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

Carsten Beta
Biologische Physik
Institut für Physik und Astronomie
Universität Potsdam
Karl-Liebknecht-Str. 24/25
D–14476 Potsdam
beta@uni-potsdam.de

Markus Bär
Physikalisch-Technische
Bundesanstalt
FB 8.4 - Modellierung und
Datenanalyse
Abbestraße 2 – 12
D–10587 Berlin
markus.baer@ptb.de

Sabine Klapp
Technische Universität Berlin
Institut für Theoretische Physik
Hardenbergstrasse 36
10623 Berlin
sabine.klapp@tu-berlin.de

The Dynamics and Statistical Physics Division covers theoretical and experimental activities in all areas of statistical physics, quantum dynamics and many-body systems, nonlinear dynamics and pattern formation, data analysis and machine learning as well as active matter, fluid physics, soft matter, and complex fluids. The DY section has strong links and joint sessions with the sections of Biological Physics (BP), Chemical Physics and Polymers (CPP), Socio- and Econophysics (SOE), and Low Temperatures (TT).

Overview of Invited Talks and Sessions

(Lecture halls A 151, BH-N 128, BH-N 243, and BH-N 334; Posters C and D)

Invited Talks

DY 3.1	Mon	9:30–10:00	A 151	**Quantum information phases in space-time: measurement-induced entanglement and teleportation on a noisy quantum processor** — •Vedika Khemani
DY 3.2	Mon	10:00–10:30	A 151	**Measurement phase transitions and universality** — •Adam Nahum
DY 3.3	Mon	10:30–11:00	A 151	**Dual-unitary circuit dynamics** — •Pieter Claeys
DY 4.1	Mon	9:30–10:00	BH-N 128	**Towards the ultimate regime in Rayleigh-Benard turbulence** — •Olga Shishkina
DY 6.1	Mon	9:30–10:00	BH-N 334	**Barrier crossing with non-Gaussian noise: Exponential transition rate gains and effects of active motion** — •Peter Sollich, Adrian Baule, Diego Tapias
DY 7.1	Mon	11:30–12:00	BH-N 128	**Critical transitions in non-autonomous complex dynamical systems: theory and applications to ecosystems and climate** — •Ulrike Feudel
DY 9.1	Mon	15:00–15:30	A 151	**Quantum Mechanics and Many Body Games** — •Shivaji Sondhi
DY 9.2	Mon	15:30–16:00	A 151	**Measurement induced phase transitions of fermions: from theory to observability** — •Sebastian Diehl
DY 9.3	Mon	16:00–16:30	A 151	**Novel quantum dynamics with superconducting qubits** — •Pedram Roushan
DY 11.1	Mon	15:00–15:30	BH-N 243	**Control of active turbulence** — •Holger Stark
DY 18.1	Tue	9:30–10:00	BH-N 128	**Phase field method to model single cell locomotion and collective cell interactions** — •Sergio Alonso
DY 20.1	Tue	9:30–10:00	BH-N 334	**Dynamics of genome replication** — •Simone Pigolotti
DY 22.1	Wed	9:30–10:00	A 151	**Boundary behavior at classical and quantum phase transitions** — •Max Metlitski
DY 22.6	Wed	11:15–11:45	A 151	**Criticality senses topology** — Oleg Vasilyev, •Anna Maciolek, Siegfried Dietrich
DY 24.1	Wed	9:30–10:00	BH-N 243	**The nonreciprocal Cahn-Hilliard model - properties and significance** — •Uwe Thiele, Tobias Frohoff-Hülsmann, Daniel Greve
DY 25.1	Wed	9:30–10:00	BH-N 334	**Emergent chemotaxis in synthetic active matter** — •Abhinav Sharma, Hidde Vuijk, Pierluigi Muzzeddu, Holger Merlitz, Jens-Uwe Sommer
DY 29.1	Wed	15:00–15:30	A 151	**Conformal boundary conditions of symmetric quantum critical states** — •Long Zhang

DY 30.1	Wed	15:00–15:30	BH-N 243	**Continuum Approach for Studying Morphological Deformations of Multiple-Phase Renewable Energy Devices** — •Arik Yochelis
DY 42.1	Thu	9:30–10:00	BH-N 243	**Is predicting chaos and extreme dynamics possible? An overview of (some) scientific machine learning approaches** — •Luca Magri
DY 43.1	Thu	9:30–10:00	BH-N 334	**Flocking by turning away** — •Ricard Alert
DY 43.7	Thu	11:30–12:00	BH-N 334	**Growth and division as drivers of complex dynamics in dense cellular matter** — •Philip Bittihn
DY 49.1	Thu	15:00–15:30	BH-N 243	**Using reservoir computing to create surrogate models** — •Lina Jaurigue
DY 49.7	Thu	17:00–17:30	BH-N 243	**Opportunities in Quantum Reservoir Computing** — •Roberta Zambrini
DY 57.1	Fri	9:30–10:00	BH-N 128	**A simulation approach for the emerging mechanical properties of multi-network systems** — •Kirsten Martens

Invited Talks of the joint Symposium SKM Dissertation Prize 2024 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H 1012	**Nonequilibrium dynamics in constrained quantum many-body systems** — •Johannes Feldmeier
SYSD 1.2	Mon	10:00–10:30	H 1012	**Controlled Manipulation of Magnetic Skyrmions: Generation, Motion and Dynamics** — •Lisa-Marie Kern
SYSD 1.3	Mon	10:30–11:00	H 1012	**Interactions within and between cytoskeletal filaments** — •Charlotta Lorenz
SYSD 1.4	Mon	11:00–11:30	H 1012	**Field theories in nonequilibrium statistical mechanics: from molecules to galaxies** — •Michael te Vrugt
SYSD 1.5	Mon	11:30–12:00	H 1012	**Lightwave control of electrons in graphene** — •Tobias Weitz

Invited Talks of the joint Symposium Advances in Ab-Initio Electronic Structure Theory of Time-Dependent and Non-Equilibrium Phenomena (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Tue	9:30–10:00	H 0105	**Light control of charge transport and phase transitions** — •Sheng Meng
SYES 1.2	Tue	10:00–10:30	H 0105	**Probing the transport of the interacting electron-phonon system self-consistently and *ab initio*** — •Nakib Protik
SYES 1.3	Tue	10:30–11:00	H 0105	**In- and out-of-equilibrium ab initio theory of electrons and phonons** — •Gianluca Stefanucci
SYES 1.4	Tue	11:15–11:45	H 0105	**Phonon screening of excitons in semiconductors and insulators from first principles** — •Marina Rucsandra Filip
SYES 1.5	Tue	11:45–12:15	H 0105	**Light-matter control of quantum materials: from Floquet to cavity engineering** — •Michael Sentef

Invited Talks of the joint Symposium Statistical Physics of Economic and Financial Systems (SYEF)

See SYEF for the full program of the symposium.

SYEF 1.1	Thu	9:30–10:00	H 0105	**Economic Complexity Theory and the General Economic Theory: Applying Synergetics** — •Wei-Bin Zhang
SYEF 1.2	Thu	10:00–10:30	H 0105	**Opinion Formation in the World Trade Network** — •Dima Shepelyansky
SYEF 1.3	Thu	10:30–11:00	H 0105	**Transfer Entropy in financial stock markets** — •Leonidas Sandoval
SYEF 1.4	Thu	11:15–11:45	H 0105	**Statistical-Physics Theory of the Long Memory in Market-Order Flows and its Empirical Validation in the Tokyo Stock Exchange** — •Kiyoshi Kanazawa
SYEF 1.5	Thu	11:45–12:15	H 0105	**Ergodicity Economics and the Insurance Problem** — •Benjamin Skjold, Ole Peters, Colm Connaughton

Invited Talks of the joint Symposium New Trends in Nonequilibrium Physics: Conservation Laws and Nonreciprocal Interactions (SYNP)

See SYNP for the full program of the symposium.

SYNP 1.1	Thu	15:00–15:30	H 0105	**Universality classes of nonequilibrium phase transitions with conservation constraints** — •Walter Zimmermann
SYNP 1.2	Thu	15:30–16:00	H 0105	**The many faces of living chiral crystals** — •Nikta Fakhri
SYNP 1.3	Thu	16:00–16:30	H 0105	**Non-reciprocal pattern formation of conserved fields** — •Fridtjof Brauns, M Cristina Marchetti
SYNP 1.4	Thu	16:45–17:15	H 0105	**Phase transitions and fluctuations of nonreciprocal systems** — •Sarah A.M. Loos
SYNP 1.5	Thu	17:15–17:45	H 0105	**Chiral matters** — •William Irvine

