as well presented at our poster. Further details can be found on our website www.morphometry.org.

DY 50.14 Thu 15:00 Poster B2

Effective Large-Scale Equations in a Model of Passive Scalar Turbulence — •Tobias Bätge[1,2] and Michael Wilczek[1] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Faculty of Physics, University of Göttingen, Germany

Turbulent flows involve dynamics across a wide range of scales. Capturing this multi-scale dynamics remains a theoretical and computational challenge. For many practical applications, a coarse-grained description of the flow is needed, in which the small scales are treated in an effective manner. How can we obtain such effective large-scale equations? Here, we address this problem at the example of a simple, one-dimensional model for the advection of a passive scalar field. Similar to the Kraichnan model, the scalar is advected by a random Gaussian field and subject to diffusion. Despite its simplicity and analytical tractability, this model shows non-trivial features such as intermittency and anomalous scaling. We propose that effective large-scale equations can be obtained by ensemble-averaging over the small-scale velocity fluctuations. We show that this procedure leads to an effective diffusivity reminiscent of phenomenological eddy viscosity models. To test our approach, we quantitatively compare the large-scale statistics of fully resolved simulations with the ones obtained from our effective large-scale equations.

DY 50.15 Thu 15:00 Poster B2

Criticality in high-degree networks — •Lorenz Baumgarten and Stefan Bornholdt — Institut für Theoretische Physik, Universität Bremen

Criticality is a topic of interest in current brain research as well as statistical physics. Recently, a previously unknown critical point was discovered in high-degree threshold networks [1]. This paper opened a new possible area of investigation in a so far barely studied region.

Therefore, we further study criticality in high-degree networks and the effects of topological variants on the details of criticality, especially in the light of real critical brain networks.

[1] S. Bornholdt, J. Neto, M. de Aguiar, J. Brum, Inhibition as a determinant of activity and criticality in dynamical networks, arXiv 2017, 1712.08816

DY 50.16 Thu 15:00 Poster B2

Estimating low dimensional dynamical models for molecules — •Max Philipp Holl and Oliver Kamps — Institut für theoretische Physik, Universität Münster, Wilhelm-Klemm-Straße 9, 48149 Münster

The dynamics of molecules is a complex problem involving many degrees of freedom. However different states of the molecular system can often be described by only a few of them. We combine two data driven techniques to calculate a low dimensional representation for these systems and estimate dynamical models for the molecules. First we reduce the dimensionality of a time series using a nonlinear dimensionality reduction algorithm, Scalable ISOMAP [1]. Secondly we estimate the deterministic drift and stochastic driving on this reduced system using a data-driven estimation method, based on the Langevin equation [2].

[1] P. Das et al. Low-dimensional, free-energy landscapes of protein-folding reactions by non-linear dimensionality reduction. Proceedings of the National Academy of Sciences, 103(26):9885-9890, 2006.

[2] R. Hegger and G. Stock. Multidimensional Langevin modeling of biomolecular dynamics. The Journal of Chemical Physics, 130(3):034106, jan 2009.

DY 50.17 Thu 15:00 Poster B2

Complex Data Workflow Management using CaosDB — •Alexander Schlemmer[1,3], Henrik tom Wörden[1,2], Timm Fitschen[1,2], Daniel Hornung[1], Ulrich Parlitz[1,2,3], and Stefan Luther[1,2,3,4,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Nonlinear Dynamics, Georg-August-Universität, Göttingen, Germany — [3]German Center for Cardiovascular Research (DZHK), partner site Göttingen, Germany — [4]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Göttingen, Germany — [5]Department of Physics and Department of Bioengineering, Northeastern University, Boston, USA

Although scientific data has been used in digital formats for a long time, the data management is in many cases flawed and highly ineffective: In many scientific workgroups data files are spread over many devices, hidden in impractical directory tree structures and rarely sufficiently documented or annotated with metadata. Concepts for overcoming these problems, like the FAIR data principles, receive a lot of attention, but practical solutions for data workflow management are far from commonly implemented. Here we propose a data workflow management based on CaosDB (https://arxiv.org/abs/1801.07653) which is able to handle big amounts of complex data. The versatile semantic data model maps various data sources and data structures, such as data from different measurement devices or computer simulation data. In particular, the software includes a powerful and intuitive query language and a system for physical units.

DY 50.18 Thu 15:00 Poster B2

Die Kräfte beim Auseinanderziehen von ineinanderlegen Telefonbüchern — •Anna Treffurth und Thomas Grillenbeck — Ignaz-Günther-Gymnasium Rosenheim

Durch das Ineinanderlegen zweier Telefonbücher, indem man eine Seite des einen auf eine Seite des anderen Telefonbuches legt, entsteht eine potenzielle Reibungskraft. Diese kann je nach Versuchsparametern relativ klein oder extrem groß sein. Sogar so groß, dass sich an unseren regionalen Büchern, die nicht besonders dick sind, sogar eine erwachsene Person hängen kann, ohne dass diese auseinander gezogen werden. Dieses Phänomen und die dafür verantwortlichen Parameter habe ich untersucht.

DY 50.19 Thu 15:00 Poster B2

Wind speed modeling by nested ARIMA processes — •So-Kumneth Sim, Philipp Maass, and Pedro Lind — Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück

Wind speed modelling is of increasing interest, both for basic research and for applications, as, e.g. for wind turbines development and strategies to construct large wind power plants. Generally, such modelling is hampered by the non-stationary features of wind speed data that, to a large extent, reflect the turbulent dynamics in the atmosphere. We study how these features can be captured by nested ARIMA models. In this approach, wind speed fluctuations in given time windows are modelled by one stochastic process, and the parameter variation between successive windows by another one. For deriving the wind speed model, we use 20 months data collected at the FINO1 platform at the North Sea and use a variable transformation that best maps the wind speed onto a Gaussian random variable. We find that wind speed increments can be well reproduced for up to four standard deviations. The distributions of extreme variations, however, strongly deviate from the model predictions.

DY 50.20 Thu 15:00 Poster B2

Global Particle Sizing and Velocimetry in Clouds — •Marcel Schröder[1], Philipp Höhne[1], Gholamhossein Bagheri[1], and Eberhard Bodenschatz[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]Laboratory of Atomic and Solid State Physics and Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, NY 14853, USA

Weather forecasts and prediction of precipitation still remain uncertain due to insufficient understanding of cloud physics. This is mainly due to the presence of the large range of spatial and temporal scales within a turbulent environment in which the moist convection, cloud droplet growth and cloud formation take place. Particularly, the role of turbulence in droplet growth between 20 μm and 100 μm in diameter, known as the size gap problem, is not yet resolved. In order to shed light on the coupling of cloud microphysics and turbulence, we have developed a new setup based on Interferometric Particle Imaging (IPI) and Multi-pulse (here four-pulse) Particle Image Velocimetry (MPIV). The combination of IPI and MPIV techniques would allow to simultaneously measure droplet size, 2D spatial distribution, phase, as well as 2D velocity and acceleration. In the first step, we have found optimal parameters for designing the experimental setup. Then, a set of synthetic IPI images is made to assess the particle detection and sizing algorithms for different droplet size distributions and concentrations typically encountered in clouds. Finally, preliminary experiments are also carried out in the lab.

DY 50.21 Thu 15:00 Poster B2

Stable subharmonic patterns in spatially modulated phase separation — •Frederik Thomsen, Mirko Ruppert, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, Deutschland

We consider the standard continuum model for phase separation, the Cahn-Hilliard model, and investigate the effects of spatially periodic modulations of the control parameter on the onset of phase separation. We find by analytical approximations and numerical solutions a reduction of the critical value of the control parameter at the onset of modulated phase separation. In addition, we find stable spatial patterns with wavenumbers subharmonic to the modulation wavenumber.

DY 50.22 Thu 15:00 Poster B2

Orientation and coexistence of stripe patterns in small rectangular domains — •Mirko Ruppert and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, Deutschland

Motivated by experiments on pattern formation in small systems, we investigate the orientation of nonlinear stripe patterns in small, rectangular domains for different boundary conditions along the domain borders. In addition the orientation of stripe patterns is investigated for spatially varying control parameter, which is only supercritical in a small domain. We characterize, how the orientation of a pattern and the coexistence between different stripe orientations depend on the aspect ratio G between the length and the width of a domain. Orientational transitions take place at different values of G for different boundary conditions as well as in the case of control-parameter variations. We present analytical considerations and numerical solutions of the Swift-Hohenberg- model and the Brusselator.

DY 50.23 Thu 15:00 Poster B2

Rectangular wrinkle patterns in modulated skin layers on compliant substrates — •Nancy Mejia Villagran, Fabian Bergmann, Lisa Rapp, and Walter Zimmermann — Universität Bayreuth

We model the post-buckling behavior of wrinkles in thin inhomogeneous solid films supported by a homogeneous substrate under biaxial

compression. In thin films on substrates with different compressional loads along the two orthogonal directions, one has a preferred direction (anisotropy). The wave vector of the wrinkles at onset points therefore along the direction with the larger load. If the elastic properties of the thin film are spatially modulated with a modulation wavelength larger than the critical one, we show that rectangular wrinkle patterns are induced for equal biaxial loads, as well as for anisotropic biaxial loads. In the latter case, we find also undulations.

DY 50.24 Thu 15:00 Poster B2

Transition from nonlinear traveling to standing waves in confined systems — •Samuel Grimm, Fabian Bergmann, Lisa Rapp, and Walter Zimmermann — TP1, Universität Bayreuth

In E. coli bacteria, for example, self-organized pole-to-pole oscillations of Min proteins - resembling a short standing wave - ensure correct positioning of the cell division site. The same biochemical reaction leads to traveling protein waves on extended membranes in in vitro experiments. We have shown in [1], that these seemingly contradictory observations can be explained by basic principles of pattern formation: For a complex Swift-Hohenberg model a transition of nonlinear traveling wave patterns in extended systems to reflection-induced standing waves takes place by reducing the system length. We show with this contribution, that the same basic principles of pattern formation cause a transition to standing waves also in the case of a subcritical bifurcation to traveling waves. We also show, how spatiotemporally chaotic traveling wave states can be supressed in favor of standing waves in short systems. We explore this behavior in terms of complex Swift-Hohenberg models with an unconserved and a conserved order-parameter field.

[1] F. Bergmann, L. Rapp, W. Zimmermann, New J. Phys. (Fast track) 20, 072001 (2018)

DY 51: Poster: Stat. Phys., Comp. Meth

Time: Thursday 15:00–18:00 Location: Poster B2

DY 51.1 Thu 15:00 Poster B2

Random Field Ising Model with spatially disorder strength gradient — •Christoph Polle and Alexander K. Hartmann — Institut für Physik, University of Oldenburg, Germany

We study numerically [1] a three-dimensional Random Field Ising Model (RFIM) in which a spatially disorder strength gradient $h(x)$ is introduced. The gradient was chosen so that $h(x)$ is equal to the critical value $h_c = 2.28$ [2] at the half of the lattice in x-direction. The actual magnetic field acting on a spin i is defined as $h_i = h(x) * n_i$, where n_i is a (0,1) quenched Gaussian number.

To investigate the system efficiently the RFIM was transformed to a network, then the maximum flow problem was solved to determine the ground state [3]. This is done for different system sizes and realizations. From the ground state the magnetization, a specific-heat like quantity and the susceptibility where calculated as a function of x. Also the system was analyzed in the spirit of gradient percolation problems[4].

[1] A.K. Hartmann, Big Practical Guide to Computer Simulations, World Scientific Publishing, Singapore 2015.
[2] A.K. Hartmann and A.P. Young, Physical Rewiew B **64**, 214419 (2001).
[3] J.-C. Picard and H.D. Ratliff, Networks **5**, 357 (1975).
[4] B. Sapoval, M. Rosso, J.-F. Gouyet, Journal de Physique Lettres **46** (4), pp.149-156 (1985).

DY 51.2 Thu 15:00 Poster B2

Semi-automatic construction of Lattice Boltzmann models — •Dominic Spiller[1] and Burkhard Duenweg[1,2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Chemical Engineering, Monash University, Melbourne, Australia

A crucial step in constructing a Lattice Boltzmann model is the definition of a suitable set of lattice velocities, and the correct assignment of the associated weights. The poster outlines the functioning of a publicly available Python script which has been written to assist researchers in that task. The speed of sound c_s is considered as a parameter, which can, within limits, be chosen at will. Under this premise, the Maxwell–Boltzmann constraint equations are a system of linear equations to determine the weights, and hence amenable to numerical solution by standard linear algebra library routines. By suitable contractions, the tensor equations are mapped to a set of equivalent scalar equations, which simplifies the treatment significantly. Using a singular-value decomposition, the software is able to distinguish between (i) no solution, (ii) one unique solution, and (iii) infinitely many solutions. Case (ii) is analyzed in detail, and the range of permitted c_s values is calculated. The script can treat arbitrary spatial dimensions, and an arbitrarily large degree of isotropy, measured in terms of tensorial velocity moments of the weights. New models that have been found in two and three dimensions are isotropic up to tenth order.

DY 51.3 Thu 15:00 Poster B2

Self-learning Monte Carlo Methods — •Kai Meinerz and Simon Trebst — ITP, University of Cologne

The application of machine learning approaches has seen a dramatic surge across a diverse range of fields that aim to benefit from their unmatched core abilities of dimensional reduction and feature extraction. In the field of computational many-body physics machine learning approaches bear the potential to further improve one of the stalwarts in the field * Monte Carlo sampling techniques. Here we explore the capability of *self-learning* Monte Carlo approaches to dramatically improve the update quality in Markov chain Monte Carlo simulations. We implement such a self-learning approach using restricted Boltzmann machines which are trained to learn the probability distribution of the configuration space and are then used to suggest updates that are almost always accepted, thereby dramatically reducing autocorrelation effects. It can, in principle, be applied to all existing Monte Carlo flavors and is tested here for both classical and quantum Monte Carlo techniques applied to a variety of many-body problems.

DY 51.4 Thu 15:00 Poster B2

Finite temperature structure of Hybrid Perovskites from ab-initio and classical MD — •Jonathan Lahnsteiner[1], Georg Kresse[1], Jurn Heinen[2], and Menno Bokdam[1] — [1]University of Vienna — [2]University of Amsterdam

Determining the finite temperature structure of the hybrid perovskite MAPbI3 is a challenge for both experimental and theoretical methods. A very powerful computational method that can resolve the atomic structure is molecular dynamics (MD). The resulting structure depends on the density functional approximation (DFA) in the case of ab-initio MD and the force field in classical MD. We compare the structure between 250 K and 400 K obtained with different DFAs and force fields in one consistent manner. In a previous study, we observed a low level of a dynamic correlation between MA molecules in large scale PBEsol MD calculations. Therefore the relative ordering of the neighboring organic molecules as well as the symmetry of the PbI3 framework is analyzed. The distribution function of the molecules is used to map out an effective energy surface for the rotation of a single molecule. This surface is accurately modeled by a pair of cubic harmonics. Available experimental data in literature are compared to the structure obtained with the different methods. The spread in these data is still too large to uniquely determine the method that *best* describes the perovskite, however promising candidates and outliers have been identified. In agreement with our previous benchmarking study based on RPA perturbation theory calculations , we find the SCAN functional is the most likely choice for the MD calculations of the hybrid perovskite.

DY 51.5 Thu 15:00 Poster B2

Entropy Production in Non Equilibrium Steady State Systems — •Timon Wittenstein, Marius Bause, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Entropy production is believed to contain structural information of non-equilibrium steady states. For further insight, the entropy production is calculated along an ensemble of stochastic off-equilibrium trajectories. By fixing start and end point, a localized entropy production for a transition between two states in conformational space is introduced. The trajectory based entropy production is compared to

statistics based Markov State Model and a theory based value on a minimal two dimensional model. This quantity is a special case of the detailed fluctuation theorem by Crooks and extends detailed balance towards non-equilibrium steady states. Trajectory based calculation of local entropy production can be used for improved sampling in simulation or as a physics based constrained for Markov Sate Modeling.

DY 51.6 Thu 15:00 Poster B2

Phase transition for parameter learning of Hidden Markov Models — •Nikita Rau[1], Jörg Lücke[2], and Alexander K. Hartmann[1] — [1]Institut of Physics, University of Oldenburg — [2]Department of Medical Physics, University of Oldenburg

We study by computer simulations [1] the learning process during which the parameters of Hidden Markov Models (HMMs) [2] are estimated from a sequence of observed data which is generated artificially. Using the Baum-Welch algorithm [3], an Expectation-Maximization algorithm from the field of Machine Learning, we are capable of observing the learning process of different sized HMMs. By changing the amount of accessible learning data and its noise level, we observe a phase-transition-like change in the performance of the learning algorithm. For bigger HMMs and more learning data, the learning behaviour improves tremendously by reaching a certain threshold in the noise strength. Before reaching the threshold, the parameter-learning is prone to errors, after exceeding it, the learning process becomes nearly perfect. This observation is strongly dependant of the amount of learning data.

[1] A. K. Hartmann, Big Practical Guide to Computer Simulations, World-Scientific, Singapore 2015)
[2] R. Durbin, S. Eddy, A. Krogh, and G. Mitchison, Biological Sequence Analysis (Cambridge University Press 2001)
[3] L. E. Baum, Ann. Math. Statist., vol. 41, 164–171, 1970

DY 51.7 Thu 15:00 Poster B2

Critical Exponent ν of the Ising Model in Three Dimensions with Long-range Correlated Disorder — •Stanislav Kazmin[1,2] and Wolfhard Janke[1] — [1]University of Leipzig — [2]Max Planck Institute for Mathematics in the Sciences

We analyze the critical behavior of the site-diluted Ising model in three dimensions using Monte-Carlo simulation techniques. The case of uncorrelated defects is compared to the long-range correlated case where the space correlation function between the defects obeys a power-law decay. We discuss different methods of critical exponent ν extraction and compare our results to theoretical predictions.

DY 51.8 Thu 15:00 Poster B2

A Theoretical Investigation of Hydrocarbon Decomposition at High Temperature and High Pressure — •Nehzat Safaei, Kurt Kremer, and Omar Valsson — Max Planck Institute for Polymer Research, Ackerman- nweg 10, 55128, Mainz, German

We have studied reaction kinetics of hydrocarbon decomposition at high pressures and temperatures using variationally enhanced sampling method. Investigation of hydrocarbons decomposition witch provides valuable information about the rate of radical creation and subsequent reactions, specially at extreme conditions where there is a serious lack of both thermodynamic and kinetic data, can reveals new insights to the synthesis of most interesting carbon-based compounds such as graphene and nanodiamond which are the promising materials for a variety of applications. In order to calculate the decomposition rate of hydrocarbons in different thermodynamics conditions, we have performed molecular dynamics simulation to explore the phase space of different systems of hydrocarbons with different chain lengths. Variationally enhanced sampling method along with metadynamics is employed to calculate the rate of decomposition reactions. In this approach, an effective bias potential is constructed and implemented as a fixed bias which speeds up the molecular dynamics time by facilitating escape over dissociation barrier. We employed metadynamics with an infrequent deposition stride to ensure that the trajectory does not stuck in any regions. We have measured the validity of the rare event assumption by the p-value test of cumulative distribution function of the data fitted to the Poisson expression.

DY 51.9 Thu 15:00 Poster B2

Non-flat histogram techniques in application to complex free energy landscapes — •Fabio Mueller, Stefan Schnabel, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

Simulation of systems with rugged free-energy landscapes such as spin glasses and polymers are intrinsically difficult and algorithmic improvements for such systems are still needed to enlighten the nature of their low-temperature phase. We developed Monte Carlo non-flat histogram methods, which base on parametric optimization of well-known flat histogram techniques in generalized ensembles, tailored explicitly for systems with complex free-energy landscapes.

DY 51.10 Thu 15:00 Poster B2

Critical properties of long-range ferromagnetic quantum Ising chains — •Stephan Humeniuk — Institut für Theoretische Physik III, Universität Stuttgart — Current address: Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

The ferromagnetic Ising chain is of great historical value, being one of the first models for which a Kosterlitz- Thouless (KT) transition was found and due to its important role in the creation of renormalization group theory [1,2]. In this work some gaps are filled in in the understanding of this well-studied model in the presence of a transverse field, notably the role of a diverging kink size for observing the KT transition in finite-size simulations. The quantum critical point of the inverse-square ferromagnet is highly anisotropic in real space and imaginary time, with a dynamical critical exponent z=1/2.

[1] Anderson et al., PRB 1, 4464 (1970); Kosterlitz, PRL 37, 1577 (1976). [2] Bhattacharjee et al., PRB 24, 3862 (1981).

DY 51.11 Thu 15:00 Poster B2

Serially-Connected Domain Model for Phase Transitions in Disordered Porous Solids — •Henry R.N.B. Enninful, Adrianna Wójciak, Dirk Enke, and Rustem Valiullin — Leipzig University, Leipzig, Germany

Detailed elucidation of the pore structure of (nano-)porous solids is important for their optimization for various applications such as energy storage, separations and catalysis. While existing characterization approaches work well for ordered, single-pore mesoporous solids, the complex morphological structure of pore network and accompanying them cooperativity effects in phase transitions render the currently used approaches inapplicable for disordered materials.

In this work, we demonstrate the potentials of a recently developed connected domain model (CDM), which intrinsically contains both the structural complexity and cooperativity effects [1]. It is essentially based on a statistical average over linear chains of pores connected to each other and takes account of the change of the transition mechanisms depending on the phases state in adjacent pores. The model is validated by comparing its predictions to the results of GCMS simulations and is further used to rationalize the freezing and melting transitions in a family of porous glasses with different pore sizes.

[1] D. Schneider; D. Kondrashova; R. Valiullin, *Phase transitions in disordered mesoporous solids*, Scientific Reports, 2017, 7, 7216.

DY 52: Poster: Active Matter, Microswimmer, Microfluidics

Time: Thursday 15:00–18:00 Location: Poster B2

DY 52.1 Thu 15:00 Poster B2

Active Rotation of Janus particles — •Burelbach Jérôme and Stark Holger — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

The active motion of Janus particles offers a wide range of interesting applications, from dynamic clustering [1] and microrotation [2] to the self-assembly of rotating micro-machines [3]. We theoretically study the rotation of active particles based on Onsager's reciprocal relations [4], by exploiting the fact that the corresponding Onsager transport coefficients are skew-symmetric. In particular, we present a theoretical model for a self-rotating particle, showing that self-rotation relies on two asymmetries, one in the interfacial interaction with the surrounding fluid, and the other in the thermodynamic field created by the particle.

[1] Pohl, O., & Stark, H. (2015). Self-phoretic active particles interacting by diffusiophoresis: A numerical study of the collapsed state and dynamic clustering. European Physical Journal E, 38(8).

[2] Jiang, Hong-Ren, Natsuhiko Yoshinaga, and Masaki Sano. "Active motion of a Janus particle by self-thermophoresis in a defocused laser beam." Physical review letters 105.26 (2010): 268302.

[3] Maggi, Claudio, et al. "Self-assembly of micromachining systems powered by Janus micromotors." Small 12.4 (2016): 446-451.

[4] Onsager, Lars. "Reciprocal relations in irreversible processes. I." Physical review 37.4 (1931): 405.

DY 52.2 Thu 15:00 Poster B2

Motion of fronts and clusters in an active Allen-Cahn model — •Fenna Stegemerten and Uwe Thiele — Institute of Theoretical Physics Westfälische Wilhelms-Universität Münster

Active matter is composed of many particles which are able to transform different types of energy into motion. This may result in motility-induced clustering or directed collective motion. Such phenomena are observable for swarming in fauna as well as for artifical microswimmers. The collective structures may consist of disordered or well ordered arrangements and are referred to as active clusters and active crystals, respectively. In order to understand aspects of the behaviour of active clusters we employ a rather simple model for active matter, namely, the active Allen-Cahn (aAC) equation: The passive Allen-Cahn equation is coupled to a polarization field similar to the active phase field model (aPFC) in [1]. We then study occurring clusters and the motion of fronts in aAC. In particular, we provide bifurcation diagrams and show that the onset of motion occurring with increasing activity corresponds to a drift-ptichfork bifurcation similar to the case of aPCF [2]. Additionally, we we find that motion is not only controlled by the activity parameter but is also affected by the chemical potential. We track the drift-pitchfork bifurcation in the corresponding parameter space. Finally, we show that depending on the chemical potential the passive AC equation generates pulled and pushed fronts and discus their existence in the active case. [1] A. M. Menzel and H. Löwen Phys. Rev. Lett. (2013) [2] L. Ophaus, et al. Phys. Rev. E (2018)

DY 52.3 Thu 15:00 Poster B2

Probing the Dynamics of Self-Electrophoretic Swimmers using Lattice Boltzmann — •Michael Kuron[1], Georg Rempfer[1], Joost de Graaf[2], and Christian Holm[1] — [1]Institut für Computerphysik, Universität Stuttgart, Deutschland — [2]Institute for Theoretical Physics, Universiteit Utrecht, Nederland

Many simulational studies are available of the rich transient and collective behavior in catalytically-propelled colloids or microswimmers. However, virtually none consider both the hydrodynamic and phoretic fields and most do not take into account even one of them. We introduce a continuum model based on the lattice Boltzmann method that incorporates both effects and is capable of simulating the dynamic behavior of many swimmers. Our swimmers propel via experimentally relevant self-electrophoretic mechanisms with bulk reactions.

DY 52.4 Thu 15:00 Poster B2

Antimargination of microparticles and platelets in branching vessels — •Christian Bächer[1], Alexander Kihm[2], Lukas Schrack[1,3], Lars Kaestner[4], Matthias W. Laschke[5], Christian Wagner[2], and Stephan Gekle[1] — [1]Biofluid Simulation and Modeling, Bayreuth, Germany — [2]Experimental Physics, Saarland University, Saarbrücken, Germany — [3]Institute for Theoretical Physics, Innsbruck, Austria — [4]Institute for Molecular Cell Biology, Research Centre for Molecular Imaging and Screening, Center for Molecular Signaling (PZMS), Medical Faculty, Saarland University, Homburg/Saar, Germany — [5]Institute for Clinical & Experimental Surgery, Saarland University, Homburg/Saar, Germany

Microparticles in red blood cell suspension are studied in a vessel confluence and a bifurcation - typical geometries for blood vessel networks. Using three-dimensional Lattice-Boltzmann simulations we find strong effects on cell and particle distribution: flowing through a confluence triggers an additional, surprisingly stable cell-free layer in the center with microparticles undergoing antimargination into this central cell-free layer. In contrast to the perturbed margination in a vessel confluence, we obtain full microparticle margination in branching vessels. Margination in branching vessels and antimargination behind confluences may explain in vivo findings of strongly different platelet distribution in arterioles (mainly bifurcations) and venules (mainly confluences).

DY 52.5 Thu 15:00 Poster B2

The role of inertia in active nematic turbulence — •Colin-Marius Koch and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen

Suspensions of active agents with nematic interactions exhibit complex spatio-temporal dynamics such as mesoscale turbulence. Continuum descriptions for such systems are typically inspired by the theory of liquid crystals and combine hydrodynamics with active nematic stresses. The resulting equations feature an advective nonlinearity which represents inertial effects. The generically low Reynolds number of such active flows raises the question of the importance of the inertial effects. To address this question, we investigate active turbulence in a two-dimensional dense suspension of active nematic liquid crystals. We quantitatively compare numerical simulations with and without nonlinear advection of the flow field. This study will help to better understand the interplay of self-induced turbulent flow and local ordering.

DY 52.6 Thu 15:00 Poster B2

Validity of the low Reynolds number approximation for collective microswimmer hydrodynamics — •Jan Cammann[1], Jörn Dunkel[2], Jonasz Słomka[3], and Michael Wilczek[1] — [1]Max Planck Institute for Dynamics and Self-Organization — [2]Department of Mathematics Massachusetts Institute of Technology — [3]ETH Zürich

Microswimmers, such as bacteria, sperm cells and motile algae, are typically found in regimes where the relevant length and velocity scales allow their hydrodynamic interactions to be studied in the limit of low Reynolds numbers (Re). This simplifies the Navier-Stokes to the Stokes equation. In this approximation inertial effects are completely neglected. For individual swimmers this approximation is known to work well, whereas for large numbers of swimmers the hydrodynamic flows produced by the individuals may interfere constructively to produce higher local values of Re. Using a combination of analytical and numerical approaches, we study the dependence of the local Reynolds number on different configurations of microswimmers modeled as extended point force dipoles acting upon the fluid. Thus, we explore the limits of low Re approximations and whether inertial effects become relevant for the collective hydrodynamics of dense microswimmer suspensions.

DY 52.7 Thu 15:00 Poster B2

Shape-anisotropic microswimmers: Influence of hydrodynamics — •Arne W. Zantop and Holger Stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Active components that constitute active matter, as for example bacteria or active filaments, are often elongated in shape. The shape and the stiffness of the active components clearly influence both their individual as well as their collective dynamics and pattern formation.

On length scales several orders larger than the size of the constituents, active materials exhibit many fascinating phenomena distinct from their passive counterparts such as the formation of vortices or turbulent structures. While these phenomena have already been

studied both in experiments and simulations [1,2], identifying the individual role of thermal fluctuations as well as direct steric and hydrodynamic interactions is still subject of current research.

In this context, we numerically model shape-anisotropic microswimmers with rod shape by composing them from overlapping spherical squirmers [3]. We simulate the hydrodynamic flow field initiated by the active rods using the method of multi-particle collision dynamics. We present results for the collective dynamics of the active rods varying their area fraction, Peclet number, and aspect ratio.

[1] Dunkel *et al.*, PRL 110.22 (2013): 228102.
[2] Wensink *et al.*, PNAS 109.36 (2012): 14308-14313.
[3] Downton *et al.*, J. of Ph.: Cond. Mat. 21.20 (2009): 204101.

DY 52.8 Thu 15:00 Poster B2

Measurement of the fluid-flow-field generated by an attached self-thermo-phoretic micro swimmer — •Nicola Söker and Frank Cichos — Leipzig University

We measure the 3D flow field induced by a heated metal caped polystyrene micro particle adherent to a glass surface in water. In current literature it is assumed, that thermo-phoresis can be well described by an induced slip flow proportional to the temperature gradient along a surface or phase boundary. The motion performed by a self thermo-phoretic micro-swimmers is then given by slip flows along the swimmers surface and boundary slip-flows in the environment. We look at an adherent micro-swimmer since then the flow field is long ranged. Also a freely moving swimmer would also sample different environmental conditions. The average fluid velocity field is recorded using gold nanoparticle tracers. Three dimensional motion is extracted from the defocused images of the gold nanoparticles. The flow fields are compared to numerical calculations of the flow field including all hydrodynamic boundaries.