Sessions

DY 1.1–1.8	Mon	9:30–13:15	H 0104	**Focus Session: Artificial Intelligence in Condensed Matter Physics I (joint session TT/DY)**
DY 2.1–2.12	Mon	9:30–12:45	H 1028	**Active Matter I (joint session BP/CPP/DY)**
DY 3.1–3.10	Mon	9:30–12:45	A 151	**Focus Session: Quantum Interactive Dynamics I (joint session DY/TT)**
DY 4.1–4.5	Mon	9:30–11:00	BH-N 128	**Fluid Physics and Turbulence**
DY 5.1–5.13	Mon	9:30–13:00	BH-N 243	**Machine Learning in Dynamics and Statistical Physics I**
DY 6.1–6.12	Mon	9:30–13:00	BH-N 334	**Statistical Physics far from Thermal Equilibrium I**
DY 7.1–7.5	Mon	11:30–13:00	BH-N 128	**Critical Phenomena and Phase Transitions**
DY 8.1–8.4	Mon	15:00–16:00	H 3025	**Artificial Intelligence in Condensed Matter Physics II (joint session TT/DY)**
DY 9.1–9.9	Mon	15:00–18:00	A 151	**Focus Session: Quantum Interactive Dynamics II (joint session DY/TT)**
DY 10.1–10.13	Mon	15:00–18:30	BH-N 128	**Nonlinear Dynamics, Synchronization and Chaos**
DY 11.1–11.12	Mon	15:00–18:30	BH-N 243	**Active Fluids and Microswimmers (joint session DY/BP/CPP)**
DY 12.1–12.8	Mon	15:00–17:00	BH-N 334	**Statistical Physics far from Thermal Equilibrium II**
DY 13.1–13.5	Mon	16:15–17:45	H 0107	**Glasses and Glass Transition (joint session CPP/DY)**
DY 14.1–14.6	Mon	16:15–18:00	H 3025	**Quantum Coherence (joint session TT/DY)**
DY 15.1–15.13	Tue	9:30–13:00	H 1028	**Active Matter II (joint session BP/CPP/DY)**
DY 16.1–16.13	Tue	9:30–13:00	H 3005	**Nonequilibrium Quantum Systems 1 (joint session TT/DY)**
DY 17.1–17.13	Tue	9:30–13:00	A 151	**Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)**
DY 18.1–18.12	Tue	9:30–13:00	BH-N 128	**Pattern Formation, Delay and Nonlinear Stochastic Systems**
DY 19.1–19.13	Tue	9:30–13:00	BH-N 243	**Machine Learning in Dynamics and Statistical Physics II (joint session DY/SOE)**
DY 20.1–20.12	Tue	9:30–13:00	BH-N 334	**Statistical Physics of Biological Systems I (joint session DY/BP)**
DY 21.1–21.5	Tue	11:45–13:00	H 3007	**Focus Session: Nanomechanical Systems for Classical and Quantum Sensing I (joint session TT/DY/HL/QI)**
DY 22.1–22.9	Wed	9:30–12:30	A 151	**Focus Session: Recent Progresses in Criticality in the Presence of Boundaries and Defects I (joint session DY/TT)**
DY 23.1–23.13	Wed	9:30–13:00	BH-N 128	**Stochastic Thermodynamics**
DY 24.1–24.12	Wed	9:30–13:00	BH-N 243	**Focus Session: New Trends in Nonequilibrium Physics – Conservation Laws and Nonreciprocal Interactions I**
DY 25.1–25.12	Wed	9:30–13:00	BH-N 334	**Active Matter III (joint session DY/BP/CPP)**
DY 26.1–26.8	Wed	15:00–17:45	H 2032	**Focus Session: Inference Methods and Biological Data (German-French Focus Session) (joint session BP/DY)**
DY 27.1–27.10	Wed	15:00–17:45	EW 202	**Focus Session: Nanomechanical Systems for Classical and Quantum Sensing II (joint session HL/DY/TT/QI)**
DY 28.1–28.13	Wed	15:00–18:30	TC 006	**Networks: From Topology to Dynamics I (joint session SOE/DY)**
DY 29.1–29.4	Wed	15:00–16:15	A 151	**Focus Session: Recent Progresses in Criticality in the Presence of Boundaries and Defects II (joint session DY/TT)**

DY 30.1–30.5	Wed	15:00–16:30	BH-N 243	**Focus Session: New Trends in Nonequilibrium Physics – Conservation Laws and Nonreciprocal Interactions II**
DY 31.1–31.24	Wed	15:00–18:00	Poster C	**Poster: Statistical Physics**
DY 32.1–32.29	Wed	15:00–18:00	Poster C	**Poster: Active Matter, Soft Matter, Fluids**
DY 33.1–33.17	Wed	15:00–18:00	Poster C	**Poster: Nonlinear Dynamics, Pattern Formation and Networks**
DY 34.1–34.16	Wed	15:00–18:00	Poster C	**Poster: Machine Learning, Data Science, and Reservoir Computing**
DY 35.1–35.22	Wed	15:00–18:00	Poster D	**Poster: Quantum Dynamics and Many-body Systems**
DY 36.1–36.5	Thu	9:30–11:00	H 0107	**Focus Session: Wetting on Adaptive Substrates I (joint session CPP/DY/O)**
DY 37.1–37.9	Thu	9:30–12:00	H 1028	**Statistical Physics of Biological Systems II (joint session BP/DY)**
DY 38.1–38.13	Thu	9:30–13:00	H 3025	**Nonequilibrium Quantum Systems 2 (joint session TT/DY)**
DY 39.1–39.8	Thu	9:30–13:00	EW 202	**Focus Session: Nanomechanical Systems for Classical and Quantum Sensing III (joint session HL/DY/TT/QI)**
DY 40.1–40.13	Thu	9:30–13:00	A 151	**Many-body Quantum Dynamics I (joint session DY/TT)**
DY 41.1–41.12	Thu	9:30–12:45	BH-N 128	**Statistical Physics: General**
DY 42.1–42.9	Thu	9:30–12:15	BH-N 243	**Focus Session: Computing with Dynamical Systems: New Perspectives on Reservoirs and Applications I – Fundamentals**
DY 43.1–43.11	Thu	9:30–13:00	BH-N 334	**Active Matter IV (joint session DY/BP/CPP)**
DY 44.1–44.5	Thu	11:30–13:00	H 0107	**Focus Session: Wetting on Adaptive Substrates II (joint session CPP/DY/O)**
DY 45.1–45.8	Thu	15:00–17:30	H 0107	**Wetting, Fluidics and Liquids at Interfaces and Surfaces (joint session CPP/DY)**
DY 46.1–46.8	Thu	15:00–17:45	H 0110	**Complex Fluids, Colloids, Micelles and Vesicles (joint session CPP/DY)**
DY 47.1–47.10	Thu	15:00–17:45	A 151	**Quantum Chaos and Coherent Dynamics (joint session DY/TT)**
DY 48.1–48.8	Thu	15:00–17:00	BH-N 128	**Granular Matter and Contact Dynamics**
DY 49.1–49.9	Thu	15:00–18:00	BH-N 243	**Focus Session: Computing with Dynamical Systems: New Perspectives on Reservoirs and Applications II – Applications and Quantum RC**
DY 50.1–50.10	Thu	15:00–17:45	BH-N 334	**Wetting, Droplets, and Microfluidics (joint session DY/CPP)**
DY 51	Thu	18:00–19:00	BH-N 243	**Members' Assembly**
DY 52.1–52.10	Fri	9:30–12:45	H 0110	**Focus Session: Wetting on Adaptive Substrates III (joint session CPP/DY/O)**
DY 53.1–53.12	Fri	9:30–13:00	H 2032	**Statistical Physics of Biological Systems III (joint session BP/DY)**
DY 54.1–54.12	Fri	9:30–13:00	H 1028	**Active Matter V (joint session BP/DY)**
DY 55.1–55.1	Fri	9:30–10:00	MA 001	**Power Grids (joint session SOE/DY)**
DY 56.1–56.4	Fri	9:30–10:30	A 151	**Many-body Quantum Dynamics II (joint session DY/TT)**
DY 57.1–57.9	Fri	9:30–12:15	BH-N 128	**Networks: From Topology to Dynamics II (joint session DY/SOE)**
DY 58.1–58.10	Fri	9:30–12:15	BH-N 243	**Complex Fluids and Soft Matter (joint session DY/CPP)**
DY 59.1–59.13	Fri	9:30–13:00	BH-N 334	**Brownian Motion and Anomalous Diffusion**
DY 60.1–60.9	Fri	10:45–13:00	A 151	**Quantum Dynamics, Decoherence and Quantum Information (joint session DY/TT)**
DY 61.1–61.1	Fri	13:15–14:00	H 0104	**Closing Talk (joint session BP/CPP/DY)**

Members' Assembly of the Dynamics and Statistical Physics Division

Thursday 18:00–19:00 BH-N 243

- Report
- Future activities of DY
- Any other business

DY 1: Focus Session: Artificial Intelligence in Condensed Matter Physics I (joint session TT/DY)

While artificial intelligence leaves an ever growing footprint in our everyday lives, it has as well inspired various new approaches in the physical sciences; for instance, one of the outstanding success stories is the prediction of protein folding with unprecedented accuracy. But what role can AI play in condensed matter physics? This symposium aims to provide an overview and discussion of recent applications of modern machine learning and its prospects for the advancement of research in this field. The increasingly data-intensive experiments with high-dimensional observations call for the development of new tools for analysis matching known strengths of machine learning algorithms. Reinforcement learning agents can be employed to precisely manipulate many-body systems, which, among other use cases, is a pivotal ingredient for quantum technologies. On the computational side, ideas from deep learning and generative modeling inspire new building blocks to boost numerical simulations. One may even ask the question whether a machine can autonomously discover physical concepts such as effective degrees of freedom or equations of motion, and reveal them in an interpretable manner to human researchers.
Please note the second part of this session which will take place this afternoon, TT 14 (15:00 − 16:00) in the lecture Hall H3025.