DY 52.9 Thu 15:00 Poster B2

Polarization of Brownian swimmers with spatially heterogeneous activity — •Sven Auschra[1], Nicola Söker[2], Paul Cervenak[1], Viktor Holubec[1], Klaus Kroy[1], and Frank Cichos[2] — [1]Institute for Theoretical Physics, University of Leipzig, 04103 Leipzig, Germany — [2]Peter Debye Institute for Soft Matter Physics, University of Leipzig, 04103 Leipzig, Germany

Janus particles fuelled by laser heating are paradigmatic autophoretic microswimmers. Their dynamics under constant driving has been well characterized [1-3]. We consider situations in which the particles' propulsion strength fluctuates in space and time, due to a variable fuel supply. Specifically, we analyze their spatial and orientational distribution experimentally, realizing prescribed spatial and temporal activity variations via the laser heating. We find depletion in regions of higher activity and polarization in activity gradients. Using Brownian dynamics simulations and a powerful numerical solver for Fokker-Planck equations [4], we can reproduce the experimental observations. A simple run-and-tumble process captures the observed features, qualitatively, and provides some analytical insights.

[1] A. Bregulla and F. Cichos: Faraday Discuss. 184, 381*391 (2015).
[2] H. Jiang, N. Yoshinaga, and M. Sano: PRL 105, 268302 (2010).
[3] A. Würger: Rep. Prog. Phys. 73, 126601 (2010).
[4] V. Holubec, K. Kroy and S. Steffenoni: arXiv:1804.01285v2 (2018).

DY 52.10 Thu 15:00 Poster B2

Brownian molecules formed by delayed harmonic interactions — •Daniel Geiss and Viktor Holubec — Institut für theoretische Physik, Uni Leipzig, Deutschland

A time-delayed response of individual living organisms to information exchange within groups or swarms leads to the formation of complicated collective behavior. A recent experimental setup where Brownian particles interact via time-delayed forces aims to mimic this behavior [1]. We study a system of N Brownian particles interacting via a harmonic, time-delayed potential. For $N < 4$, we model the problem analytically by linear stochastic delay differential equations, and for $N > 3$ we use Brownian dynamics simulations. The particles form molecular-like structures which become increasingly unstable with the number of particles and the length of the delay. We evaluate the entropy fluxes in the system and develop an appropriate time-dependent transition state theory to characterize transitions between different isomers of the molecules.

[1] U. Khadka, V. Holubec, H. Yang, and F. Cichos: Nat. Commun. 9, 3864 (2018)

DY 52.11 Thu 15:00 Poster B2

Isotropic - Nematic Phase Transition of Active Rods — •Felix Winterhalter and Matthieu Marechal — Theroetische Physik I - Friedrich Alexander Universität Erlangen, Erlangen, Deutschland

The Isotropic - Nematic transition of spherocylinders is a well studied phenomenon. This transition gets modified for spherocylinders with active motion along its orientation axis. We found that for short rods the Isotropic-Nematic transition is shifted to higher packing fractions depending on the velocity.

DY 52.12 Thu 15:00 Poster B2

Passive swimming of deformable particles in shaken fluids — Matthias Laumann[1], •Andre Förtsch[1], Eva Kanso[2], and Walter Zimmermann[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Aerospace and Mechanical Eng., University of Southern California, Los Angeles, California 90089, USA

It was demonstrated recently that deformable, passive and asymmetric particles of different mass density than the fluid exhibits in a shaken fluid a net motion [1] with respect to the fluid. We give an explanation in terms of semi-analytical calculations why passive elastic particles show a net motion in shaken fluids. We also demonstrate that common symmetric particles can display a net motion if the time-dependence of the fluid motion is nonsymmetric with respect to an half-period of fluid oscillation. We further show results from simulations of capsules and provide parameters for which a capsule allows to rise in shaken fluid against gravity. The results may be helpful to assemble artificial microswimmers or may be useful for cell sorting and manipulation in microfluidic devices.

DY 52.13 Thu 15:00 Poster B2

Oscillatory bifurcations in active particle systems — •Andreas Förtsch, Fabian Bergmann, Lisa Rapp, and Walter Zimmermann — Theoretische Physik, Universität Bayreuth, 95440 Bayreuth

We introduce a model with two types of interacting active species A and B. We assume A-A attraction, A-B attraction and B-B repulsion/attraction. The use continuum and Brownian dynamics modelling of the two chemotactically interacting active particles. The continuum model for the two interacting species shows either a stationary or an oscillatory instability of the homogeneous particle distribution. Since the both particle types are conserved the instabilities lead either to a non-oscillatory active phase separation [1] or to an oscillatory type of active phase separation. Above the oscillatory onset of active phase separation, we find in simulations traveling and spatio-temporal dynamics of clusters.

[1] F. Bergmann, L. Rapp, W. Zimmermann, Active phase separation: A universal approach, Phys. Rev. E 98, 020603(R) (2018)

DY 53: Poster Quantum Systems

Time: Thursday 15:00–18:00 Location: Poster B2

DY 53.1 Thu 15:00 Poster B2

Resonance–assisted tunneling in 4D normal–form Hamiltonians — •Markus Firmbach[1,2], Felix Fritzsch[1], Roland Ketzmerick[1,2], and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

Dynamical tunneling is a paradigmatic example of the interplay of classical phase-space structures and the quantum effect of tunneling. In particular the presence of classical nonlinear resonances leads to significant enhancement of tunneling known as resonance–assisted tunneling. We describe this resonance–assisted tunneling in a 4D normal–form Hamiltonian as it captures all fundamental features. Focusing on the case of a double resonance we study the morphology of the quantum states. Quantitatively we describe tunneling in terms of the weight of these states in classically disconnected regions. By applying perturbative methods we reveal the underlying mechanism and obtain excellent qualitative and quantitative agreement with numerical data.

DY 53.2 Thu 15:00 Poster B2

Entanglement in bipartite systems with a mixed phase space — •Maximilian Kieler[1] and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

The entanglement of pure states in a bipartite system can be characterized by the von Neumann entropy. We consider the case of two coupled quantized standard maps, where one map is chosen to be integrable while the other is fully chaotic. By increasing the coupling a transition to nearly maximal entanglement is found. We investigate the implications of the integrable part on the transition of the spectral statistics and the von Neumann entropy. The analytical description will be based on a suitable random matrix model and the identification of the relevant transition parameter.

DY 53.3 Thu 15:00 Poster B2

Geometry of complex instability in 4D symplectic maps — •Jonas Stöber[1] and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

In dynamical systems with more than two degrees of freedom periodic orbits may show many different types of stabilities. For 4D symplectic maps so-called complex instability commonly occurs, which is not possible for 2D symplectic maps. For a specific 4D map we investigate the transition from elliptic to complex unstable dynamics of a fixed point under parameter variation. The change in the geometry of regular structures is visualized using 3D phase space slices and in frequency space. The chaotic dynamics is studied using escape time plots and by computations of the 2D invariant manifolds associated with the complex unstable fixed point.

DY 53.4 Thu 15:00 Poster B2

A microwave realization of the chiral GOE — •Aimaiti Rehemanjiang[1], Martin Richter[2,3], Ulrich Kuhl[2], and Hans-Jürgen Stöckmann[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]InPhyNi, Université Côte d'Azur, 06100 Nice, France — [3]School of Mathematical Sciences, University of Nottingham, Nottingham NG7 2RD, UK

The universal features of the spectra of chaotic systems are well reproduced by the corresponding quantities of the random matrix ensembles [1]. Depending on symmetry with respect to time reversal and the presence or absence of a spin 1/2 there are three ensembles: the Gaussian orthogonal (GOE), the Gaussian unitary (GUE), and the Gaussian symplectic ensemble (GSE). With a further particle-antiparticle symmetry there are in addition the chiral variants of these ensembles [2]. Relativistic quantum mechanics is not needed to realize the latter symmetry. A tight-binding system made up of two subsystems with only interactions between the subsystems but no internal interactions, such as a graphene lattice with only nearest neighbor interactions, will do it as well. First results of a microwave realization of the chiral GOE (the BDI in Cartan's notation) will be presented, where the tight-binding system has been constructed by a lattice made up of dielectric cylinders [3].

[1] O. Bohigas, M. J. Giannoni, and C. Schmit. PRL **52**, 1 (1984).
[2] C. W. J. Beenakker. Rev. Mod. Phys. **87**, 1037 (2015).
[3] S. Barkhofen, M. Bellec, U. Kuhl, and F. Mortessagne. PRB **87**, 035101 (2013).

DY 53.5 Thu 15:00 Poster B2

Stickiness in the volume-preserving Arnold-Beltrami-Childress map — •Swetamber Das[1] and Arnd Bäcker[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Technische Universität Dresden, Institut für Theoretische Physik, Dresden

Stickiness and power-law behavior of Poincaré recurrence statistics for higher-dimensional systems is still unexplained, while for systems for two degree-of-freedom, the mechanism is fairly well understood. We study such intermittent behavior of chaotic trajectories in three-dimensional volume-preserving systems using the example of the Arnold-Beltrami-Childress map. If two action-like variables of the map are nearly conserved, the phase space displays tubular regular structures surrounded by a chaotic sea. Stickiness occurs around these tubes and manifestations of partial barriers to transport are observed. We investigate this dynamics in phase space and in frequency space to identify the underlying origin of stickiness.

DY 53.6 Thu 15:00 Poster B2

Localization and transport in coupled kicked rotors — •Sanku Paul[1] and Arnd Bäcker[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden 01187, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, Dresden 01069, Germany

Coupled kicked rotors are a prototypical example of a periodically driven system. It consists of two one-dimensional rotors receiving periodic kicks as well as interacting with each other at the time of the kicks. We investigate the classical diffusion and quantum transport and its dependence on the strength of the coupling between the rotors.

DY 53.7 Thu 15:00 Poster B2

Relaxation dynamics after the removal of a static force: Binary operators and impact of eigenstate thermalization — •Jonas Richter[1], Jacek Herbrych[2], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]University of Osnabrück, Germany — [2]The University of Tennessee, USA

We study the relaxation dynamics of expectation values under unitary time evolution for a certain class of initial states. The latter are thermal states of the quantum system in the presence of an additional static force which, however, become nonequilibrium states when this force is eventually removed. While for weak forces the dynamics is well captured by linear response theory (LRT), the case of strong forces, i.e., initial states far away from equilibrium, is highly nontrivial. Employing a combination of analytical arguments as well as numerical calculations for interacting quantum lattice models, we unveil that the nonequilibrium dynamics at high temperatures can, in various cases, be universally generated by a single correlation function in the entire regime close to and far away from equilibrium. Specifically, we consider so-called binary operators and study, as an example, the dynamics of spinless fermions in a random potential. In addition, we discuss the role of the eigenstate thermalization hypothesis (ETH) and establish a connection between ETH and LRT.

[1] J. Richter, J. Herbrych, R. Steinigeweg, Phys. Rev. B **98**, 134302 (2018).
[2] J. Richter, R. Steinigeweg, arXiv:1711.00672.
[3] J. Richter, J. Gemmer, R. Steinigeweg, arXiv:1805.11625.

DY 53.8 Thu 15:00 Poster B2

Correlational latent heat by nonlocal quantum kinetic theory — •Klaus Morawetz — M\"unster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universit\'ario Lagoa nova,59078-970 Natal, Brazil

The nonlocal kinetic equation unifies the achievements of the transport in dense quantum gases with the Landau theory of quasiclassical transport in Fermi systems. Large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors [1]. The remaining corrections are expressed in terms of shifts in space and time that characterize the non-locality of the scattering process [2]. In

this way quantum transport is possible to recast into a quasi-classical picture [3]. The balance equations for the density, momentum, energy and entropy include besides quasiparticle also the correlated two-particle contributions beyond the Landau theory [4]. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy. For Maxwellian particles a sign change of the latent heat is reported at a universal ratio of scattering length to the thermal De Broglie wavelength. This is interpreted as a change from correlational heating to cooling [5]. [1] Ann. Phys. 294 (2001) 135, [2] Phys. Rev. C 59 (1999) 3052, [3] "'Interacting Systems far from Equilibrium -Quantum Kinetic Theory"', Oxford University Press, (2017), ISBN 9780198797241, [4] Phys. Rev. E 96 (2017) 032106, [5] Phys. Rev. B 97 (2018) 195142

DY 53.9 Thu 15:00 Poster B2

Dynamics and equilibration of the finite spin-boson model — •Sebastian Wenderoth, Ulrich Wärring, Tobias Schätz, and Michael Thoss — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany

The study of thermalization processes in finite quantum systems has been of great interest recently. Of particular importance in this context is the eigenstate thermalization hypothesis, which states that the expectation values of few-body observables in an energy eigenstate are, under certain conditions, indistinguishable from microcanonical expectation values [1].
Recent experimental progress in the field of cold atoms and trapped ions, has made it possible to study these questions in tailored quantum systems. Inspired by a recent experimental realization of a finite version of the spin-boson model in a trapped ion experiment [2], we have theoretically investigated the dynamics of such a system.
Employing the Multiconfiguration time-dependent Hartree approach [3], which allows us to treat a large number of bosonic modes in a numerically exact way, we analyze the relaxation dynamics. In particular we investigate the dependence of the dynamics on the number of bosonic modes and the influence of a thermal initial state.
[1] M. Rigol *et al.*, Nature **452**, 854 (2008).
[2] G. Glos *et al.*, Phys. Rev. Lett. **117**, 170401 (2016).
[3] H. Wang *et al.*, New J. Phys. **10**, 115005 (2008).

DY 53.10 Thu 15:00 Poster B2

Equilibration and thermalization in the XXZ model — •Philipp Jaeger[1,2], Andreas Klümper[2], and Jesko Sirker[1] — [1]University of Manitoba, Department of Physics and Astronomy, Winnipeg, MB, Canada — [2]Bergische Universität Wuppertal, Fachbereich C - Fachgruppe Physik, Wuppertal, Germany

The quantum XXZ model is an integrable lattice model, hence exact solutions are available via Bethe ansatz (BA). For many ground-state properties or correlation functions, explicit expressions are available. Expectation values of observables at late times after a quench can be calculated for example using the generalized Gibbs ensemble (GGE) formalism. However, particular dynamical correlation functions (DCF) are notoriously hard to calculate from BA, and perturbations of the XXZ model can not be treated directly. Using numerics, it is possible both to obtain DCF relatively easy and to include perturbations. Here, we present numerical results obtained employing the light-cone renormalization group algorithm.

DY 53.11 Thu 15:00 Poster B2

Modelling cells as pressurized elastic shells — •Behzad Golshaei[1], Renata Garces[1], Samaneh Rezvani[1], Octavio E. Albarran[1], and Christoph F. Schmidt[1,2] — [1]Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen, 37077 Göttingen — [2]Department of Physics, Duke University, Durham, NC 27708, USA

Animal cells and bacteria are enveloped and sealed by lipid membranes and mechanically protected by cortical polymer networks. Cells typically maintain a small (eukaryotic cells) or large (bacteria) positive osmotic pressure against their environment. Volume and shape regulation also impact the mechanical properties of cells. The mechanical properties of cells can be probed by exerting external force and measuring cell response. To better understand micromechanical optical trapping experiments with suspended rounded cells, and AFM experiments on bacteria, we employed finite element simulations and modelled cells as pressurized elastic shells.

DY 54: Poster: Complex, Fluids, Glasses, Granular

Time: Thursday 15:00–18:00 Location: Poster B2

DY 54.1 Thu 15:00 Poster B2

A Phase Field Crystal Approach for Patchy Colloids — •Robert F. B. Weigel and Michael Schmiedeberg — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany

Patchy colloids are particles with discrete rotational symmetry and anisotropic interaction, thus preferring certain bond angles. Finding the complex equilibrium phases in systems with patchy colloids is challenging.