Prof. Dr. Simon Trebst, Universität Köln
Prof. Dr. Florian Marquardt, Max-Planck-Institut Erlangen
Dr. Markus Schmitt, FZ Jülich

Time: Monday 9:30–13:15 Location: H 0104

Invited Talk DY 1.1 Mon 9:30 H 0104
Exploring artificial intelligence for engineered quantum matter — •Eliska Greplova — Kavli Institute of Nanoscience, Delft University of Technology, Netherlands

In research labs worldwide, quantum physics is making unprecedented strides. The realization of robust quantum systems holds tremendous promise for applications in secure communication and computing. Yet, as physicists, our most exciting pursuit lies in experimentally testing quantum phenomena predicted over the past century within highly controlled environments. In this talk, I will explore artificial intelligence approaches in the field of engineered quantum matter. Throughout the seminar, we will uncover how these approaches can be effectively deployed in contemporary quantum experiments. As one example, I will show how we can utilize generative models for parameter prediction of engineered topological systems known as Kitaev chains. Using this result and similar examples, I will discuss how we can use ML techniques to pave the way for advancing our control and understanding of real quantum experiments.

Invited Talk DY 1.2 Mon 10:00 H 0104
Communicability as a criterion for interpretable representations — •Renato Renner — ETH Zürich, Zürich, Switzerland

We propose an autoencoder architecture that can generate representations of data from physical experiments which are operationally meaningful and thus interpretable. The architecture is based on the paradigm of "communicability". Roughly, the idea is that the encoder orders the data into several parts that may be communicated separately to agents, whose task is to answer different questions about the data. The encoding is then optimised so that this communication is minimised, i.e., each agent receives precisely the information that is relevant to its task. Using some toy examples, including ones from quantum state tomography, we show that this approach leads to a separation of parameters, which can be regarded as a step towards interpretability.

Invited Talk DY 1.3 Mon 10:30 H 0104
Disentangling Multiqubit States using Deep Reinforcement Learning — •Marin Bukov — Max Planck Institute for the Physics of Complex Systems

Quantum entanglement plays a central role in modern quantum technologies. It is widely perceived as a proxy for the quantum nature of physical processes and phenomena involving more than one particle. In this talk, we will revisit the problem of disentangling 4-, 5-, and 6-qubit quantum states with the help of machine learning techniques. We use policy gradient algorithms to train a deep reinforcement learning agent which, given access to the pure state of a multiqubit system, has to find the shortest sequence of disentangling two-qubit gates that brings it to a product state. We leverage the agent's interpolation and extrapolation capabilities to learn (approximately) optimal strategies to disentangle Haar-random states that lack any obvious spatial entanglement structure in the computational basis. Analyzing the protocols found by the agent, we show that any 4-qubit state can be prepared using at most 11 CNOT gates. Last, we also demonstrate the robustness of our agent to various sources of stochasticity common for present-day NISQ devices.

15 min. break

Invited Talk DY 1.4 Mon 11:15 H 0104
Neural Quantum States For The Many-Electron Problem — •Giuseppe Carleo — EPFL, Lausanne, Switzerland

This presentation explores recent strides in using neural quantum states [1] to represent many-body fermionic quantum wave functions for the many-electron problem [2]. I will delve into a message-passing-neural-network-based Ansatz designed for simulating strongly interacting electrons in continuous space [3]. This approach achieves unprecedented accuracy in the electron gas problem, pushing the boundaries of system sizes previously inaccessible to neural network states. I will also discuss a Pfaffian-based neural-network quantum state for ultra-cold Fermi gases, outperforming traditional methods and enabling exploration of the BCS-BEC crossover region [4]. Finally, I will provide insight into ongoing work on the entanglement properties of Helium 4 and Helium 3, and discuss open problems in the field [5].
[1] Carleo and Troyer, Science 355, 602 (2017)
[2] Hermann et al., Nature Reviews Chemistry 7, 692 (2023)
[3] Pescia et al., arxiv:2305.07240 (2023)
[4] Kim et al., arxiv:2305.08831 (2023)
[5] Linteau et al., in preparation (2024).

Invited Talk DY 1.5 Mon 11:45 H 0104
Neural quantum states for strongly correlated systems: learning from data and Hamiltonians — •Annabelle Bohrdt[1], Hannah Lange[2], Schuyler Moss[3], Fabian Döschl[2], Felix Palm[2], Giulia Semeghini[4], Mikhail Lukin[4], Sepehr Ebadi[4], Tout Wang[4], Fabian Grusdt[2], Juan Carrasquilla[5], and Roger Melko[3] — [1]Universität Regensburg — [2]LMU München — [3]UWaterloo — [4]Harvard University — [5]Vector Institute

Neural quantum states have emerged as a new tool to efficiently represent quantum many-body states with two main use cases: 1.) efficiently reconstruct a quantum state by training on measured data. For states with a non-trivial sign structure, measurements in many different basis configurations are necessary. I will present an active learning

scheme which adaptively chooses the next measurement basis in order to maximize the information gain. 2.) The second main application of neural quantum states is to apply variational Monte Carlo to find e.g. the ground state of a system. I will present some of our recent results on ground states of strongly correlated systems, such as t-J type systems and fractional quantum Hall states. Finally, we combine both approaches: by first training on experimental data from a Rydberg atom tweezer array, we initialize the neural quantum state closer to the ground state. By then switching to variational Monte Carlo to minimize the energy in the second stage of training, we find a speedup in convergence. This showcases how limited datasets from experiments can be combined with numerical methods in a hybrid approach to yield more accurate results than either could provide on their own.

Invited Talk DY 1.6 Mon 12:15 H 0104

Towards an Artificial Muse for new Ideas in Quantum Physics — •Mario Krenn — Max Planck Institute for the Science of Light, Erlangen, Germany

Artificial intelligence (AI) is a potentially disruptive tool for physics and science in general. One crucial question is how this technology can contribute at a conceptual level to help acquire new scientific understanding or inspire new surprising ideas. I will talk about how AI can be used as an artificial muse in quantum physics, which suggests surprising and unconventional ideas and techniques that the human scientist can interpret, understand and generalize to its fullest potential.

[1] Krenn et al., Phys. Rev. X 11 (2021) 031044.
[2] Krenn et al., Nat. Rev. Phys. 4 (2022) 761.
[3] Krenn et al., Nat. Mach. Intell. 5 (2023) 1326

DY 1.7 Mon 12:45 H 0104

Adversarial Hamiltonian learning of quantum dots in a minimal Kitaev chain — •Rouven Koch[1], David van Driel[2,3], Alberto Bordin[2,3], Jose L. Lado[1], and Eliska Greplova[3] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]QuTech, Delft University of Technology, Delft, The Netherlands — [3]Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands

Knowledge of the underlying Hamiltonian in quantum devices is key for tuning and controlling experimental quantum systems. Here we demonstrate an adversarial machine learning framework capable of Hamiltonian learning of a quantum dot chain from noisy experimental measurements. We train a convolutional conditional generative adversarial network with simulated data of the differential conductances based on a Kitaev chain model. The trained model is able to predict the parameters determining the sweet spot conditions of the two-quantum-dot system at which the predicted mid-gap bound state emerges. This gives us a fast and numerically efficient way to explore the phase diagram describing the transition between elastic co-tunning and Andreev reflection regimes and thus is suitable to assist the sweet-spot tuning of the Kitaev chains. The application of our methodology to experimental measurements in an InSb nanowire shows promising results in extracting Hamiltonians from measurements, potentially supporting the hard task of tuning quantum-dot systems into distinct Hamiltonian regimes.

DY 1.8 Mon 13:00 H 0104

Machine determination of a phase diagram with and without deep learning — •Burak Çivitcioğlu[1], Rudolf A. Römer[2], and Andreas J. Honecker[1] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, CY Cergy Paris Université, France — [2]University of Warwick, Coventry, UK

We study the performance of unsupervised learning in detecting phase transitions in the J_1-J_2 Ising model on the square lattice. We use variational auto encoders (VAE) and the reconstruction error, defined as the mean-squared error between two configurations, to explore the phase diagram of the system. Moreover, we propose as simple alternative method a direct spin comparison. The results of the spin comparison are contrasted with that of the VAEs. Our findings highlight that for certain systems, the simpler method can yield results comparable to a much more complex model, namely the VAE. This work contributes to the broader understanding of machine-learning applications in statistical physics and introduces an efficient approach to the detection of phase transitions using machine determination techniques.

DY 2: Active Matter I (joint session BP/CPP/DY)

Time: Monday 9:30–12:45 Location: H 1028

DY 2.1 Mon 9:30 H 1028

Active Colloids as Tunable Swarmalators — •Veit-Lorenz Heuthe[1,2] and Clemens Bechinger[1,2] — [1]Fachbereich Physik, Universität Konstanz — [2]Centre for the Advanced Study of Collective Behaviour, Universität Konstanz

The complexity and functional advantages in various systems from groups of organisms to robotic swarms and digital networks hinge on spatiotemporal patterns arising from the interactions of their constituents. One approach to gain understanding of how these patterns emerge are so-called swarmalators. In this conceptual framework, individual entities exhibit both oscillatory behavior and translational motion, coupled based on their relative phase and position, yielding a diverse array of complex patterns. Here, we introduce a system of active colloids that both oscillate and translate and are coupled to each other in both speed and phase through hydrodynamic interactions. Despite the physical nature of the interactions, the system retains tunability, enabling us to systematically study the behavior of swarmalators in a real system.

DY 2.2 Mon 9:45 H 1028

Electric field driven active colloids moving in polymeric environments — •venkata manikantha sai ganesh tanuku, peter vogel, and thomas palberg — Institute of Physics, Johannes Gutenberg University

A dilute suspension of Janus particles (JPs) in a dense viscoelastic fluid, forms a natural setting to study their dynamics in surrounding doped with macromolecules such as polymers is crucial, as most of the target application media are complex in nature. In this study, we investigate the motion of AC electric field driven SiO2-Au JPs in the presence of concentrated amounts of poly (ethylene glycol) (PEG). The transport of active particles is strongly influenced by the viscous medium and shows a dynamical jamming transition as a function of activity and medium density. For low activity, the active particle gets self-trapped in a cavity of its own making. Conversely, higher activity causes JP to push through the fluid, leaving behind a porous trail. At the given concentration of the PEG studied within these experiments two intriguing outcomes emerge: firstly, a JP can be immobilized and secondly, when two JPs move in the same direction, an unusual attraction occurs, causing the trailing JP to eventually catch up with the leading one in finite time.

DY 2.3 Mon 10:00 H 1028

Lorentz reciprocal theorem in fluids with odd viscosity — •Yuto Hosaka[1], Ramin Golestanian[1,2,3], and Andrej Vilfan[1,4] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom — [3]Institute for the Dynamics of Complex Systems, University of Göttingen, 37077 Göttingen, Germany — [4]Jozef Stefan Institute, 1000 Ljubljana, Slovenia

The Lorentz reciprocal theorem – that is used to study various transport phenomena in hydrodynamics – is violated in chiral active fluids that feature odd viscosity with broken time-reversal and parity symmetries. Here we show that the theorem can be generalized to fluids with odd viscosity by choosing an auxiliary problem with the opposite sign of the odd viscosity [1]. We demonstrate the application of the theorem to two categories of microswimmers. Swimmers with prescribed surface velocity are not affected by odd viscosity, while those with prescribed active forces are. In particular, a torque-dipole can lead to directed motion.

[1] Y. Hosaka, R. Golestanian, and A. Vilfan, Phys. Rev. Lett. 131, 178303 (2023).

DY 2.4 Mon 10:15 H 1028

A Stochastic Bubble Model in MIPS Active systems — •Mingqi Yan[1,2,3,4], Erwin Frey[1,4], Marcus Müller[2,4], and Stefan Klumpp[3,4] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany — [2]Institut für Theoretische Physik, Department of Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [3]Institut für Dynamik komplexer Systeme, Department of Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [4]Max Planck School Matter to Life, Hofgartenstraße 8, D-80539 München, Germany

Motility-Induced Phase Separation (MIPS) is a notable phenomenon in which self-propelled particles undergo phase separation solely due to their intrinsic motility. This behavior starkly contrasts with passive systems, where active systems constantly form bubbles in liquids. Here, we introduce a stochastic bubble model to elucidate the changes in bubble area within Active Brownian Particle systems. We demonstrate that the bubble-area evolution can be described by a Langevin equation. Notably, this equation characterizes a unique category of stochastic systems: while it possesses an absorbing state, it concurrently maintains a stable nonequilibrium steady state distribution of areas.

DY 2.5 Mon 10:30 H 1028

Dynamics and phase separation of active Brownian particles on curved surfaces and in porous media — •Priyanka Iyer, Roland Winkler, Dmitry Fedosov, and Gerhard Gompper — Theoretical Physics of Living Matter (IBI-5/IAS-2), Forschungszentrum Jülich

In biophysical systems, active particles are often exposed to curved geometries and confinement. This prompts a crucial question: How does curvature influence the emergent collective behavior of active particles? We study this question by considering the effect of curvature on an ensemble of repulsive active Brownian particles (ABPs) moving on a spherical surface. Surface curvature affects the dynamics of ABPs, as it introduces a new time scale $\tau = R/v_0$, with curvature radius R and propulsion velocity v_0, in addition to the rotational diffusion time τ_r. The time scale τ is related to a stop-and-go motion caused by the recurrent alignment of the propulsion direction with the surface normal. This implies that motility-induced phase separation (MIPS) disappears for large curvature. Moreover, the phase-separation boundary at low area fraction ϕ attains a turning point for small R, allowing for the possibility of a re-entrant behavior. The findings also have implications for understanding how curvature influences ABP dynamics in porous media, as demonstrated through a paradigmatic example involving two connected pores. Surprisingly, it is found that the different curvatures of the two pores can facilitate particle flux towards regions of high particle density and induce transient MIPS states.

[1] Iyer et al. Phys. Rev. Res. **5**, 033054 (2023).

DY 2.6 Mon 10:45 H 1028

Giant Activity-Induced Stress Plateau in Entangled Polymer Solutions — Davide Breoni[1], Christina Kurzthaler[2], Benno Liebchen[3], Hartmut Löwen[2], and •Suvendu Mandal[3] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöhnitzer Straße 38, 01187 Dresden, Germany — [3]Technische Universität Darmstadt, Karolinenplatz 5, 64289 Darmstadt, Germany

Highly entangled active polymer solutions play vital roles in various biological processes, spanning from the intricate mechanisms of cell mitosis to the regulation of genetic transcription. We study the viscoelastic properties of highly entangled, flexible, self-propelled polymers using Brownian dynamics simulations. Our results show that the active motion of the polymer increases the height of the stress plateau by orders of magnitude due to the emergence of grip forces at entanglement points. Identifying the activity-induced energy of a single polymer and the ratio of polymer length to self-propulsion velocity as relevant energy and time scales, we find the stress autocorrelation functions collapse across Peclet numbers [1]. We predict that the long-time viscosity scales with polymer length squared, in contrast to equilibrium counterparts that scale with the cube of the polymer length [1]. These insights offer prospects for designing new materials with activity-responsive mechanical properties.

[1] D. Breoni, C. Kurzthaler, B. Liebchen, H. Löwen, and S. Mandal, https://doi.org/10.48550/arXiv.2310.02929

15 min. break

DY 2.7 Mon 11:15 H 1028

Gravitactic bioconvection drives emergent transport and mixing in harmful algal blooms — •Soumitree Mishra[1] and Anupam Sengupta[1,2] — [1]Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg — [2]Institute for Advanced Studies, University of Luxembourg

Bioconvection, the active self-sustaining transport phenomenon triggered by the accumulation of motile microbes, has been long studied. Yet, if and how this collective behavior, driven by competing physico-chemical cues, impacts ecological processes including Harmful Algal Blooms (HABs) remains unexplored. Here, using a bloom-forming model phytoplankton, we present a comprehensive mechanistic study on the biophysical factors governing the emergent collective patterns and capture the eco-physiological implications of bioconvective flows. Leveraging our Ocean-On-Chip platform, together with particle tracking velocimetry (PTV) and particle image velocimetry (PIV), we uncover flow fields around isolated self-organized microbial plumes, using which we extract the spatial range of active transport. Using data-backed fluid dynamic simulations, we extract the Lyapunov exponents, revealing the mixing capacity of such plumes in confined environments. Our findings significantly advance our understanding of bioconvection's functional role in ecological contexts[1], providing a novel playground where ecology meets active matter. [Reference 1] Bioconvection mediates transport and mixing dynamics within harmful algal blooms: S. Mishra & A. Sengupta (manuscript in preparation).

DY 2.8 Mon 11:30 H 1028

Energetic cost of microswimmer navigation: the role of body shape — •Lorenzo Piro[1,2], Andrej Vilfan[1,3], Ramin Golestanian[1,4], and Benoît Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Goettingen, Germany — [2]Department of Physics and INFN, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy — [3]Jozef Stefan Institute, 1000 Ljubljana, Slovenia — [4]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We study the energetic efficiency of navigating microswimmers by explicitly taking into account the geometry of their body. We show that, whereas arguments based solely on propulsion efficiency lead to the conclusion that needle-like swimmers are most energetically efficient, disk-like swimmers rotated by flow gradients naturally follow time-optimal trajectories. The coupling between body geometry and hydrodynamics thus leads to a generic trade-off between the energetic costs associated with propulsion and navigation, which is accompanied by the selection of a finite optimal aspect ratio. We derive from optimal control theory the steering policy ensuring overall minimum energy dissipation and characterize how navigation performances vary with the swimmer shape. Our results highlight the important role of the swimmer geometry in realistic navigation scenarios.

DY 2.9 Mon 11:45 H 1028

Optimal motility strategies for self-propelled agents to explore porous media — •Christoph Lohrmann and Christian Holm — Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany

Micro-robots for, e.g., biomedical applications, need to be equipped with motility strategies that enable them to navigate through complex environments. Inspired by biological microorganisms we recreate motility patterns such as run-and-reverse, run-and-tumble or run-reverse-flick applied to active rod-like particles in silico. We investigate their capability to efficiently explore disordered porous environments with various porosities and mean pore sizes ranging down to the scale of the active particle. By calculating the effective diffusivity for the different patterns, we can predict the optimal one for each porous sample geometry. We find that providing the agent with the ability to sense position for a certain time and to make a decision based on its observation yields a motility pattern outperforming the biologically inspired patterns for all investigated porous samples[1].