We propose and study a mean field model for patchy colloids that is motivated by the phase field crystal theory for systems with particles exhibiting 2-fold rotational symmetry as in liquid crystals for which a theory has been proposed in [1]. In such an approach the free energy $F[\psi, U]$ is given as a functional of a real-valued density-like field ψ and a complex-valued orientation field U, which encodes the intensity and direction of the orientation. As usual in phase field crystal models, F is composed of a Landau-like power series in the fields along with an expansion with respect to the gradients as well as coupling terms respecting the rotational symmetry of the particles. Numerical minimization of F yields a rich phase diagram of complex structures. Our special interest is to find out how orderings with non-crystallographic symmetries, such as in quasicrystals, can be obtained.
[1] Achim *et al.*, Phys. Rev. E **83**, 061712 (2011)

DY 54.2 Thu 15:00 Poster B2

X-ray Particle Tracking of Granular Materials — •Luis Torres-Cisneros[1], Kit Windows-Yule[2], Patric Müller[1], and Thorsten Pöschel[1] — [1]Institute for Multiscale Simulation, Cluster of Excellence "Engineering of Advanced Materials", Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Deutschland — [2]School of Physics and Astronomy, University of Birmingham, Edgbaston, United Kingdom

Nowadays the fundamental understanding of granular materials (a finite amount of macroscopic fragmented matter that interacts mainly by dissipative collisions and friction) flowing is one of the most exciting challenges. We could find these systems present in nature as in industry; i. e., in a rock avalanche or in silo downloading corn grains. Given that there are in the literature many theoretical studies done in order to understand its underlying rules an experimental setup capable to corroborate it is needed.

In the last years the X-ray tomography appeared to let us able to have an insight in granular materials at static conditions, as a non-invasive technique. But given that we could find a granular system in a fluid-like state the present tools used to study granular materials at static conditions are not suitable. In this way the present research is aimed in order to establish the main ideas concerning the features needed in an X-Ray machine capable to track the trajectories in a granular system at non-static conditions.

DY 54.3 Thu 15:00 Poster B2

Rheology of a model composite of liquid crystals and magnetic nanoparticles — •Nima H. Siboni, Gaurav P. Shrivastav, and Sabine H. L . Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36 D-10623 Berlin

Liquid crystals (LC) functionalized with nano-to-micro sized magnetic particles (MNP) have attracted much recent attention due to their rich self-assembly, dynamics and a wide range of applications [1]. Using molecular dynamics (MD) simulations, we show that the flow properties of the LC matrix can be modified by the inclusion of spherical MNPs.

We study the rheology of an 80:20 binary mixture of LCs and MNPs in the isotropic phase for various dipolar coupling strengths of the MNP by shearing it via Lees-Edwards periodic boundary conditions with constant shear rates. The mixture shows a shear thinning be-

havior for the considered range of the dipolar coupling strength. The extent of the non-Newtonian region in the flow curve increases with increasing dipolar coupling strength of the MNPs. The nematic order in LC and MNP both increases with strain, however, the degree of ordering in MNPs is higher than in LCs.

References:

[1] G. P. Shrivastav, and S. H. L. Klapp, arXiv:1809.08288 (2018).
[2] G. P. Shrivastav, N. H. Siboni and S. H. L. Klapp, in preparation.

DY 54.4 Thu 15:00 Poster B2

Investigation of the glassy dynamics of charged Lennard-Jones systems with molecular dynamics simulations — •Lukas Hecht, Robin Horstmann, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstraße 6, 64289 Darmstadt, Germany

The explanation of the glass transition is one of the most challenging topics in physics of condensed matter. To get ahead, recent work investigated systematically altered water and silica variants in bulk and confinement to ascertain the glass transition behavior via molecular dynamics simulations [1]. A strong relation between the activation energy in the simple liquid regime at high temperatures and the glass transition temperature was found. Moreover, it proved useful to decompose the activation energy into a temperature independent part and a temperature dependent part associated with cooperative dynamics, which is an exponential function of temperature [2].

Since water and silica have a complex structure with prefered order, it is difficult to ascertain basic mechanisms behind the glass transition. Therefore, we focus on simpler systems, explicitly mixtures of charged Lennard-Jones atoms. We vary the mixing ratio of the atoms as well as their partial charges and analyze their dynamics in wide temperature ranges. In this way, it is possible to strongly vary the high-temperature activation energy and the glass transition temperature and, thus, to obtain further insights into their relation.

[1] J. Geske et al., Z. Phys. Chem., 2018, 232(7-8), pp 1187-1225
[2] B. Schmidtke et al., Phys. Rev. E, 2012, 86, 041507

DY 54.5 Thu 15:00 Poster B2

Thermodynamic bond-angular instability drives glass formation — •Andrii Babich[1,2], Maria Göbel[1,5], Volodymyr Bugaev[2,3], Johannes Roth[3], Gerhard Grübel[1,4], and Peter Wochner[2] — [1]Center for Ultrafast Imaging,University of Hamburg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Institute for Functional Matter and Quantum Technologies, University of Stuttgart — [4]DESY, Hamburg — [5]Max Planck Institute for Intelligent Systems, Stuttgart

Glasses are indispensable in everyday life and technology. However, the microscopic mechanisms generating this state of matter remain subject to debate. Within MD simulations and the original statistical-thermodynamic ring approximation, we revealed that at the vitrification the 4-point positional correlations caused by the configurational entropy create an instability with respect to formation of a structural state with angular order. This state is described in terms of only one dominant orientational mode in the angular statistical variance of the density fluctuations, which results in a mesoscopic-scale mutual ordering of the polytetrahedral clusters. Their lifetime exhibits the well-known slowdown at approaching the glass transition point. Our results can be tested by coherent diffraction experiments at the newly developed light sources and will be an essential guide to determine the best conditions for successful experiments in a broad range of glassy systems, e.g. colloidal, metallic glasses and water.

DY 54.6 Thu 15:00 Poster B2

The Quest for Spontaneous Core Rotation in Ferrofluid Pipe Flow — •Max Fabian Steudel, Ingo Rehberg, and Reinhard Richter — Experimentalphysik 5, Universität Bayreuth, Bayreuth, Germany

Ferrofluidic pipe flow in a constant [1] or alternating [2] axial magnetic field has attracted much interest because the flow can conveniently be controlled by the parameters of the applied field. More recently, for a flow in a static field, a transition from a purely axial flow to a steady swirling one has been unveiled in analytical and numerical studies [3]. The swirl appearance is predicted to yield a sharp increase of the flow rate [3]. To uncover this transition we measure the flow rate of different types of ferrofluid as a function of the applied magnetic field.

[1] M. A. Martsenyuk, Y.L. Raikher and M. I. Shliomis, Sov. Phys. JETP **38**, 413 (1994).
[2] A. Zeuner, R. Richter and I. Rehberg, Phys. Rev. E **58**, 6287 (1998).
[3] Alexei Krekhov and Mark Shliomis, Phys. Rev. Lett. **118**, 114503 (2017).

DY 54.7 Thu 15:00 Poster B2

Structural and mechanical properties of sodium, magnesium, and calcium metaphosphate glasses: insights from molecular dynamics simulations — •Achraf Atila and Erik Bitzek — Materials Science & Engineering, Institute I, Friedrich-Alexander Universität Erlangen-Nürnberg (FAU)

Phosphate glasses are of great interest in various industrial, technological and clinical applications. Compared to silicate glasses, they have a lower glass transition and melting temperatures. Doping phosphate glasses by alkali or alkaline earth ions reduces the glass transition temperature and makes them more chemically durable. Metaphosphate glasses, defined as the composition in which the ratio O/P is three, have a chain-like structure made of PO_4 tetrahedra. These glasses are usually isotropic due to the random orientation of the chains. Until now, there are few atomistic simulations studies on the mechanical and structural properties of binary metaphosphate glasses. Here, we present molecular dynamics simulations regarding the effect of different non-framework cations (Na^+, Ca^{2+}, Mg^{2+}) on the structural and the mechanical properties of the metaphosphate glasses using a Morse-type pair potential with Coulomb interactions (J. Phys. Chem. B, 2006, 110 (24), pp 11780−11795). We investigate and compare the mechanical properties of these glasses by applying tension, compression, and shear. Radial distribution functions, their projections on spherical harmonics and angular distribution functions are used for analyzing the glasses structure.

DY 54.8 Thu 15:00 Poster B2

Molecular dynamics study of structural and dynamic properties of ionic liquids at amorphous silica surfaces — •Robin Koester, Tamisra Pal, and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

Structural and dynamic properties of imidazolium-based ionic liquids change severely in presence of rigid interfaces. Previous molecular dynamics studies of [Bmim][NTf_2] revealed layered structures and a considerable slowdown of dynamics in the layers next to amorphous silica surfaces [1]. In recent simulation studies of [Bmim][PF_6] and [Bmim][BF_4] similar effects for systems confined by amorphous silica slit pores were found [2]. For both anions preferential localization at irregularly distributed sites at the interface can be observed. While these sites differ in volume and number of associated silanol groups, favourable local structures appear to be a major determinant. Building on the preceding studies, we relate the residence time to the structural properties of the silica surface near the adsorption sites to obtain a microscopic understanding for the mechanism of the slowdown in the interfacial layer. Additionally, we examine anion dynamics by means of spatially resolved analysis of correlation functions. Further investigations aiming for a better understanding of the slowed down dynamics involve the examination of anion dynamics in terms of hopping motion required to change site.

[1] Li et al., Langmuir, 2013, 29, pp. 9744-9749
[2] T. Pal and M. Vogel, J. Phys. Chem. C, 2018, 122, pp. 624-634

DY 54.9 Thu 15:00 Poster B2

Electrohydrodynamic instabilities of droplets suspended in highly viscous liquids — Sebastian Rühle, •Martin Brinkmann, and Ralf Seemann — Experimental Physics, Saarland University

Motivated by recent experimental results we study electroconvective flows in poorly conducting droplets that are suspended in an ambient liquid with high viscosity and conductivity. The coupled electrostatic and Stokes problem for a homogeneous external field is solved numerically for both 2d and axially symmetric 3d droplets using a boundary element approach. A number of dynamical flow regimes and instabilities are observed whose appearance is controlled by the contrast of viscosity, conductivity, and dielectric permittivity, as well as the magnitude of the applied field. If the timescale of charging or discharging of the 2d droplets is comparable or larger than the timescale of flow, the droplets may display transient shape oscillations and rotational flows.

DY 54.10 Thu 15:00 Poster B2

Fast calculation method for determining the shape of static liquid/liquid or liquid/vapor interfaces under the influence of electrical fields — •Sebastian Bohm and Erich Runge — Technische Universität Ilmenau, FG. Theoretische Physik 1, Weimarer Straße 25, 98693 Ilmenau

Due to the constant trend towards smaller systems new methods for the manipulation of liquids on the micro-scale are required. One important and frequently used technique to manipulate liquids on small scales is the so called Electrowetting-on-Dielectrics (EWOD) effect. EWOD based microfluidic devices provide high-throughput platforms for a wide range of applications in biology, chemistry and nanotechnology. For the design and optimization of such devices, the shape of liquid/vapor or liquid/liquid interfaces needs to be determined. However, the numerical simulation presents a great challenge due to the coupling of fluidics and electrodynamics.

This work reports a new and fast method for the determination of the shape of static three-dimensional interfaces under the influence of electrical fields. Additionally, the influence of interface effects and gravity are considered. The simulation also allows to determine the shape of the interface near the contact line with high accuracy and verify that the local contact angle at the contact line is voltage independent. The simulation results are confirmed by EWOD experiments on systems with different geometries.

DY 54.11 Thu 15:00 Poster B2

Self-assembly in magnetic filament systems: impact of internal factors — •Elena Pyanzina, Tatjana Belyaeva, Marina Kashpurova, and Ekaterina Novak — Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia

The fundamental understanding of the self-assembly properties of colloidal systems is one of the key topics in current research on novel microstructured soft materials and technologies. In this work we investigate self-assembly of magnetic filaments of different topology with different additional interaction and particles polydispersity. We performed molecular dynamics simulations using a Langevin thermostat. Cluster analysis based on graph theory is used to analyze the obtained data. At the moment we are analyzing the results, but we can already say that the introduction of additional attraction and particles polydispersity significantly expands the structural diversity of the self-assembly of magnetic filaments, and the effect of magnetic dipole-dipole interaction remains substantial. All these results will pave the way for the development of analytical models and identify the most interesting building block candidates for the design of new magnetoresponsive materials.

DY 55: Poster: Noneq. Stat. Phys., Stat. Bio. Phys., Brownian

Time: Thursday 15:00–18:00 Location: Poster B2

DY 55.1 Thu 15:00 Poster B2

Coherent oscillations in periodically driven systems — •Lukas Oberreiter[1], Andre Cardoso Barato[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Department of Physics, University of Houston, Houston, Texas 77204, USA

Biochemical oscillations are prevalent in living organisms. Organisms count time with biochemical oscillators to properly time their functions. Since these oscillations rely on a stochastic process fluctuations in the period of oscillation lead to a finite precision. The latter is quantified by the number of coherent oscillations. A former study [1] revealed that the number of coherent oscillations of an autonomous system is bounded by the topology of the network of states and the thermodynamic force that drives the system out of equilibrium. Here, we extend the analysis to *periodically* driven systems. We construct a specific external protocol showing that the number of coherent oscillations is not necessarily bounded. Moreover, the trade-off between the number of coherent oscillations and its costs, the entropy production rate, is investigated.

[1] A. C. Barato and U. Seifert, Phys. Rev. E **95**, 062409 (2017)

DY 55.2 Thu 15:00 Poster B2

Coarse-grained toy model for ring polymer melts — •Stanard Mebwe Pachong[1], Jan Smrek[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]University of Vienna, Austria

Nonconcatenated and unknotted rings in melt subdiffuse on length scales several times larger than their gyration radius [1]. It has been hypothesised that ring threadings [2,3], although they might be quantitatively marginal [4]. On the other hand, the prolonged onset of diffusion can be observed also in a dense system with a small number of particles with a relatively deep correlation hole. Due to a finite-size effect, a significant rearrangement would be necessary for large particle displacements which results in longer sub-diffusion regime. As the simulated ring melts [1] were composed of only 200 rings and have deep correlation holes, the effect can be at play. In order to understand the cause of the subdiffusion of the rings melt, we attempt to falsify the threading hypothesis. We constructed a simple coarse-grained (soft-sphere) model of rings that (trivially) cannot thread, but can exhibit the correlation hole effect. We have not found a sign of subdiffusion. This goes in line with a recent observation that threading and diffusion relax on similar time scales[4].

References

[1] J. D. Halverson et al., J. Chem. Phys., 134,204905(2011) [2] Michieletto et al. ACS Macro Lett.,3,255-259(2014) [3] J. smrek and A. Y. Grosberg,ACS Macro Lett.5,750-754(2016) [4] J. Smrek, K. Kremer, A. Rosa ,unpublished(2018)

DY 55.3 Thu 15:00 Poster B2

Field Theoretic Thermodynamic Uncertainty Relation for the Kardar-Parisi-Zhang Equation — •Oliver Niggemann and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

In this poster I will present a way to show the validity of the thermodynamic uncertainty relation in the setting of the one-dimensional Kardar-Parisi-Zhang (KPZ) equation with white in time, spatially colored Gaussian noise for weak coupling, i.e. $\partial_t h(x,t) = \nu\partial_x^2 h(x,t) + \lambda/2(\partial_x h(x,t))^2 + \eta(x,t)$ with $\langle\eta(x,t)\rangle = 0$ and $\langle\eta(x,t)\eta(x',t')\rangle = D(|x-x'|)\delta(t-t')$. Within Hilbert space theory of stochastic partial differential equations the height field $h(x,t)$ is regarded as a trajectory $t \mapsto h(x,t)$, $h(x,t) \in \mathcal{H}$. On a finite spatial interval $[0,L]$, $\mathcal{H} = \mathcal{L}_2(0,L)$ is a suitable choice, and the eigenfunctions of the differential operator $\mathcal{A} \equiv \nu\partial_x^2$ with periodic boundary conditions form an orthonormal base of $\mathcal{H}$. The height $h(x,t)$ and the noise $\eta(x,t)$ are expressed then by means of eigenfunction expansions. In this setting, the following thermodynamic uncertainty relation has been derived for the non-equilibrium steady state: $\Delta s_{\mathrm{tot}}^{\mathrm{stat}}\epsilon^2 > 2 + O(\lambda^2)$. Here $\Delta s_{\mathrm{tot}}^{\mathrm{stat}} \equiv \int_0^t dt' \left((\partial_x h(x,t'))^2, \hat{D}^{-1}(\partial_x h(x,t'))^2\right)_{\mathcal{L}_2}$ is the stationary state total entropy production, and $\epsilon^2 \equiv \langle\|h(x,t) - \langle h(x,t)\rangle\|_{\mathcal{L}_2}^2\rangle / \|\langle h(x,t)\rangle\|_{\mathcal{L}_2}^2$ is the squared variation coefficient of $h(x,t)$, evaluated for $t \gg 1$. $\hat{D}^{-1}$ is the inverse of the integral covariance operator with kernel $D(|x-x'|)$. The uncertainty relation holds for $D(x)$ describing a class of regular spatially colored noise, which, in a suitable limit, approximates white noise and for white noise itself, i.e. $D(x) = \delta(x)$.

DY 55.4 Thu 15:00 Poster B2

Hot Brownian Motion on Short Time Scales — •Xiaoya Su — Molecular Nanophotonics, Peter Debye Institute for Soft Matter Physics, University Leipzig, Linnéstraße 5, 04103, Leipzig

Hot Brownian motion describes the motion of a heated microsphere in a liquid. It is a fundamental issue for thermal non-equilibrium. A temperature field is created around the heated particle decaying with 1/r and a stationary temperature and viscosity field is moving with the particle through the liquid. The non-equilibrium dynamics of the particle now differs from the unheated particles and an effective temperature and viscosity is introduced to describe the system. Here we report on a study of the fluctuations of a heated particle in an optical trap with nanosecond and nanometer resolution. We calculated the mean squared displacement MSD and the autocorrelation function of velocity(VACF) of the heated particle and found evidence that the short time motion is influenced by the temperature increase.

DY 55.5 Thu 15:00 Poster B2

Characterizing non-equilibrium steady states via invariant manifolds — •Prakhar Godara, Jens Lucht, Marco Mazza, and Stephan Herminghaus — MPI für Dynamik und Selbstorgani-

sation, Göttingen

It is still an unsolved question whether there is a general way to predict the steady state of a driven (non-equilibrium) system (a convection roll, a spiral wave, spatiotemporal chaos etc.) solely from its microscopic physics. The main obstacle is that detailed balance is breached in such systems. However, by describing the system not in state space, but instead in the space of all possible closed cycles in that space, detailed balance reappears. We demonstrate for the two-dimensional Fokker-Planck equation that the transition rates in this 'cycle space' can be obtained from simple integrals of the drift field and the diffusion field, yielding a general potential in cycle space. The occupation probabilities of the non-equilibrium steady states, which correspond to the invariant manifolds of the drift field, are then given by a Boltzmann factor containing this potential. We corroborate our findings numerically.

DY 55.6 Thu 15:00 Poster B2

Large deviations for a driven underdamped particle in a periodic potential — •Lukas P. Fischer and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Germany

Large deviation theory is a versatile tool that proved useful for establishing connections between current fluctuations and thermodynamic steady state properties, e.g. the thermodynamic uncertainty relation [1]. Previous studies, however, were limited to systems which are diffusive in all variables, i.e. overdamped Brownian motion or Markov jump processes. In a previous study we extended the work to underdamped Brownian motion of a single, driven particle in a periodic potential and derived an expression for the large deviation functional of the empirical phase space density [2]. This functional replaces the level 2.5 functional used for overdamped dynamics. Although bounds can be derived from the underdamped level 2 functional in general, a straightforward proof of the thermodynamic uncertainty relation for underdamped dynamics is not possible. In this contribution we revisit the underdamped large deviation function for a driven particle in a periodic potential with focus on the thermodynamic uncertainty relation. We present some ansatzes for thermodynamic bounds and discuss the problems arising from them. Furthermore we outline difficulties which have to be faced following other techniques.

[1] A.C. Barato, U. Seifert, Phys. Rev. Lett. **114**, 158101 (2015)
[2] L.P. Fischer, P. Pietzonka, U. Seifert, Phys. Rev. E **97**, 022143, (2018)

DY 55.7 Thu 15:00 Poster B2

Dynamic ordering of driven spherocylinders in a non-equilibrium suspension of small colloidal spheres — •Anton Lüders, Ullrich Siems, and Peter Nielaba — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The ordering effects of driven spherocylinder-shaped rods in a colloidal suspension of small spheres confined to a two-dimensional channel geometry are observed via Brownian Dynamics simulations without hydrodynamics. To describe the ordering, an order parameter and an expression for a potential of mean force of an equivalent equilibrium system are defined and analyzed. By varying the application point of the external force along the rods and thus the resulting lever, a transition from a preferred orientation parallel to the direction of the force to a preferred orientation perpendicular to the direction of the force was observed. It is shown that this effect can only be found, if the spheres and multiple rods are present. Furthermore, a dependency of the order parameter on the absolute value of the force was discovered. The analysis of the potential of mean force further indicates a transition between two different phases of mean orientation. The observation of the flow equilibrium mean velocity in channel direction led to a s-shaped progression regarding the lever dependency, also marking a transition between two states linked to the mean orientation of the rods. By means of a finite size analysis it was possible to show that the transition between the two orientation states is a general phenomenon of the observed rod-sphere mixture.

DY 55.8 Thu 15:00 Poster B2

Stochastic rotor engine based on the electron shuttling mechanism — •Christopher W. Wächtler[1], Philipp Strasberg[2], and Gernot Schaller[1] — [1]Institute of Theoretical Physics, Berlin, Germany — [2]Física Teòrica: Informació i Fenòmens Quàntics, Barcelona, Spain

The single electron shuttle is an example of a nano-scale system exhibiting a transition towards self-oscillation, where mechanical oscillations of a metallic grain are achieved by sequential electron tunnelling between the grain and two connecting leads. We theoretically investigate how one can use this shuttling mechanism to build a stochastic rotor engine which converts between chemical and mechanical work by applying a bias voltage between the two leads. Furthermore, we show that this rotor engine can also be used as a heat engine by applying a temperature bias between the electronic leads and the heat reservoir connected to the rotor. Besides the average thermodynamic quantities we additionally study the fluctuations of these quantities.

DY 55.9 Thu 15:00 Poster B2

A generalization of the thermodynamic uncertainty relation to periodically driven systems — •Timur Koyuk[1], Udo Seifert[1], and Patrick Pietzonka[1,2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, CambridgeCB3 0WA, United Kingdom

The thermodynamic uncertainty relation expresses a universal trade-off between precision and entropy production, which applies in its original formulation to current observables in steady-state systems. We generalize this relation to periodically time-dependent systems and, relatedly, to a larger class of inherently time-dependent current observables [1]. In the context of heat engines or molecular machines, our generalization applies not only to the work performed by constant driving forces, but also to the work performed while changing energy levels. The entropic term entering the generalized uncertainty relation is the sum of local rates of entropy production, which are modified by a factor that refers to an effective time-independent probability distribution. The conventional form of the thermodynamic uncertainty relation is recovered for a time-independently driven steady state and, additionally, in the limit of fast driving. We illustrate our results for a simple model of a heat engine with two energy levels.

[1] T. Koyuk, U. Seifert, and P. Pietzonka, A generalization of the thermodynamic uncertainty relation to periodically driven systems, J. Phys. A: Math. Theor. (2018), arXiv:1809.02113, in press.

DY 55.10 Thu 15:00 Poster B2

Unravelling the energetics of stochastic surface growth with artificial neural networks — •Thomas Martynec[1], Stefan Kowarik[2], and Sabine H.L. Klapp[1] — [1]Institut fuer Theoretische Physik, Technische Universitaet Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut fuer Physik, Humboldt-Universitaet zu Berlin, Newtonstrasse 15, 12489 Berlin, Germany

Stochastic surface growth by means of molecular beam epitaxy (MBE) is one of the most widely used techniques to fabricate thin film devices for various technological applications. It involves a competition between the adsorption of particles and various diffusion processes. Initially, particles like atoms, colloids or organic molecules are adsorbed on an ideally flat and defect free discrete substrate at rate F. This is followed by thermally activated Arrhenius-type diffusion processes to neighboring lattice sites. Once clusters are formed, nucleation on top of these clusters sets in. Depending on the strength Ees of the Ehrlich-Schwoebel barrier that reduces the interlayer transport rate of particles, surface growth proceeds either in a smooth or rough fashion. We demonstrate that an artificial neural network can precisely determine the value of the interlayer transport barrier from images of the growing islands with a 'wedding cake' morphology.

[1] C. M. Bishop, Rev. Sci. Instr. 65 1803 (1994)
[2] T.Martynec and S.H.L. Klapp Phys. Rev. E 98, 042801 (2018)

DY 55.11 Thu 15:00 Poster B2

The role of interactions in a in a quantum heat pump for fermionic atoms — •Manuel Alamo, Arko Roy, and Andre Eckardt — Max-Planck-Institut für Physik komplexer Systeme

We design and investigate a quantum heat pump for fermionic atoms in a structured optical potential. It is based on a structure given by two quantum dots hosting two levels each. By applying periodic driving, we engineer an energy-selective transport between both dots. Coupling each of them to a different fermionic reservoir, particles and heat is transported. We investigate the role of interactions on the performance of this device as a heat pump by employing Floquet-Born-Markov theory.

DY 55.12 Thu 15:00 Poster B2

Non-equilibrium dynamics of open systems exchanging particles — •JunHyuk Woo[1], Segun Goh[2], Jean-Yves Fortin[3],

and MooYoung Choi[1] — [1]Department of Physics and Center for Theoretical Physics, Seoul National University, Seoul 151-747, Korea — [2]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany — [3]Institut Jean Lamour, Groupe de Physique Statistique, Département de Physique de la Matière et des Matériaux, CNRS-UMR 7198, Vandoeuvre-lès-Nancy, F-54506, France

We consider an open system in contact with a reservoir, where particles as well as energies can be exchanged between them, and present a description of the dynamics in terms of mixed (pseudo)spin and state variables. Specifically, a master equation is constructed out of the exchange rates for particles and for energies, which allows us to probe the system in the grand canonical description. In particular, by means of the state resummation analysis, we obtain coupled time evolution equations for the probability distributions of the system as well as the environment. This is exemplified by a standard growth model, where the steady-state density function exhibits power-law behavior with the exponent depending on the microscopic parameters of the rate equations.

DY 55.13 Thu 15:00 Poster B2

Diffusion of solitons — •Tony Albers and Günter Radons — Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

Solitons propagating in nonlinear dissipative media have properties different from the ones in conservative media. One of the special features of these solitons are explosions, i.e., transient enlargements of the soliton that can lead to a spatial shift of the center of mass of the soliton if the explosion is asymmetric. A long sequence of such asymmetric explosions leads to a random walk of the soliton which is reminiscent of a diffusion process [1,2]. In this contribution, we use a simple but prototypical model, namely the one-dimensional cubic-quintic complex Ginzburg-Landau equation, to investigate the dynamical behavior of the solitons. We will characterize the random motion with quantities known from diffusion theory and, especially, we will pay attention to the ergodic properties of the soliton motion. We introduce two stochastic models, one discrete in time and one continuous in time, which are able to reproduce the observed features of the soliton motion.

[1] J. Cisternas, O. Descalzi, T. Albers, and G. Radons, Phys. Rev. Lett. **116**, 203901 (2016)
[2] J. Cisternas, T. Albers and G. Radons, Chaos **28**, 075505 (2018)

DY 55.14 Thu 15:00 Poster B2

Nonlinear response theory in classical systems — •Fenna Müller and Matthias Krüger — Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

The fluctuation-dissipation theorem describes the linear response of a system in relation to equilibrium fluctuations. However, there is no corresponding general theorem or scheme to do the same for the nonlinear response. Here, we develop a coarse grained scheme for computation of nonlinear responses based on path integrals [2]. Comparing the time reversed system to its original, one can identify several components, such as entropy flux in the first order, as done e.g. in [1]. In experiments it is oftentimes impossible or impractical to observe the whole system with all its microstates, however. Therefore, we extend the path integral formalism to include a coarse graining, see [2]. All response formula describe the system in terms of coarse grained variables and direct access to microscopic variables is not necessary. We explore using this method for time dependent pertubations by applying it to the analytically solvable two state model.

[1] Basu, U., Krüger, M., Lazarescu, A., & Maes, C. (2015). Frenetic aspects of second order response. Physical Chemistry Chemical Physics, 17(9), 6653-6666. [2] Basu, U., Helden, L., & Krüger, M. (2018). Extrapolation to Nonequilibrium from Coarse-Grained Response Theory. Physical review letters, 120(18), 180604.

DY 56: Annual General Meeting of the Dynamics and Statistical Physics Division

Time: Thursday 18:30–19:30 Location: H3

Duration 60 min.

DY 57: Talk Alberto Fernandes-Nieves

Time: Friday 9:30–10:00 Location: H3

Invited Talk DY 57.1 Fri 9:30 H3

Toroidal droplets, active nematics and topological defects — •Alberto Fernandez-Nieves — School of Physics, Georgia Tech (USA) — Department of Condensed Matter Physics, University of Barcelona (Spain) — ICREA - Institució Catalana de Recerca i Estudis Avançats, Barcelona (Spain)

In this talk, I will briefly discuss our recent work with toroidal droplets: How to make them, how they evolve, and how to stabilize them. I will then discuss how active nematics organize on a torus and show that despite the activity and inherent out-of-equilibrium nature of our experimental system, we see traces of the ground-state expectations –curvature induced defect unbinding– for passive nematics. However, activity augments the behavior leading to completely unexpected positive and negative defect distributions and a very rich overall dynamic behavior.

DY 58: Active matter II (joint session BP/CPP/DY)

Time: Friday 9:30–12:00 Location: H11

DY 58.1 Fri 9:30 H11

Dynamics of an active model microswimmer in an anisotropic fluid — •Abdallah Daddi-Moussa-Ider and Andreas M Menzel — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Düsseldorf

Several recent experiments investigate the orientational behavior of self-propelled bacteria and colloidal particles in anisotropic fluids such as nematic liquid crystals. Correspondingly, we study theoretically the dynamics of a simple model microswimmer in a uniaxially anisotropic fluid. The behavior of both puller- and pusher-type swimmers in the anisotropic fluid is analyzed. Depending on the propulsion mechanism as well as the relative magnitude of different involved viscosities, we find alignment of the microswimmer parallel or perpendicular to the anisotropy axis. The observed swimmer reorientation results from the hydrodynamic coupling between the self-induced fluid flow and the anisotropy of the host fluid. Our theoretical predictions are found to be in qualitative agreement with recent experiments on swimming bacteria in nematic liquid crystals. They support the objective of utilizing the anisotropy of a surrounding fluid to guide individual swimmers and self-propelled active particles along a requested path, enabling controlled active transport.