[1] Lohrmann, Holm: Optimal motility strategies for self-propelled agents to explore porous media, arXiv:2302.06709, 2023

DY 2.10 Mon 12:00 H 1028

Chemotaxis of an active particle attached to a semiflexible cargo — •Shashank Ravichandur[1], Abhinav Sharma[2,1], and Jens-Uwe Sommer[1] — [1]Leibniz-Institut für Polymerforschung, Dres-

den, Germany — [2]Universität Augsburg, Augsburg, Germany

The chemotaxis of synthetic active particles in activity gradients, achieved by connecting them to other active/passive particles to form simple dimers, has been demonstrated in recent studies. These studies have been extended to synthetic active particles connected to each other to form polymer chains, which also exhibit chemotaxis. However, the study of these polymer chains in activity gradients has been limited to the Rouse model, wherein the particles are connected to each other via springs, and the excluded volume interactions are ignored. To obtain a more realistic description, we consider an active synthetic particle connected to a passive tail that is semiflexible. In such a system, the configuration of the passive tail affects the motion of the active particle. Using Langevin dynamics simulations, we show that these polymers also exhibit chemotaxis in activity gradients despite the coupling between the active particle and the passive tail. We also study the effects of the chain length and bending rigidity on the chemotactic behavior.

DY 2.11 Mon 12:15 H 1028

How cell shape guides gliding motility — •Leon Lettermann[1], Falko Ziebert[1], Mirko Singer[1], Friedrich Frischknecht[2], and Ulrich S. Schwarz[2] — [1]IPT & Bioquant, Heidelberg University — [2]CIID, Heidelberg University

Cell motility comes in many different types, including swimming, crawling and gliding. The latter term denotes movement on surfaces or through tissues without appreciable changes in cell shape and is usually based on some kind of surface flow. Gliding motility is often used by cells that need to accomplish high speeds, including myxo- or flavobacteria as well as eukaryotic parasites from the phylum apicomplexa, in particular the causative agents of malaria and toxoplasmosis. We have developed an active particle theory which connects the self-organized surface dynamics to the global motility patterns of the glider. Our theory demonstrates that the resulting trajectories depend strongly on glider shape. Our analytical solutions and numerical simulations show that straight motion to get from A to B is unstable and predict the rotational and helical trajectories which are observed experimentally for gliding bacteria and apicomplexan parasites.

DY 2.12 Mon 12:30 H 1028

Impact of non-reciprocity on the self-aggregation of an anisotropic colloidal system — •Salman Fariz Navas and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Non-reciprocal interactions have been demonstrated to introduce interesting collective behaviour in many-body systems[1]. Recent studies involving non-reciprocal colloidal particle systems have shown to induce propulsion mechanisms[2] and cause enhanced diffusion of tracer particles[3]. Such effects can have an impact on aggregation mechanisms as well[2]. Here, we introduce non-reciprocal interactions to a self-aggregating colloidal system with direction dependent, field-induced interactions[4]. In stark contrast to the passive (reciprocal) case, non-reciprocity induces a propulsion mechanism when a pair of particles belonging to different species come in contact. We show that at low degrees of non-reciprocity the aggregation is accelerated. At higher degrees of non-reciprocity, the system even tends to phase separate leading to the coexistence of dilute, freely moving particles and dense clusters.

[1] M. Fruchart, R. Hanai, P. B. Littlewood, and V. Vitelli, Nature 592, 363 (2021).
[2] S. Fehlinger and B. Liebchen, Phys. Rev. Research 5, L032038 (2023).
[3] A. Benois, M. Jardat, V. Dahirel, V. Démery, J. Agudo-Canalejo, R. Golestanian, and P. Illien, Phys. Rev. E 108, 054606 (2023).
[4] F. Kogler, O. D. Velev, C. K. Hall, and S. H. L. Klapp, Soft Matter 11, 7356 (2015).

DY 3: Focus Session: Quantum Interactive Dynamics I (joint session DY/TT)

Quantum many-body systems out of equilibrium represent a challenging frontier and have been shown to exhibit extremely rich phenomena. Recent experimental advances in building Noisy Intermediate-Scale Quantum (NISQ) devices have opened up a completely new territory in this context. The natural evolution implemented by NISQ devices is a quantum interactive dynamics generated by a combination of unitary gates and measurements. These platforms provide an opportunity to explore vastly larger parts of the Hilbert space and go beyond what can be realized in purely unitary systems. In pioneering works, an entanglement phase transition was identified in the dynamics of circuits of random unitary gates interleaved with local projective measurements. This phase transition separates a disentangling phase, obeying an area law, and an entangling phase obeying a volume law. Successively, it has been shown that additional phase transitions between different area phases can occur and new kinds of quantum phase transitions have been discovered. This session aims to give an overview of recent theoretical and experimental developments within this very active field and point towards the open questions.

Organized by Roderich Moesser (Dresden) and Frank Pollmann (München)

Time: Monday 9:30–12:45 Location: A 151

Invited Talk DY 3.1 Mon 9:30 A 151

Quantum information phases in space-time: measurement-induced entanglement and teleportation on a noisy quantum processor — •Vedika Khemani — Stanford University, USA

I will discuss the dynamics of monitored systems combining the ingredients of unitary evolution, measurements, and adaptive classical control. I will present various novel dynamical phases and phase transitions that arise in these systems, ranging from entanglement and teleportation phase transitions to "learnability" transitions in the ability to reconstruct quantum information from measurements. I will also discuss experimental realizations of these phenomena in noisy quantum processors.

Invited Talk DY 3.2 Mon 10:00 A 151

Measurement phase transitions and universality — •Adam Nahum — ENS Paris & CNRS

Repeated measurement can lead to a phase transition in quantum many-body dynamics. A subcritical rate of measurement allows complex, entangled states to evolve, while a supercritical measurement rate kills long-range entanglement. These phase transitions allow formal analogies with standard ordering transitions, but they are fundamentally different, partly as a result of the role played by quantum mechanical measurement randomness. Obtaining exact results for generic versions of the problem is challenging. I will sketch limits in which progress can be made (for example mean-field-like models, models in high dimensions, and noninteracting analogs).

Invited Talk DY 3.3 Mon 10:30 A 151

Dual-unitary circuit dynamics — •Pieter Claeys — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden

Dual-unitary circuits are minimal models of many-body quantum dynamics characterized by an underlying space-time duality. This duality makes them amenable to exact analysis, while remaining chaotic, and in recent years dual-unitary circuits have been used to study e.g. aspects of operator dynamics, quantum chaos, operator scrambling, entanglement dynamics, and the interplay between unitary dynamics and projective measurements. In this work I will give an overview of recent developments in dual-unitary circuits, focusing on the connection with many-body dynamics.

DY 3.4 Mon 11:00 A 151

Truncated Hilbert space approach for simulating dynamics in perturbed Ising chains — •Nico Albert[1] and Hong-Hao Tu[2] — [1]Technische Universität Dresden, Dresden, Germany — [2]Ludwig-Maximilians-Universität München, Munich, Germany

Simulating dynamics in interacting quantum many-body systems is a challenging problem. We develop a truncated Hilbert space approach (THSA) and apply it to the quantum Ising chain with both transverse and longitudinal fields for studying its spectrum and quench dynamics. We find that the characteristic features of this model, such as E_8 particles with universal mass ratios, are well captured in the truncated Hilbert space approach. We also use this new method to study the confinement dynamics of domain-wall bound states in the ferromagnetic phase.

DY 3.5 Mon 11:15 A 151

Entanglement Transitions in Unitary Circuit Games — •Raúl Morral-Yepes[1,2], Adam Smith[3], Shivaji L. Sondhi[4], and Frank Pollmann[1,2] — [1]Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [3]University of Nottingham, Nottingham, UK — [4]University of Oxford, Oxford, UK

Repeated projective measurements in unitary circuits can lead to an entanglement phase transition as the measurement rate is tuned. In this work, we consider a different setting in which the projective measurements are replaced by dynamically chosen unitary gates that minimize the entanglement. This can be seen as a one-dimensional unitary circuit game in which two players get to place unitary gates on randomly assigned bonds at different rates: The "entangler" applies a random local unitary gate with the aim of generating extensive (volume law) entanglement. The "disentangler", based on limited knowledge about the state, chooses a unitary gate to reduce the entanglement entropy on the assigned bond with the goal of limiting to only finite (area law) entanglement. In order to elucidate the resulting entanglement dynamics, we consider three different scenarios: (i) a classical discrete height model, (ii) a Clifford circuit, and (iii) a general $U(4)$ unitary circuit. We find that both the classical and Clifford circuit models exhibit phase transitions as a function of the rate that the disentangler places a gate. In contrast, the entangler always wins when using Haar random unitary gates and we observe extensive, volume law entanglement for all non-zero rates of entangling.

DY 3.6 Mon 11:30 A 151

Entanglement phases, localization and multifractality of monitored free fermions in two dimensions — •Karim Chahine and Michael Buchhold — Institut für Theoretische Physik, Universität zu Köln, D-50937 Cologne, Germany

We investigate the entanglement structure and wave function characteristics of continuously monitored free fermions with $U(1)$-symmetry in 2D. By deriving the fermion replica-Keldysh field theory and a bosonic effective long-wavelength action, we explore the similarities and differences between entanglement phase transitions in 2D monitored fermions and Anderson-type localization transitions in 3D. Using exact numerical simulations, we establish the phenomenology of entanglement transitions in 2D monitored fermions, examining entanglement entropy, mutual information, and inverse participation ratio. At weak monitoring, we observe characteristic $L \log L$ entanglement growth and multifractal dimension $D_q = 2$, resembling a metallic Fermi liquid. At strong monitoring, exponentially localized wave functions lead to saturation, following an area law for entanglement. In between, the critical point exhibits entanglement scaling consistent with emergent conformal invariance and strong multifractality. Our numerical findings align well with mean-field analysis and a one-loop renormalization group treatment of the field theory, shaping the understanding of a monitoring-induced metal-to-insulator transition in entanglement content. This establishes 2D monitored fermions as a unique platform to explore the connection between non-unitary quantum dynamics in D dimensions and quantum statistical mechanics in $D+1$ dimensions.