Reference: A. Daddi-Moussa-Ider and A. M. Menzel. Dynamics of a simple model microswimmer in an anisotropic fluid: Implications for alignment behavior and active transport in a nematic liquid crystal, Phys. Rev. Fluids 3, 094102 (2018).

DY 58.2 Fri 9:45 H11

Dynamics of bottom-heavy squirmers — •Felix Ruehle and Holger Stark — Institut für Theoretische Physik, Technische Uni-

versität Berlin, Germany

The self-propulsion of biological or synthetic microswimmers is often influenced by a gravitational field [1,2], where a density mismatch leads to sedimentation and an offset center of mass triggers reorientation along the direction of gravity so that they swim upwards [2]. Combining these passive effects with the non-equilibrium properties of active motion creates novel and interesting dynamics, both in dense and dilute suspensions [3]. In particular, a large variety of dynamical behaviours has been observed for the squirmer microswimmer model [4,5].

In this contribution we focus on bottom-heavy squirmers and determine their state diagram, depending on the gravitational force and acting torque. For strong gravitational forces we observe conventional sedimentation, whereas the density profile is inverted for weaker forces. Additionally, we find stable convective plumes for neutral squirmers that become metastable as the torque increases. We also observe spawning clusters at the bottom if the sedimentation velocity almost equalizes the swimming speed. Spawning clusters and continuous plumes do not occur for pusher and puller type swimmers.

[1] J. Palacci, et al., *Phys. Rev. Lett.* **105**, 088304 (2010).
[2] K. Drescher et al., *Phys. Rev. Lett.* **102**, 168101 (2009).
[3] K. Wolff, A. M. Hahn and H. Stark, *EPJE* **36**, 1 (2013).
[4] J.-T. Kuhr et al., *Soft Matter* **13**, 7548 (2017).
[5] F. Rühle et al., *New J. Phys.* **20**, 025003 (2018).

DY 58.3 Fri 10:00 H11

Bead-spring modelling of triangular microswimmers — •Sebastian Ziegler[1], Alexander Sukhov[2], Jens Harting[2,3], and Ana-Sunčana Smith[1,4] — [1]PULS Group, Institute for Theoretical Physics, Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Germany — [3]Dep. of Applied Physics, Eindhoven University of Technology, The Netherlands — [4]Division of Physical Chemistry, Ruder Bošković Institute Zagreb, Croatia

A customary approach to model mechanical micropropulsion is to prescribe the swimming stroke. However, with this approach, the hydrodynamic features of the motion are in essence smoothed over and the problem becomes a purely geometrical one. The alternative approach, yet significantly more demanding, is to impose not the stroke itself but the forces driving the device. The swimming stroke then emerges as a result of the various forces acting in the system. We use a perturbative approach to examine a triangular swimmer's behaviour in the Stokes regime that is also eligible for general geometries of bead-spring swimmers. The device shows a multifaceted comportment dependent on a number of therefore identified effective parameters. The triangular swimmer is further used as a prototype to study the influence of variations in the viscosity of the surrounding fluid on its motion.

DY 58.4 Fri 10:15 H11

Simple Swimmers Reverse Direction near a Surface — •Michael Kuron[1], Philipp Stärk[1], Joost de Graaf[2], and Christian Holm[1] — [1]Institut für Computerphysik, Universität Stuttgart, Deutschland — [2]Institute for Theoretical Physics, Universiteit Utrecht, Nederland

The motion of a microswimmer can change substantially in the presence of a surface. Sperm are known to move in circular trajectories near a wall, paramecia move in sinusoidal trajectories through a tube, and chemical swimmers can orbit around spherical obstacles. Spherical squirmers are one of the simplest model microswimmers, commonly defined by the first two Legendre modes of their surface slip velocity. In this talk, we use the squirmer to numerically investigate the effect of the environmental geometry. We discuss how the transition between scattering and orbiting/hovering depends on the strength of the squirmer's hydrodynamic dipole moment. Interestingly, we observe cases where the squirmer orbits/hovers along a surface in a direction opposite to that observed in bulk. This effect is present both in a far-field theoretical model and our lattice Boltzmann calculations, which accurately account for the near-field flow. These results extend the understanding of the effect of geometry on microswimmer motion and show the importance of finite swimmer size and associated near-field effects.

DY 58.5 Fri 10:30 H11

Bacterial Swarming Dynamics — •Hannah Jeckel[1,2,3], Eric Jelli[1,2], Raimo Hartmann[1], Praveen Singh[1], Rachel Mok[3,4], Jan Frederik Totz[5], Lucia Vidakovic[1], Bruno Eckhardt[2], Jörn Dunkel[3], and Knut Drescher[1,2] — [1]Max Planck Institute for Terrestrial Microbiology, Marburg, Germany — [2]Department of Physics, Philipps-University Marburg, Germany — [3]Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA — [4]Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA — [5]Institute for Theoretical Physics, Technical University Berlin, Germany

Coordinated dynamics of individual components in active matter are an essential aspect of life on all scales. Establishing a comprehensive, causal connection between intracellular, intercellular, and macroscopic behaviors has remained a major challenge due to limitations in data acquisition and analysis techniques suitable for multiscale dynamics. Here, we combine a high-throughput adaptive microscopy approach with machine learning, to identify key biological and physical mechanisms that determine distinct microscopic and macroscopic collective behavior phases which develop as *Bacillus subtilis* swarms expand over five orders of magnitude in space. Our experiments, continuum modeling, and particle-based simulations reveal that macroscopic swarm expansion is primarily driven by cellular growth kinetics, whereas the microscopic swarming motility phases are dominated by physical cell-cell interactions. These results provide a unified understanding of bacterial multi-scale behavioral complexity in swarms.

DY 58.6 Fri 10:45 H11

Effects of collective bacterial motility on their chemotactic navigation — •Remy Colin and Victor Sourjik — Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

At high cell density, swimming bacteria exhibit collective motility patterns, self-organized through physical interactions of a however still debated nature. Although high-density behaviors are frequent in natural situations, it remains unknown how collective motion affects chemotaxis, the main physiological function of motility that enables bacteria to follow chemical and other gradients in their environment. Here, we systematically investigated this question in the model organism *Escherichia coli*, varying cell density, cell length and suspension confinement. The characteristics of the collective motion indicated that its emergence is dominated by hydrodynamic interactions between swimmers. We observed that moderate increase in cell density enhanced the chemotactic drift of bacteria, whereas it was suppressed at higher densities, because the collective motion disturbed the choreography necessary for chemotactic sensing. We suggest that this physical hindrance imposes a fundamental constraint on high-density behaviors of motile bacteria, including swarming as well as the formation of multicellular aggregates and biofilms.

DY 58.7 Fri 11:00 H11

Feedback Control of Active Microswimmers — •Alexander Fischer[1], Haw Yang[2], and Frank Cichos[1] — [1]Uni Leipzig — [2]Princeton University

Collective motion created by the interaction of autonomous individuals plays a major role in flocks of birds, bacterial growth or the motion of robotic swarms. Sensing and reacting to signals is a fundamental issue of life. Microswimmers, which are artificial objects that mimic the active motion of biological systems, do not have such sensing and response features built in yet, but may gain them through an external control of their propulsion. Here we explore an information exchange between artificial microswimmers by computer-controlled feedback processes. We have created a setup where multiple active microswimmers can react to their position in space or their distance to other microswimmers. We investigate the influence of different interaction potentials or a delay in the information exchange. Our results demonstrate so far that particles can be coupled to each other by the used feedback by designed virtual potentials. The collective motion of such coupled particles reveals oscillating modes with emergent features like spontaneous rotation. The experiments shall help to understand the emergence of complex behavior in biological systems.

DY 58.8 Fri 11:15 H11

Out-of-plane beating components of active axonemes isolated from Chlamydomonas reinhardtii — Azam Gholami[1], •Soheil Mojiri[2], Eberhard Bodenschatz[1], and Jörg Enderlein[2] — [1]Max-Planck Instiute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August Universität, Göttingen, Germany

Cilia and flagella are ubiquitous in the living world. They are essential for micro-scale driven transport of fluids or cells by cilia/flagellar beating. Their slender bodies are composed of a microtubule/molecular motor structure that when taken independently are called an axoneme.

Axonemes move by bending waves that emerge from the interplay between internal stresses generated by dynein motor proteins . Here we use the novel multi-plane phase contrast imaging technique to record the three dimensional beating pattern of isolated axonemes from Chlamydomonas reinhardtii that beat in the vicinity of a substrate. We measure the torsion of the axoneme along the contour length with high spatiotemporal resolution. High precision information on out-of-plane beating component of axonemes allows us to check the validity of the resistive-force theory.

DY 58.9 Fri 11:30 H11

Nanoscale chemotaxis of enzymes and small molecules — •Jaime Agudo-Canalejo[1,2], Tunrayo Adeleke-Larodo[1], Pierre Illien[3], and Ramin Golestanian[4,1] — [1]University of Oxford, Oxford, UK — [2]Penn State University, State College, USA — [3]ESPCI Paris, Paris, France — [4]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

We present a microscopic theory for the observed chemotaxis of enzymes and other small molecules. [1,2] We find that two distinct mechanisms contribute to enzyme chemotaxis: a diffusiophoretic mechanism due to non-specific interactions, and a new type of mechanism due to binding-induced changes in the diffusion coefficient of the enzyme. For a typical enzyme, the two mechanisms compete against each other, one dominating at high substrate concentration, the other at low concentration. The competition between the two mechanisms may be used to engineer nanovehicles that move towards or away from regions with a specific substrate concentration. Finally, we include the effects of anisotropy and flexibility of the enzyme, [3] and show that enzymes can be aligned by gradients, and shape fluctuations lead to corrections in the diffusion and chemotactic mobility of enzymes. [1] Agudo-Canalejo, J., Adeleke-Larodo, T., Illien, P., & Golestanian, R. (2018) Acc. Chem. Res. 51, 2365 [2] Agudo-Canalejo, J., Illien, P., & Golestanian, R. (2018) Nano Lett. 18, 2711 [3] Adeleke-Larodo, Agudo-Canalejo, J., & Golestanian, R. (2018) arXiv:1811.09631

DY 58.10 Fri 11:45 H11

High-motility visible light-driven Ag/AgCl Janus microswimmers interacting with passive beads — •xu wang[1], larysa baraban[2], vyacheslav r misko[3,4], franco nori[4,5], petre formanek[6], tao huang[2], gianaurelio cuniberti[2], jürgen fassbender[1], and denys makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorfe.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Universiteit Antwerpen, B-2610 Antwerpen, Belgium — [4]RIKEN Cluster for Pioneering Research, 351-0198 Saitama, Japan — [5]University of Michigan, 48109-1040 Michigan, USA — [6]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany

Visible light driven nano/micro swimmers typically show mean squared displacement (MSD) values in the range of up to 200 μm^2 (over 10 s) under favorable UV light illumination.[1] Here, we demonstrate Ag/AgCl-based spherical Janus micromotors that reveal an efficient propulsion with a MSD to 3000 μm^2 (over 10 s) in pure H_2O under visible blue light illumination (λ = 450-490 nm).[2] Furthermore, we show the micromotors reveal efficient exclusion effect to their surrounding passive polystyrene beads in pure H_2O experimentally and using numerical simulations of the Langevin equations.[3]

1. Simmchen, J., et al., ChemNanoMat 2017, 3, 65.
2. Wang, X., et al., Small DOI: 10.1002/smll.201803613.
3. Wang, X., et al., Small 2018, 14, 1802537 (Frontispiece paper)

DY 59: Talk Michael Schmiedeberg

Time: Friday 9:30–10:00 Location: H19

Invited Talk DY 59.1 Fri 9:30 H19

Energy landscape exploration approach for non-ergodic soft matter systems — •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Motivated by the successful studies [1] of the athermal jamming transition by exploring the configuration space of soft colloidal particles that interact according to finite-ranged repulsive interactions, we have proposed an energy landscape exploration method of such a system at small but non-zero temperatures [2]. We find that the system can become effectively non-ergodic if the packing fraction is increased. The ergodicity breaking transition is in the universality class of directed percolation [2] and therefore is fundamentally different from athermal jamming. Our approach can be used to predict how the glass transition density depends on temperature [3].

In future we want to extend our energy exploration method to other soft matter systems that might be trapped in metastable states because the dynamics is effectively non-ergodic. For example, the dynamics of gel networks in colloid-polymer mixtures slows down and ageing can be observed if both the breaking of colloidal bonds is rare and the network is directed percolated in space [4].

[1] C.S. O'Hern et al., Phys. Rev. Lett. 88, 075507 (2002).
[2] M. Maiti and M. Schmiedeberg, Scientific Reports 8, 1837 (2018).
[3] M. Maiti and M. Schmiedeberg, ArXiv:1812.02503.
[4] M. Kohl et al., Nature Communications 7, 11817 (2016).

DY 60: Statistical Physics in Biological Systems III

Time: Friday 10:00–11:45 Location: H3

DY 60.1 Fri 10:00 H3

Charting the hydrophobic effect: Computing spatially resolved absolute hydration shell entropies — •Leonard Heinz and Helmut Grubmüller — Department of Theoretical and Computational Biophysics, Max Planck Institute for Biophysical Chemistry, Göttingen

Biophysical systems are governed by their free energy and thus depend on a fine-tuned interplay between enthalpy and entropy. E.g. for protein folding, the solvation contributions are crucial, as they give rise to the hydrophobic effect. A quantitative understanding of the thermodynamics of solvation, and in particular the associated entropies, is therefore essential. While a variety of methods allow assessing the solute entropy, solvation shell entropies are notoriously difficult to obtain from computer simulations, because the shallow energy landscape requires sampling of an extremely large configuration space. Here we solve the sampling problem by exploiting the permutation symmetry of the solvent particles which reduces the configuration space that needs to be sampled by the Gibbs factor 1/N!, leaving the physics of the system unchanged. We perform a mutual information expansion to obtain translational and rotational solvent entropy values from the permutationally reduced trajectory. The expansion yields entropy contributions of individual solvent particles as well as of groups of particles, such as different solvation shells, thereby providing spatial resolution. We tested our method by assessing the solvation of small molecules, such as n-alkanes and small peptides and obtained agreement with other methods and experimental values.

DY 60.2 Fri 10:15 H3

GTPase cascades can perform as both robust switches and biochemical oscillators — •Andreas Ehrmann, Basile Nguyen, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

GTPases regulate a wide range of cellular processes, such as intracellular vesicular transport, signal transduction, and protein translation. These hydrolase enzymes operate as biochemical switches by toggling between an active guanosine triphosphate (GTP)-bound state and an inactive guanosine diphosphate (GDP)-bound state. We compare two switch models, a single-species switch and an interlinked switch that consists of two species coupled through positive and negative feedback

loops. We find that interlinked switches are closer to the ideal all-or-none switch and are more robust against input fluctuations. While the single-species switch can only achieve bistability, interlinked switches can be converted into oscillators by tuning the cofactor concentrations. These regimes can only be achieved with sufficient chemical driving, which is associated with GTP hydrolysis. In this study, we provide a minimal thermodynamically consistent model that can achieve bistability and oscillations with the same feedback structure.