DY 3.7 Mon 11:45 A 151

Temporal Entanglement in Dual-Unitary Clifford Circuits with Probabilistic Measurements — •Jiangtian Yao and Pieter Claeys — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We study temporal entanglement in dual-unitary Clifford circuits with probabilistic measurements preserving spatial unitarity. We present exact results on characterizing the temporal entanglement barrier in the measurement-free regime. In the finite-measurement-rate regime, we numerically study the interplay between measurement rate and bath size. We connect the initial diffusive growth of temporal entanglement with bath size to a persistent random walk model and present an exact transfer-matrix approach for understanding how the system approaches the perfect-dephaser limit.

DY 3.8 Mon 12:00 A 151

Universal correlations in mesoscopic many-body systems: Berry's Random Wave Model in Fock space — •Florian Schöppl[1,2], Rémy Dubertrand[2], Juan Diego Urbina[2], and Klaus Richter[2] — [1]Northumbria University, NE1 8ST Newcastle upon Tyne, United Kingdom — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

A complete characterization of quantum signatures of (mean-field) chaos in interacting many-body systems requires, besides the widely used universality of spectral correlations, the analysis of the corresponding universality for eigenstate correlations in Fock space.

We lift the concepts and techniques that characterize this universality in first-quantized systems, introduced by Berry [1] into the realm of interacting bosonic fields in [2]. The existence of a classical (mean-field) limit allows us to use of many-body semiclassical methods [3].

We employ them to investigate the universal statistical features of eigenstate correlations in Bose-Hubbard models.

[1] M. V. Berry, "Regular and irregular semiclassical wavefunctions", Journal of Physics A: Mathematical and General 10, 2083 (1977). [2] R. Dubertrand, F. Schöppl, J. D. Urbina, K. Richter, "Universal correlations in chaotic many-body quantum states: Fock space formulation of Berry*s random wave model", preprint (2023). [3] K.Richter, J.D. Urbina, S. Tomsovic. "Semiclassical roots of universality in many-body quantum chaos",J. Phys. A: Math. Theor. 55 453001 (2022)

DY 3.9 Mon 12:15 A 151

Efficient Learning of Matrix Product States for Approximation of Purities in Quantum Many-Body Systems — •Dmytro Kolisnyk, Raimel Medina, and Maksym Serbyn — Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria

The defining feature of quantum many-body systems is an exponential scaling of the Hilbert space with the number of degrees of freedom. This exponential complexity naïvely renders the complete characterization of state, for instance via the complete set of bipartite Renyi entropies, a challenging task. Recently, the compact way of storing subregions' purities by encoding them as amplitudes of a fictitious quantum wave function, known as the entanglement feature (EF), was proposed. Matrix product state (MPS) encoding of such EF was obtained for Haar random states, however, the general applicability and practical usage of such encoding remained unclear. In this work, we demonstrate that EF can be efficiently learned using only polynomial amount of samples in the number of degrees of freedom through the so-called TTcross algorithm, assuming it is expressible as a finite bond dimension MPS. We benchmark this learning process on Haar and random MPS states, utilizing analytic insights. Additionally, we devise novel applications for the learned EF, such as quantifying the distance between different entanglement patterns and finding the optimal one-dimensional ordering of physical indices in a given state, highlighting the potential utility of proposed learning method in characterizing quantum many-body systems.

DY 3.10 Mon 12:30 A 151

Quantum complexity phase transitions in monitored random circuits — •Ryotaro Suzuki[1], Jonas Haferkamp[2], Jens Eisert[1], and Philippe Faist[1] — [1]Freie Universität Berlin — [2]Harvard University

Recently, the dynamics of quantum systems that involve both unitary evolution and quantum measurements have attracted attention due to the exotic phenomenon of measurement-induced phase transitions. At the same time, quantum complexity emerged as a key quantity for the identification of complex behaviour in quantum many-body dynamics. Quantum complexity of a quantum state is defined as the minimum number of unitary gates to generate the state by a quantum circuit. In this work, we investigate the dynamics of the quantum state complexity in monitored random circuits, where n qubits evolve according to a random unitary circuit and are individually measured with a fixed probability at each time step. We find that the growth behaviour of the exact quantum state complexity undergoes a phase transition when

changing the measurement rate. Below a critical measurement rate, the complexity grows linearly in time until an exponential time in n. Above, the complexity does not grow more than polynomially in n. We lower bound the exact state complexity in the former regime using recently developed techniques based on algebraic geometry.

DY 4: Fluid Physics and Turbulence

Time: Monday 9:30–11:00 Location: BH-N 128

Invited Talk DY 4.1 Mon 9:30 BH-N 128

Towards the ultimate regime in Rayleigh-Benard turbulence — •Olga Shishkina — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Rayleigh-Benard convection – a fluid flow in a container heated from below and cooled from above – is one of the paradigmatic systems in fluid dynamics. Here the key response of the system is the heat transport (Nusselt number Nu) and the key question is: how does Nu depend on the thermal driving strength (Rayleigh number Ra), in particular for extremely large Ra – the case which is relevant in many astrophysical and geophysical systems? We will start with a brief digression into the history of the theory of heat transport scaling relations for large Ra, and in particular for the so-called ultimate regime, where the scaling laws do not change anymore with the further growing Ra. We will discuss the assumptions and outcomes of the various scaling models as well as the factors that influence the transition to the ultimate regime, including the container shape, wall roughness, specific thermal boundary conditions, and possible non-Oberbeck–Boussinesq effects, as well as the multiple-state nature of turbulent thermal convection.

DY 4.2 Mon 10:00 BH-N 128

Statistical modeling of Burgers turbulence with a superposition of characteristic functionals — •Gabriel B Apolinário and Michael Wilczek — Theoretical Physics I, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

We study an ensemble of random fields, each with statistics described by a general characteristic functional. The typical length scale of these fields is a random variable and is used to model intermittency. This ensemble decomposition approach [Wilczek, *New J. Phys.* **18**, 125009 (2016)] allows for an analytically tractable approximation to turbulent statistics, and is applied to the Burgers equation. By choosing smooth correlation functions and an appropriate distribution for the typical length scale, we build a description of Burgers turbulence at an infinite Reynolds number, in which the velocity statistics are Gaussian, but increment and gradient statistics are bifractal. Skewness, a hallmark of turbulent fields, is obtained by truncating a Taylor-expanded cumulant generating functional, and this is shown to be a useful approximation.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 101001081).

DY 4.3 Mon 10:15 BH-N 128

Ensemble modeling of large-scale intermittency in turbulence — •Lukas Bentkamp and Michael Wilczek — Theoretical Physics I, University of Bayreuth, Germany

Turbulent flows at high Reynolds number are often assumed to have universal small-scale statistics, independent of the precise structure of the large scales. However, many experimental and numerical studies show a large scatter of statistical quantities, in particular with respect to higher-order moments. One reason for this may be large-scale intermittency, i.e. very slow variations of the large scales whose effect is still detectable at the small scales. At the example of homogeneous, isotropic turbulence simulations with sinusoidally varying energy injection rate, we investigate how ensembles of statistically stationary flows can be used to model the impact of large-scale intermittency. In order to build an accurate ensemble model, we find that not only the time series of the mean energy dissipation rate but also statistical fluctuations around it have to be incorporated.

DY 4.4 Mon 10:30 BH-N 128

Low-dimensional description of turbulent superstructures in three-dimensional Kolmogorov flow — •Fabián Álvarez-Garrido and Michael Wilczek — Theoretische Physik I, Universität Bayreuth, Bayreuth, Germany

Certain flows display the coexistence of small-scale turbulence and large-scale turbulent superstructures. Despite the ubiquity of these structures, their interplay with the smaller scales is not yet fully understood. We investigate the three-dimensional Kolmogorov flow as a model flow displaying turbulent superstructures, namely, it features large-scale quasi-two-dimensional vortex pairs. Moreover, we observe non-periodic transitions between states with one and two pairs of these large-scale vortices. We identify these different large-scale states as remnants of two solutions that emerge when a laminar solution looses stability at low Reynolds number where no turbulent fluctuations are present. This allows us to characterize the dynamics of the large scales by keeping track of two complex amplitudes. Through conducting direct numerical simulations, we gathered statistics on these two complex amplitudes and constructed a set of stochastic amplitude equations. The statistical properties of this low-dimensional system can reproduce, up to a fair agreement, the ones observed in the fully three-dimensional Kolmogorov flow. Based on these results, we discuss how the transfer of energy from the large to the smaller scales can stabilize the large-scale vortices, and how the fast-evolving fluctuations can enable the switching between large-scale states, mimicking the mechanism behind noise-induced transitions.

DY 4.5 Mon 10:45 BH-N 128

Dual energy cascade in ocean macroscopic turbulence: Kolmogorov self-similarity in surface drifter observations and Richardson-Obhukov constant — •Julia Dräger-Dietel and Alexa Griesel — Institut für Meereskunde, Universität Hamburg, Hamburg, Germany

We combine two point velocity and position data from surface drifter observations in the Benguela upwelling region off the coast of Namibia. The compensated third order longitudinal velocity structure function $<u^3(s)>/s$ shows a positive plateau for inertial separations s roughly between 9 km and 120 km revealing an inverse energy cascade with energy transfer rate ϵ=1.2 10^-7 m^3/s^2. For scales roughly below 800 m a negative plateau for $<u^3(s)>/s$ indicates to a direct energy cascade with energy-transfer rate 30 times smaller. For both regimes the second order longitudinal velocity structure function $<u^2(s)>$ scales as s^(2/3), as theoretically predicted. Deviations from Gaussianity of the corresponding probability distributions are stronger for the direct cascade in accordeance with theoretical expectation, for instance the kurtosis is 3 times larger. The combination of the energy transfer rate ϵ with Richardson dispersion $<s^2(t)>=g\,\epsilon\,t^3$, where $<s^2(t)>$ is the mean squared pair separation at time t, reveals a Richardson-Obhukov constant of g=0.11 for the inverse cascade regime [1].

[1] Draeger-Dietel et al. https://arxiv.org/abs/2311.13560

DY 5: Machine Learning in Dynamics and Statistical Physics I

Time: Monday 9:30–13:00 Location: BH-N 243

DY 5.1 Mon 9:30 BH-N 243

Active-Learning Training of Accurate Machine-Learned Interatomic Potentials for Strongly Anharmonic Materials — •Kisung Kang, Thomas A. R. Purcell, Christian Carbogno, and Matthias Scheffler — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin

Machine-learned interatomic potentials (MLIP) promise numerically efficient access to long time and large length scales in molecular dynamics (MD) simulations while retaining an accuracy that is on par with *ab initio* MD. To this end, it is necessary that MLIPs provide reliable predictions even for geometries that are largely unaccounted for in the original training, e.g., for rare dynamic events. For instance, this is required for thermal transport calculations, for which the creation of defects and phase transition precursors can profoundly affect anharmonic effects [1]. To this end, we propose an active learning ($\mathcal{AL}$) technique, in which uncertainty estimates are used to iteratively incorporate strongly anharmonic configurations into the MLIP training. At variance with traditional approaches, this $\mathcal{AL}$ method is thereby able to accurately capture those (meta-stable) configurations that are only seldom explored, as demonstrated in the cases of CuI and $AgGaSe_2$. Eventually, we show that this approach results in improved training and data acquisition efficiency for strongly anharmonic materials, whereas virtually no overhead is needed for more harmonic compounds.

[1] F. Knoop, *et al.*, *Phys. Rev. Lett.* **130**, 236301 (2023).

DY 5.2 Mon 9:45 BH-N 243

Machine-learned Potentials for Vibrational Properties of Acene-based Molecular Crystals — •Shubham Sharma and Mariana Rossi — Max Planck Institute for the Structure and Dynamics of Matter

Machine-learning potentials (MLPs) have allowed the efficient modelling of complex atomistic systems with ab-initio accuracy. Normally, the construction of sufficiently large and diverse reference datasets, using first-principles calculations, is a bottleneck for training. Therefore, several active-learning strategies have been proposed, which aim to make the training more efficient, especially when used together with molecular-dynamics techniques [1]. In this work, we explore building protocols for training sets of high-dimensional neural network potentials (HDNNPs), targeting specifically an accurate description of the vibrational properties of weakly-bound condensed-phase systems. For that, we show how we can use and augment the committee-model framework within the i-PI code [2]. We show results for acene-based molecular crystals and discuss the advantages and limitations of different learning strategies to treat different crystal polymorphs, at various thermodynamic conditions. [1] C. Schran et. at., J. Chem. Phys. 153, 104105 (2020). [2] V. Kapil et. al., Comput. Phys. Commun. 236, 214 (2019).

DY 5.3 Mon 10:00 BH-N 243

Sampling free energies with deep generative models — •Maximilian Schebek[1], Michele Invernizzi[2], Frank Noé[1,2,3,4], and Jutta Rogal[5,1] — [1]Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany — [2]Department of Mathematics and Computer Science, Freie Universität Berlin, 14195 Berlin, Germany — [3]Department of Chemistry, Rice University, 77005 Houston, Texas, USA — [4]AI4Science, Microsoft Research, 10178 Berlin, Germany — [5]Department of Chemistry, New York University, New York, NY 10003, USA

Evaluating free energy differences is a computationally demanding task, that requires a rigorous sampling of the phase space. Here, we train generative machine learning models based on normalizing flows to map between probability distributions of condensed phase systems at different thermodynamic conditions. Using the trained model, uncorrelated configurations can easily be generated. The model architecture incorporates permutation invariance and periodic boundary conditions, which improves convergence and enables the treatment of solid and liquid systems on the same footing. Training the flow model in a conditional way allows us to assess free energy differences over a wide range of temperatures and pressures, needed to evaluate the relative stability of different phases and reconstruct phase diagrams. The developed approach is applied to determine the coexistence line between liquid and solid as well as two different solid phases of a Lennard-Jones system. Our results are in excellent agreement with state-of-the-art methods, while the computational costs are significantly reduced.

DY 5.4 Mon 10:15 BH-N 243

Generative deep neural networks for topological defects and their microstructure reconstruction in two-dimensional spin systems — •Kyra Klos[1], Karin Everschor-Sitte[2], and Friederike Schmid[1] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg- Essen (CENIDE), University of Duisburg-Essen, Germany

Topological defects are stable localized perturbations of an underlying ordering field characterized by their winding number. These microscopic structures have an intrinsic multi-scale character and can be described as point like quasi-particles in the macroscopic picture. Due to long range interaction patterns and their complex implications, like the phase transition induced by topological defects, the so called Berezinskii-Kosterlitz-Thouless phase transition [1] in the two-dimensional XY Model, simulations are of high interest but difficult to realize for large system sizes. To overcome this problem we develop a generative neural network tool based on an Wasserstein Generative Adversarial Network (WGAN) [2] bridging between the microscopic and macroscopic scale. Through physics induced constraints this WGAN tool provides the opportunity to construct physical realistic representative sets of spin configuration of magnetic materials from a given defect distribution and physics input parameters.

[1] J. M. Kosterlitz, Rev. Mod. Phys. 89 (2017)
[2] M. Arjovsky et al. arXiv:1701.07875v3 (2017)

DY 5.5 Mon 10:30 BH-N 243

Automated large-scale chemical breakdown simulations with machine learned reaction rates — •Joe Gilkes[1], Mark Storr[2], Reinhard J. Maurer[1], and Scott Habershon[1] — [1]University of Warwick, United Kingdom — [2]AWE plc, United Kingdom

Degradation of organic materials occurs over many years and involves rare reaction events over expansive networks of elementary processes.

Building such networks and propagating them in time to evaluate the mechanisms by which materials break down requires tackling combinatorially large chemical spaces and accurately calculating the rates at which thousands of reactions proceed. Such a process comes with a high computational cost, and kinetic simulation of such networks is made prohibitively difficult when variable experimental conditions must be considered, as reaction rates must also vary over the duration of a simulation.

We demonstrate a workflow for the automated construction and solution of chemical breakdown networks using machine-learned reaction rates and a discrete kinetic update approximation when propagating networks in time. This allows for rapid iterative exploration of chemical reaction space with arbitrary variable experimental conditions. We demonstrate this by constructing and simulating a detailed reaction network for the pyrolysis of ethane.

DY 5.6 Mon 10:45 BH-N 243

Machine learning of a density functional for anisotropic patchy particles — •Alessandro Simon[1,2], Martin Oettel[1], and Georg Martius[2] — [1]University of Tübingen, Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

Anisotropic patchy particles have become an archetypical statistical model system for associating fluids. Here we formulate an approach to the Kern-Frenkel model via classical density functional theory to describe the positionally and orientationally resolved equilibrium density distributions in flat wall geometries. After investigating the orientational structure of the fluid close to the wall, we bring the anisotropic part of the free energy into a kernel-form suitable for machine learning, through an expansion into orientational invariants and the proper incorporation of the tetrahedral single-particle symmetries. The mean-field kernel is constructed via machine learning on the basis of hard wall simulation data and a robust and numerically stable method that is able to condition neural networks on fixed points of their output. Results are compared to other well-known mean-field approximations,

which strongly underestimate orientational correlation. Finally, we propose more general machine-learning methods that are able to go beyond the mean-field approximation.

DY 5.7 Mon 11:00 BH-N 243

Systematic construction of velocity gradient models for turbulence — Maurizio Carbone[1,2], Vincent Peterhans[3,2], Alexander Ecker[4,2], and •Michael Wilczek[1,2] — [1]Theoretical Physics I, University of Bayreuth — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [3]Faculty of Physics, University of Göttingen — [4]Institute of Computer Science and Campus Institute Data Science, University of Göttingen

The dynamics and statistics of small-scale turbulence can be described in terms of velocity gradients, which makes them an appealing starting point for low-dimensional modeling approaches. Modeling velocity gradients in turbulence requires formulating closures for nonlocal pressure contributions and viscous effects based on modeling hypotheses about the small-scale dynamics and statistics of turbulence.