DY 60.3 Fri 10:30 H3

Force-dependent diffusion coefficient of molecular Brownian ratchets — •Matthias Uhl and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

We study the mean velocity and diffusion constant in models of molecular Brownian ratchets. Brownian ratchets can be used to describe translocation of biopolymers through nanopores in cells in the presence of molecules that prevent backwards transitions if bound to the polymer strand. We provide an analytical expression for the diffusion constant in the classical model of a translocation ratchet that was first proposed by Peskin et al. [1]. This model is only applicable if the binding and unbinding of the blocking molecules are much faster than the diffusion of the strand. We propose a modified model that is also applicable if the (un)binding rates are finite [2]. Our analysis shows that for large pulling forces the predictions of both models can differ strongly even if the (un)binding rates are large in comparison to the diffusion timescale but still finite. Implications of the thermodynamic uncertainty relation on the efficiency of Brownian ratchets are also discussed.

[1] C. S. Peskin, G. M. Odell, and G. F. Oster, Biophys. J. 65, 316 (1993).
[2] M. Uhl and U. Seifert, Phys. Rev. E 98, 022402 (2018).

DY 60.4 Fri 10:45 H3

Structures and Dynamics of Growing Semi-Flexible Polymer Chains — •Jörn Appeldorn and Reiner Kree — Inst. f. Theo. Physik, Univ. Göttingen, Friedrich-Hund Pl. 1, 37077 Göttingen

Numerous studies have investigated both, the conformational dynamics of semi-flexible polymer chains with fixed length and the dynamics of the chemical growth separately. Here, we study the combined effects, if both processes are characterized by comparable time scales.
We consider irreversible chain growth of a Gaussian semi-flexible polymer with growth laws $\langle N(t)\rangle = \left(\frac{t}{\tau_0}\right)^{\alpha}$ characterized by a power law exponent $0 < \alpha \leq 1.1$. In particular, we study the end-to-end distance, mean square radius of gyration, mean square displacement of monomers, and center of mass position. Results are obtained from numerical simulations using a modified Brownian dynamics algorithm, which makes use of the exact solvability of the Gaussian dynamics and allows us to perform simulations on very long timescales.
For small growth parameters, the polymer chains reach their equilibrium state in between the growth events for all bending stiffnesses. With increasing α, the conformational properties are influenced by the chemical growth and the polymer chains never reach their equilibrium state. The resulting non-stationary properties are systematically studied as a function of ν and α .

DY 60.5 Fri 11:00 H3

Reactive paths and record statistics in complex energy landscapes — David Hartich and •Aljaz Godec — Mathematical Biophysics Group, Max-Planck-Institute for Biophysical Chemistry, Göttingen (GER)

When considering reaction kinetics in a single-molecule setting paradigmatic kinetic rate-based approaches often fail, and an explicit consideration of trajectory-to-trajectory fluctuations is required for a correct theoretical description. Exploiting a recently proven duality between relaxation and first passage processes (Hartich & Godec, *New J. Phys.* **20**, 112002 (2018)) we will review our recent results on the full statics of reactive trajectories. We will demonstrate that traditional rate-based approaches counter-intuitively reflect delocalized and indirect reactive trajectories. We will highlight the striking difference between diffusion-controlled reactions in chemical systems and kinetics in the so-called few-encounter limit relevant for nucleation-limited phenomena. As a second application of the duality we will present large deviation results for the statistics of records. On the hand of selected examples we will discus the relevance of our results for emerging biophysical phenomena at low-copy numbers.

DY 60.6 Fri 11:15 H3

NK Fitness Landscapes Interpolated between K=2 and K=3 — James E Sullivan, Dmitry Nerukh, and •Jens Christian Claussen — Department of Mathematics, Aston University, Birmingham B4 7ET, U.K.

The NK model was introduced by Stuart Kauffmann and coworkers [1] as a model for fitness landscapes with tunable ruggedness, to understand epistasis and pleiotropy in evolutionary biology. It has also raised interest in combinatorial optimisation, study of spinglasses and in organizational theory. In the original formulation, fitness is defined as a sum of fitness functions for each locus, each depending on the locus itself and K other loci. Varying K from $K = 0$ to $K = N - 1$ leads to different ruggedness of the landscape. Here we introduce a generalization that allows to interpolate between integer values of K by allowing K_i to assume different values for each locus. We focus on the interpolation between the most widely studied cases of $K = 2$ and $K = 3$ and characterize the landscapes by study of their local minima. While we largely see a linear interpolation, small deviations are observed. Finally we discuss applications of this approach in economic systems and biology.

[1] Kauffman, S.; Levin, S., Journal of Theoretical Biology. 128, 11 (1987); Kauffman, S.; Weinberger, E., Journal of Theoretical Biology. 141, 211 (1989).

DY 60.7 Fri 11:30 H3

Transport and Free Energy Transduction in Chemical Reaction Pathways far from Equilibrium — •Artur Wachtel and Massimiliano Esposito — Complex Systems and Statistical Mechanics, Physics and Materials Science, University of Luxembourg

The metabolism of living cells extracts useful energy and matter from their food. Recent progress in the understanding of the nonequilibrium thermodynamics of chemical reaction networks [1, 2, 3] allows us to address the thermodynamics in biochemical reaction pathways in a systematic and rigorous way.

In this talk I address two important points: transport far from thermodynamic equilibrium and the transduction of free energy. For the first point I draw a similarity to electrical circuits. This similarity is remarkable because the reactions may operate far from the linear regime, thus currents and thermodynamic forces are no longer linearly related.

Transduction is the defining feature of all thermodynamic machines. In living systems it allows building up of nonequilibrium free energy against its natural tendency to degrade. Here, I provide a systematic identification of free energy transduction in nonlinear biochemical reaction pathways, which also leads to a formal definition of its efficiency.

[1] Polettini & Esposito, J Chem Phys 141, 024117 (2014)
[2] Rao & Esposito, Phys Rev X 6, 041064 (2016)
[3] Wachtel, Rao, & Esposito, New J Phys 20, 42002 (2018)

DY 61: Microfluidics (joint session DY/CPP)

Time: Friday 10:00–12:15 Location: H6

DY 61.1 Fri 10:00 H6

Tunable stirring of the interior of biofluid microdroplets in a microfluidic channel — •Pierre-Yves Gires, Mithun Thampi, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Studying dynamic changes of and within fluid droplets with biomimetic or biological composition, e.g. produced in microfluidic devices, is a key technique for biotechnology. However, due to their small dimensions, a controlled and gentle stirring of the droplets' interior has been very challenging. Here we report on an approach that allows for performing such a tunable stirring of microdroplets via home-made magnetic nano-stir bars. In particular, we have used a PDMS-based microfluidic junction with a hydrophobic carrier fluid to produce aqueous biofluid droplets with 10-100 microns diameter into which magnetic nano-stir bars were incorporated. By subsequent stimulation with an alternating magnetic field, nano-stir bars performed a rotational motion with tunable frequencies in the range 0.01-10 Hz. The differential effect of this stirring on particle diffusion and on the undulation of semiflexible biofilaments, i.e. microtubules, was then quantified via quantitative fluorescence microscopy to dissect thermal and active noise contributions.

DY 61.2 Fri 10:15 H6

Soft particles in inertial microchannel flow — •Christian Schaaf and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Particles immersed in an inertial microchannel flow at intermediate Reynolds numbers move towards discrete equilibrium positions in the channel cross section. This Segré-Silberberg effect can be explained by the inhomogeneous shear profile of Poiseuille flow and particle-wall interactions. While rigid particles assemble around halfway between channel walls and channel center, deformable capsules move closer towards the center [1]. In addition to this lateral inertial focusing, rigid particles at low densities also assemble on 1D lattices along the flow [2]. In this contribution we aim to understand how the deformability of elastic capsules influences the lattice formation and what novel structures now develop.

To study this problem we conduct lattice-Boltzmann simulations. As a first step we focus on the dynamics of a flowing particle pair and see how inertia changes the dynamics of a pair of deformable capsules. For a pair of rigid particles we have recently found that the dynamics is dominated by viscous forces at small distances and by inertial forces at larger distances [3].

In the end these results are used to explain the behavior of soft particle trains and to analyze their dynamics and stability.

DY 61.3 Fri 10:30 H6

Focusing and splitting of particle streams in microflows via viscosity gradients — •Matthias Laumann and Walter Zimmermann — University of Bayreuth, Germany

Microflows are intensively used for investigating and controlling the dynamics of particles, including soft particles such as biological cells and capsules. A classic result is the tank-treading motion of elliptically deformed soft particles in linear shear flows, which do not migrate across straight stream lines in the bulk. However, soft particles migrate across straight streamlines in Poiseuille flows. In this talk we present a new mechanism of cross-streamline migration of soft particles. If the viscosity varies perpendicular to the stream lines then particles migrate across stream lines towards regions of a lower viscosity, even in linear shear flows. An interplay with the repulsive particle-boundary interaction causes then focusing of particles in linear shear flows with the attractor stream line closer to the wall in the low viscosity region. Viscosity variations perpendicular to the stream lines in Poiseuille flows leads either to a shift of the particle attractor or even to a splitting of particle attractors, which may give rise to interesting applications for particle separation. The location of attracting streamlines depend on the particle properties, like their size and elasticity. The cross-stream migration induced by viscosity variations is explained by analytical considerations, Stokesian dynamics simulations with a generalized Oseen tensor and Lattice-Boltzmann simulations.

DY 61.4 Fri 10:45 H6

Synchronization between two boiling bubbles — •Claus-Dieter Ohl[1,2], Dang Minh Nguyen[1,2], Muttikulangara Swaminathan Sanathanan[3], Jianmin Miao[3], and David Fernandez Rivas[4] — [1]Otto-von-Guericke University, Institute for Physics, Magdeburg. — [2]School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore. — [3]School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore. — [4]Mesoscale Chemical Systems, Faculty of Science and Technology, University of Twente, Enschede, The Netherlands

Acoustically driven bubbles are nonlinear oscillators showing a wide range of behaviours such as period-doubling bifurcations, deterministic chaos, and synchronization to an external signal. Here we demonstrate that bubbles driven with a constant heat source can couple with each other and yield in-phase synchronization, even in the absence of an external sound field. Besides perfect synchronization we resolve the parameter space where independent oscillations and bubble merging occurs. The main finding that only weakly oscillating bubbles synchronize provides a path for experimental scale-up to study spatiotemporal synchronization. In the wider scope the findings are relevant for heat transfer applications from structured heaters where complex multi-bubble oscillations are expected.

DY 61.5 Fri 11:00 H6

Dissipative particle dynamics simulation for viscosity behavior induced by self-assembly of surfactants confined in nanotubes — •Yusei Kobayashi and Noriyoshi Arai — Kindai University, Higashiosaka, Japan

Self-assembly is one of the most studied branches of materials chemistry, and has attracted a lot of attention due to its diverse potential applications in electronics, engineering, biomedical, and optical fields. Thus far, many previous studies have reported on the self-assembly of surfactants in solution for developing various functional materials. On the other hand, the chemical nature of the wall surface on the nano/micro scale is another key parameter which can drastically change the self-assembled structures. To study such wall-induced effects on the self-assembled structures and their rheological properties, we performed computer simulations of surfactant solutions in chemically distinct nanotubes under pipe flow. In particular, we determined the shear viscosity as a function of (local) shear rate in hydrophilic, hydroneutral, and hydrophobic nanotubes at different surfactant concentrations. Here, we found that the addition of surfactant molecules led to characteristic viscosity behaviors with rich steady-state morphologies.

15 min. break

DY 61.6 Fri 11:30 H6

Particle trajectory entanglement in confined fluidic systems — •Alvaro Marin[1], Massimiliano Rossi[2], and Christian J. Kähler[2] — [1]Physics of Fluids, University of Twente, The Netherlands — [2]Bundeswehr University Munich, Germany

Suspensions in motion can show very complex and counterintuitive behavior, particularly at high concentrations. However, in this work we show how suspensions at substantially lower dilute concentrations can develop complex dynamics. Such non-trivial dynamics appear when particles tend to interlace their trajectories, only bonded by hydrodynamic interactions. Using a fairly simple system of non-Brownian particles flowing in a confined channel, we reveal a rich complexity in the particle dynamics due to the dominance of short-range particle-particle and particle-wall hydrodynamic interactions. Such rich dynamics are revealed and studied via experiments and particle dynamics simulations, resulting in a very good quantitative comparison.

DY 61.7 Fri 11:45 H6

Aligning beads with boxing gloves — •Archit Bhatnagar[1], Anatol Fritsch[1], Matthäus Mittasch[1], Michael Nestler[2], Matthias Loidolt[1], Axel Voigt[2], and Moritz Kreysing[1] — [1]MPI of Cell Biology, Dresden — [2]Department of Mathematics, TU Dresden

Recently we have described that we can move the cytoplasm of cells and developing embryos in a non-invasive manner. For this we made use of thermoviscous flows (1).

Here we ask the question if these long-ranged flow fields can in principle also be used for the precision alignment of colloids, an endeavor that seems as reasonable as trying to align small beads while wearing boxing gloves. Simulations, however, suggest that series of flow fields can be found to align multiple colloids at the same time, even if these particles are closely spaced.

We follow this strategy experimentally and will report the feasibility, precision limits due to the brownian motion of particles, and prospects for colloidal physics and applications in biology.

References: (1) Mittasch et al., " Non-invasive perturbations of intracellular flow reveal physical principles of cell organization", Nature Cell Biology 1 (2018)

DY 61.8 Fri 12:00 H6

Anisotropic thermophoresis and thermal orientation of elongated colloids — •Marisol Ripoll and Zihan Tan — Institute of Complex Systems, Forschungszentrum Jülich, Germany

Anisotropic phoresis refers to the different phoretic response that elongated particles can have as a function of their relative orientation with a gradient of temperature or concentration. These effects can further be enhanced when the surface of the system is not homogeneous, case in which an additional phoretic orientation can appear for non-fixed colloids [1]. Investigations are performed by a hydrodynamic mesoscale simulation approach [2]. The anisotropic phoresis can furthermore be applied to the design of phoretic micromachines and micropums, which shows to provide an alternative to the conventional application of external forcing in order to pump fluids at the microscale [3].

[1] Z. Tan, M. Yang, and M. Ripoll, Soft Matter 13, 7283 (2017) Z. Tan, PhD thesis, Universität zu Köln (2018)

[2] D. Lüsebrink, M. Yang, and M. Ripoll, J. Phys.: Condens. Matter 24, 284132 (2012) M. Yang, and M. Ripoll, Soft Matter 9, 4661 (2013)

[3] M. Yang, R. Liu, M. Ripoll, and K. Chen, Nanoscale 6, 13550 (2014); Lab Chip, 15, 3912 (2015)

DY 62: Glasses and Glass transition (joint session DY/CPP)

Time: Friday 10:00–11:45 Location: H19

DY 62.1 Fri 10:00 H19

Unified Formulation of Fractional Relaxation — •Tillmann Kleiner and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart

Susceptibility functions that involve stretching exponents which are derived from fractional dynamics [1] reproduce the excess wing of α-relaxation peaks that has been observed in dielectric spectra of glass forming materials [2]. The contemporary formulation of fractional dynamics requires two distinct approaches to describe the relaxation motion and the response of the system to periodic excitations. The former uses fractional Liouville-Caputo derivatives in the time domain and the latter multiplication with the susceptibility function in the frequency domain. Both approaches impose severe restrictions on the past history of the involved electric field that are unrealistic in an experimental situation. Due to the occurrence of memory effects this poses a serious problem. In this contribution a unified description of fractional dynamics is presented where fractional derivatives are defined using distributional convolution. The resulting response functions are stretched multinomial Mittag-Leffler functions. This formulation extends the mentioned approaches to all experimentally relevant situations in a consistent way and exposes a high degree of convenience.

[1] R. Hilfer, Analysis **36**, 49-64 (2016)

[2] F. Kremer and A. Loidl, The Scaling of Relaxation Processes, Springer, (2018)

DY 62.2 Fri 10:15 H19

Ion and Molecule Transport in Nanopores - a NMR Study — •Christoph Säckel, Sarah Schneider, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

We analyze ion and molecule transport in aqueous salt solutions confined to nanopores as part of a project that aims to develop a new generation of nanosensors by combining biological and synthetic nanopores. While biological ion channels are highly selective and sensitive, they lack the robustness for technological applications. In contrast, silica pores are well-established in industrial environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favourable properties of both types of pores. It is therefore necessary to understand the influence of the confinement on the temperature-dependent ion and molecule transport. We systematically vary the pore parameters and study effects on the dynamics with ^{1}H, ^{2}H and ^{7}Li nuclear magnetic resonance (NMR). We combine homogeneous and gradient field NMR to selectively investigate water and ion dynamics on broad time and length scales in the supercooled regime. Both the local and long-range dynamics of ions and water show a slowdown with decreasing pore size. In addition, our data indicates more heterogeneous dynamics for the liquid in confinement than in bulk. Both the slowdown and heterogeneity can be explained by a slower layer of solution at the pore walls and bulk-like dynamics in the pore centre. Self-diffusion shows an Arrhenius-like behaviour of the solution in confinements, while bulk samples are best described by a VFT fit.

DY 62.3 Fri 10:30 H19

Glass transition of water-like models in bulk and confinement — •Robin Horstmann and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

Tetrahedral network formers have a special position among glass-forming liquids. Their well defined local prefered structures cause significant structural changes with temperature but often render the transfer of models of supercooled liquids, e.g. density scaling, difficult. We use molecular dynamics simulations to examine two families of water-like molecules, based on the SPC/E and TIP4P/2005 water models, that vary only in their partial charges to systematically alter the strength of the hydrogen-bonds and, hence, the relevance of tetrahedral order.[1] The varied inter-molecular interactions spread dynamics over a wide temperature range with the glass transition temperature T_g and the high temperature activation energy E_∞ both changing by a factor of five. Additionally, we study water-like systems in neutral confinements and find unchanged tetrahedral structure but slowed molecular dynamics. To describe the glassy slowdown, we assume that the activation free energy can be split into a constant value E_∞ and an exponentially growing contribution $E_c(T)$.[2] Common ratios of E_∞/T_g and $E_c(T)/T_g$ are found indicating that the high temperature results can be used to rescale the glassy slowdown in bulk and confinement.

[1] R. Horstmann and M. Vogel, J. Chem. Phys. **147**, 034505 (2017)

[2] B. Schmidtke et al., Phys. Rev. E **86**, 041507 (2012)

DY 62.4 Fri 10:45 H19

Effects of fractional freezing on the structure and dynamics of deeply cooled confined water — •Sebastian Kloth and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

The properties of confined water are of enormous importance in nature and technology. In particular, the effects of partial freezing on structure and dynamics is largely relevant for, e.g. geology, cryopreservation and our understanding of the glass transition of water [1]. To obtain a better understanding of the properties of the liquid fraction molecular dynamic simulations were performed with the TIP4P/Ice water model. This model was chosen for its good agreement with several water and ice properties. A series of frozen confinements with different pore diameters were made to analyze the structure and dynamics of the water layer remaining liquid upon deeply cooling, between pore wall and ice crystals. The partial freezing results in altered water dynamics, most importantly, the non-Arrhenius behavior of weakly supercooled bulk water is replaced by an Arrhenius behavior. Confined and bulk water have in common that the structure is disturbed at low temperatures. Either trough the existence of two interfaces in the case of the frozen confinement or through partly forming ice nuclei in the bulk.

[1] Cerveny, S. et al., Chem. Rev., **2016**, *116* (13)

DY 62.5 Fri 11:00 H19

Decoding of the Toric Code: A High Temperature Series Analysis — •Benedikt Placke[1], Nikolas Breuckmann[2], and Ananda Roy[1,3] — [1]JARA Institute for Quantum Information, RWTH Aachen University — [2]Department of Physics and Astronomy,

University College London — [3]Insitut de Physique Théorique, CEA Saclay

The decoding of several topological quantum codes (TQC) can be mapped onto statistical physics models (SPM). This mapping relates the successful decoding of the error syndrome of the TQC to a certain phase of the respective SPM. The error-correction performance of several TQC-s have been analyzed using Monte Carlo (MC) simulations of the corresponding SPM. We, on the other hand, use high-temperature series expansion (HTSE) to analyze the decoding performance of the toric code. In contrast to zero temperature simulations, which estimate the threshold of the minimum-weight perfect-matching decoder, our method naturally provides an estimate of that of the maximum-likelihood decoder. First, we analyze the full phase diagram of the 2D random-bond Ising model by computing HTSE to a higher order than previously performed. From our analysis, we estimate the accuracy threshold of the toric code in absence of measurement imperfections. We compare our result to those obtained by MC simulations and network model analysis. Then, we perform HTSE of the zero-field free-energy and the Wilson loop order parameter in the 3D Ising gauge theory in the presence of quenched disorder. The latter model describes the decoding of the toric code subject to measurement errors.

DY 62.6 Fri 11:15 H19

Local and translational dynamics of water in various confinements investigated via ^{1}H and ^{2}H NMR — •Simon Schoner, Max Weigler, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

Confined water is interesting for several reasons. On the one hand the topic is highly relevant in biology or geology where water is often found in soft or hard confinements, water around proteins or in rods being prime examples. On the other hand confined water allows one to investigate liquid water at low temperatures, where normally crystallization would occur, and, in this way, to obtain insights into the heavily debated glass transition of water. We investigate the dynamics of water confined in various rigid matrices using ^{1}H and ^{2}H NMR experiments. One goal is to obtain information on the influence of different kinds of confinements and pore sizes on the self diffusion and the structural relaxation of water. Especially, we address the question whether translational diffusion and local reorientation are affected by confinement in a comparable way. First measurements with D_2O and H_2O indicate similar correlation times and diffusion coefficients for both MCM-48 and MCM-41 confinements with comparable pore sizes between 2 and 3 nm.

DY 62.7 Fri 11:30 H19

Universal hidden order in amorphous cellular geometries — •Gerd E Schröder-Turk — Murdoch University, Perth, School of Engineering and IT, WA 6150, Murdoch, Australia

Partitioning space into cells is central to many fields of science and technology, as well as to resource distribution problems in economics and telecommunication. The nature of cellular partitions is often defined by optimization with respect to certain properties, such as interface area in the Kelvin problem, packing density in the Kepler problem, or cell centrality in the Quantizer problem. In all known cases, the optimal solutions are crystalline configurations with long range order. To date, no optimization problem has been identified where the optimal solution is a disordered configuration. Amorphous, or disordered, structures are generally considered to be intermittent meta-stable states that prevent the system from attaining the optimal ordered structures. Here we use Lloyd's iteration to demonstrate the existence and stability of a special disordered state in the three-dimensional Quantizer problem, despite the existence of lower-energy crystalline configurations. Akin to a thermodynamic phase, this state is universal. Specifically, irrespective of the level and type of disorder in the initial configurations, we find a convergence to the same amorphous state, representing configurations characterized by the same structure factor and energy distributions. This highly degenerate state is characterised by an anomalous suppression of long-wavelength density fluctuations, known as hyperuniformity.

DY 63: Modeling and Data Analysis

Time: Friday 10:00–11:30 Location: H20

DY 63.1 Fri 10:00 H20

Analyzing stochastic time serieses via Bayesian parameter estimation of Langevin models with correlated noise — Oliver Kamps and •Clemens Willers — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany

Over the last years, the estimation of stochastic evolution equations of complex systems has been applied in many scientific fields ranging from physics to biology and finance. Especially, Langevin models with delta-correlated noise terms, which realize a Markovian dynamic, have been used successfully in this context [1]. However, many real world data sets exhibit correlated noise and a non-Markovian dynamic, for example data sets from turbulence [2].

To tackle this problem, we use Langevin models containing an added hidden component which realizes a driving correlated noise. We develop a method for the systematic estimation of the drift- and diffusion functions, parameterized through spline functions. The method is based on a likelihood function which is constructed by a short-time propagator for the measured values of the visible component. A Markov Chain Monte Carlo procedure makes it possible to get access to both the parameters and their reliability. The method is demonstrated using the example of turbulent real world data sets as the country-wide wind power production [3].

[1] Friedrich et al., Phys. Rep. 506, 87 (2011) [2] Friedrich and Peinke, Phys. Rev. Lett. 78, 863 (1997) [3] Kamps O., in Wind Energy-Impact of Turbulence, edited by Hölling M. et al. (Springer) 2014, p. 67.

DY 63.2 Fri 10:15 H20

Phase walk analysis of leptokurtic time series — •Christoph Räth[1], Heike Modest[1], and Korbinian Schreiber[2] — [1]Institut für Materialphysik im Weltraum, DLR, Münchener Str. 20, 82234 Weßling, Germany — [2]Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

A very general definition of nonlinearity in data sets can be obtained from their representation in Fourier space: From the Wiener-Khintchine theorem and the bijectivity of the Fourier transformation it follows that the linear information is entirely represented by the Fourier amplitudes. Hence, all nonlinear information is contained solely in the Fourier phases. Yet, the direct study of the Fourier phases has so far attracted only little attention. Here, we present a novel method to quantify the phase information. In close analogy to random walk analyses, we propose the phase walk statistics as a way to quantify the phase information. We apply it to the analysis of nonlinearities in intermittent, leptokurtic time series like turbulent wind data, the Dow Jones (DJ) day-to-day returns and synthetic leptokurtic data. Testing for nonlinearities by means of surrogates shows that the new method yields strong significances for nonlinear behavior. Due to the drastically decreased computing time as compared to embedding space methods, the number of surrogate realizations can be increased by orders of magnitude [1]. Thereby, the probability distribution of the test statistics can very accurately be derived and parameterized, which allows for much more precise tests on nonlinearities. [1] K. Schreiber et al., Chaos, 28, 063120 (2018)

DY 63.3 Fri 10:30 H20

Data Science based Magnesium Corrosion Engineering — Tim Würger[1] and •Robert Meissner[1,2] — [1]MagIC Magnesium Innovation Centre, Institute of Materials Research, Helmholtz Zentrum Geesthacht, Geesthacht, Germany — [2]Hamburg University of Technology, Institute of Polymer and Composites, Hamburg, Germany

Magnesium is a material with high potential for a wide range of applications in areas such as transport, energy, and medicine. However, the corrosion properties of magnesium still limit its practical application. It is, therefore, necessary to develop new approaches that can prevent or control corrosion and degradation in order to adapt to the specific needs of the application. One way to accomplish this is to use inhibitor molecules that block or trap corrosive species that would otherwise further promote corrosion. As it is not possible to obtain a

detailed atomistic understanding of the inhibition mechanisms for each additive due to the variety of different molecules, other inhibition prediction measures are required. We present a concept combining high throughput calculations with dimensionality reduction algorithms and corrosion experiments. Physical properties, e.g. HOMO/LUMO gaps or corrosion inhibition of inhibitor molecules, are presented next to a two-dimensional sketch map of the molecules based on their molecular similarity. This approach facilitates the search for new molecules with a positive or negative influence on corrosion inhibition efficiency by out-of-sample mapping and could thus contribute significantly to a better understanding of corrosion inhibition mechanisms and control of magnesium/electrolyte interface properties.

DY 63.4 Fri 10:45 H20

DyCA - Dynamical Component Analysis — Steffen Hartmann, •Katharina Korn, Bastian Seifert, and Christian Uhl — Center for Signal Analysis of Complex Systems, University of Applied Sciences Ansbach, Residenzstr. 8, 91522 Ansbach

Spatio-temporal patterns emerging from a certain class of low-dimensional differential equations can be decomposed by dynamical component analysis (DyCA), a new algorithm proposed in [1]. We present the method, which is based on a least-square-optimization leading to a generalized eigenvalue problem of correlation matrices of the signal and its derivative. The application of DyCA to simulated and real world data is demonstrated and the power of the algorithm is shown by comparing the results to principal and independent component analysis (PCA, ICA).

[1] B. Seifert, K. Korn, S. Hartmann, and C. Uhl, Dynamical Component Analysis (DyCA): Dimensionality reduction for high-dimensional deterministic time-series, 2018 IEEE 28th International Workshop on Machine Learning for Signal Processing (MLSP), Aalborg, 17.-20.09.2018

DY 63.5 Fri 11:00 H20

Data-driven modelling of spatio-temporal dynamics by means of artificial neural networks — •Sebastian Herzog[1,2], Florentin Wörgötter[2], and Ulrich Parlitz[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Germany — [2]Third Institute of Physics and Bernstein Center for Computational Neuroscience, University of Göttingen, Germany

We present a data driven modeling ansatz [1] which combines deep convolutional neural networks (CNNs) for feature extraction and dimension reduction with an adapted conditional random field (CRF) in order to model the properties of temporal sequences. To validate the proposed method we used the BOCF model describing electrical excitation waves in cardiac tissue where chaotic dynamics is associated with cardiac arrhythmias. Running the trained network in a closed loop(feedback) configuration iterated prediction provided forecasts of the complex dynamics that turned out to follow the true evolution of the BOCF simulation. The direct comparison between the forecasted data from the network and the real data from the BOCF simulation clearly shows that machine learning methods like those employed here provide faithful models of the underlying complex dynamics of excitable media that, when suitably trained can provide powerful tools for predicting the spatio-temporal evolution and for cross-estimating not directly observed variables. [1] S. Herzog, F. Wörgötter, U. Parlitz, Data-driven modelling and prediction of complex spatio-temporal dynamics in excitable media, in: Front. Appl. Math. Stat. - Dynamical Systems (2018), doi: 10.3389/fams.2018.00060

DY 63.6 Fri 11:15 H20

Estimating model parameters by attractor comparison — •Ulrich Parlitz — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — Institute for Nonlinear Dynamics, Georg-August-Universität, Göttingen, Germany

Time series based methods for estimating parameters of dynamical models are discussed which are based on a comparison of the asymptotic dynamics given by (reconstructed) attractors underlying the observed data and those generated by the model. The similarity of both distributions of (reconstructed) states is quantified by different measures of (dis-)similarity or "distance" (e.g., ordinal pattern distributions, nearest neighbor distances) and a good set of model parameters minimizes their "distance" or dissimilarity. We present different implementations of this approach for parameter estimation and evaluate their performance with several dynamical examples.

DY 64: Closing talk (joint session BP/CPP/DY)

Time: Friday 12:30–13:15 Location: H1

Invited Talk DY 64.1 Fri 12:30 H1

Pattern formation in active cytoskeletal systems — •Andreas R. Bausch — Lehrstuhl für Biophysik, Technische Universität München, 85747 Garching

Living cells rely on the self-organization mechanisms of cytoskeleton to adapt to their requirements. In processes such as cell division, or cellular motility rely on the controlled self-assembly and disassembly of well defined active cytoskeletal structures interacting with lipid membranes. One important and promising strategy to identify the underlying governing principles is to quantify the underlying physical processes in model systems mimicking functional units of living cell. Here I*ll present in vitro minimal model systems consisting of active microtubule and actin filament systems which show pattern formation resulting from active transport processes. I will discuss how small variations in local interactions results in nematic or polar patterns in high density motility essays. With the example of reconstituted active vesicles I will discuss how to relate local force exertion and tension generation to shape transformations, blebbing, invagination or tethering of lipid membranes