Here, we discuss an alternative, data-driven approach to derive a velocity gradient model that captures given velocity gradient statistics by construction. By analyzing the velocity gradient PDF equation, we distinguish contributions to the single-time statistics from those that impact temporal correlations. We then systematically construct a closure to reproduce a given velocity gradient PDF by design. We use the 'normalizing flow' machine learning approach to estimate the full eight-dimensional velocity gradient PDF from direct numerical simulation (DNS) data. Comparisons with Lagrangian velocity gradient data from DNS confirm that statistical features of small-scale turbulence statistics can be quantitatively captured by our low-dimensional dynamical model.

15 min. break

DY 5.8 Mon 11:30 BH-N 243

Quantum Phase Transitions with Neural Network Quantum States and a Lee-Yang Method — •Pascal M. Vecsei, Jose L. Lado, and Christian Flindt — Aalto University, Otakaari 1, 02150 Espoo, Finland

Predicting the phase diagram of interacting quantum many-body systems is a central problem in condensed matter physics and related fields. A variety of quantum many-body systems, ranging from unconventional superconductors to spin liquids, exhibit complex competing phases whose theoretical description has been the focus of intense efforts. Here, we show that neural network quantum states can be combined with a Lee-Yang method to investigate quantum phase transitions and predict the critical points of strongly correlated spin lattices [1,2]. Specifically, we implement our approach for quantum phase transitions in the transverse-field Ising model on different lattice geometries in one, two, and three dimensions. We show that the Lee-Yang method combined with neural network quantum states yields predictions of the critical field, which are consistent with large-scale quantum many-body methods. As such, our results provide a starting point for determining the phase diagram of more complex quantum many-body systems, including frustrated Heisenberg models.

[1] Pascal M. Vecsei, J. L. Lado, C. Flindt, Phys. Rev. B **106**, 054402 (2022)
[2] Pascal M. Vecsei, C. Flindt, J. L. Lado, Phys. Rev. Research **5**, 033116 (2023)

DY 5.9 Mon 11:45 BH-N 243

A Study of Quantum Non-Equilibrium Relations with Imaginary Path Integrals — •Jorge Castro, Eszter Pos, and Mariana Rossi — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Several processes at the atomic scale occur in strongly out-of-equilibrium conditions. When such processes involve atomic motion at low temperatures or with light nuclei, it is expected that nuclear quantum effects play a pronounced role. However, theories that can rigorously treat quantum dynamics out of equilibrium are typically impossible to apply to explicit atomistic simulations of systems with many degrees of freedom. In this contribution, we study the protocols proposed in Ref.[1], where path-integral molecular dynamics simulations are used to evaluate quantum free energy differences through the Jarzynski and Crooks relations. We developed a code capable of generating non-equilibrium trajectories from path integral molecular dynamics. With this code, we investigated the efficiency and realm of validity of the work calculation employing driven path-integral molecular dynamics simulations. Our findings, based on 1D potentials, compare performance at various switching rates and varying coordinate shifts between the minima of starting and ending anharmonic potentials. We investigate the extend to which machine-learning methods targeting the inference of work distribution can speed up the statistical convergence of these protocols.

[1] R. van Zon, L. Hernández de la Peña, H. Peslherbe, and J. Schofield, *Phys. Rev. E* **78**, 041103 (2008)

DY 5.10 Mon 12:00 BH-N 243

Mean-field theories are simple for neural quantum states — •Fabian Ballar Trigueros, Tiago Mendes-Santos, and Markus Heyl — Universität Augsburg

The utilization of artificial neural networks for representing quantum many-body wave functions has garnered significant attention, however, quantifying state complexity within this neural quantum states framework remains elusive. In this study, we address this key open question from the complementary point of view: Which states are simple to represent with neural quantum states? Concretely, we show on a general level that ground states of mean-field theories with permutation symmetry only require a limited number of independent neural network parameters. We analytically establish that, in the thermodynamic limit, convergence to the ground state of the fully-connected transverse-field Ising model (TFIM), the mean-field Ising model, can be achieved with just one single parameter. Expanding our analysis, we explore the behavior of the 1-parameter ansatz under breaking of the permutation symmetry. For that purpose, we consider the TFIM with tunable long-range interactions, characterized by an interaction exponent α. We show analytically that the 1-parameter ansatz for the neural quantum state still accurately captures the ground state for a whole range of values for $0 \leq \alpha \leq 1$, implying a mean-field description of the model in this regime. We also comment on a potential method to identify and extract information from the neural network weight matrix that can give insight into the complexity of the state representation.

DY 5.11 Mon 12:15 BH-N 243

Tensor-network-based reinforcement learning for quantum many-body systems — •Giovanni Cemin — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The exploration of quantum many-body systems is a widely pursued field. However, the exponential growth of the Hilbert space dimension makes it challenging to classically simulate quantum many-body systems and, consequently, to extract meaningful information. In this context, we present a novel framework for efficiently controlling quantum many-body systems based on reinforcement learning (RL). Our framework addresses the complexities of the quantum control problem by utilizing matrix product states to represent the many-body state within the trainable machine learning architecture of our RL agent. This novel methodology enables the control of systems on a scale beyond the capabilities of neural-network-only architectures, while retaining the advantages of deep learning, such as generalizability and robustness to noise. Notably, our research demonstrates the ability of RL agents to accurately handle previously unseen many-body states.

DY 5.12 Mon 12:30 BH-N 243

Derivative learning of tensorial quantities – Predicting infrared spectra from first principles — •Bernhard Schmiedmayer[1] and Georg Kresse[1,2] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Sciences, Vienna, Austria — [2]VASP Software GmbH, Vienna, Austria

In this talk, we present a novel computational framework that integrates machine learning with first-principles calculations to achieve accurate predictions of infrared spectra. Our method demonstrates its ability to reliably generate infrared spectra for complex systems at finite temperatures. The efficiency of the method is highlighted in challenging scenarios such as the analysis of water and the organic-inorganic halide perovskite MAPbI3. Our method is in good agreement with experimental results. A unique feature of our technique is the use of derivative learning, which is essential for obtaining accurate polarization data in bulk materials and facilitates the training of a symmetry-adapted machine learning framework. Using derivative learning, we are able to predict the anti-derivative with an accuracy of about 1%.

DY 5.13 Mon 12:45 BH-N 243

Stellar evolution forecasting with a timescale-adapted evolutionary coordinate and machine learning — •Kiril Maltsev and et al. — Heidelberger Institut für Theoretische Studien, Schloss-Wolfsbrunnenweg 35, 69118 Heidelberg

Many astrophysical applications require efficient yet reliable forecasts of stellar evolution tracks. One example is population synthesis, which generates forward predictions of models for statistical comparison with observations. The majority of state-of-the-art rapid population synthesis methods are based on approximate analytic fitting formulae to stellar evolution tracks that are computationally cheap to sample statistically over a continuous parameter range. The computational costs of running detailed stellar evolution codes over wide and densely sampled parameter grids are prohibitive, while stellar-age based interpolation in-between sparsely sampled grid points leads to intolerably large systematic prediction errors. In this work, we use supervised learning methods to construct an emulator of stellar evolution at a satisfactory trade-off between cost-efficiency and accuracy. We construct a timescale-adapted evolutionary coordinate and use it in a two-step interpolation scheme that traces the evolution of stars from zero age main sequence all the way to the end of core helium burning while covering a mass range from red dwarfs to very massive Wolf-Rayet stars. The feedforward neural network regression model that we train to predict stellar surface variables can make millions of predictions within tens of seconds on a 4-core CPU, with a mean prediction error that is an order of magnitude lower than typical observational uncertainties.

DY 6: Statistical Physics far from Thermal Equilibrium I

Time: Monday 9:30–13:00 Location: BH-N 334

Invited Talk DY 6.1 Mon 9:30 BH-N 334

Barrier crossing with non-Gaussian noise: Exponential transition rate gains and effects of active motion — •Peter Sollich[1], Adrian Baule[2], and Diego Tapias[1] — [1]Institute for Theoretical Physics, University of Goettingen, Friedrich-Hund-Platz 1, D-37077 Goettingen, Germany — [2]School of Mathematical Sciences, Queen Mary University of London, London E1 4NS, UK

Noise-induced escape from metastable states governs a plethora of transition phenomena in physics, chemistry, and biology. While the escape problem for thermal Gaussian noise has been well understood since the seminal works of Arrhenius and Kramers, many systems, in particular living ones, are effectively driven by non-Gaussian noise for which the conventional theory does not apply. Here we present a theoretical framework based on path integrals that allows the calculation of both escape rates and optimal escape paths for a generic class of non-Gaussian noises. We find that non-Gaussian noise always leads to more efficient escape and can enhance escape rates by many orders of magnitude compared with thermal noise, highlighting that away from equilibrium escape rates cannot be reliably modelled based on the traditional Arrhenius-Kramers result. Our analysis also identifies a new universality class of non-Gaussian noises, for which escape paths are dominated by large jumps. We outline finally how the approach can be extended to barrier crossing by self-propelled particles with active Brownian or run-and-tumble motion, and show that dynamical phase transitions can be used to sort such particles according to the persistence of their active motion.

DY 6.2 Mon 10:00 BH-N 334

Minimum-dissipation principle for synchronised stochastic oscillators far from equilibrium — •Jan Meibohm[1,2] and Massimiliano Esposito[3] — [1]Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [2]Department of Mathematics, King's College London, London WC2R 2LS, United Kingdom — [3]Complex Systems and Statistical Mechanics, Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We study driven q-state Potts models with thermodynamically consistent dynamics and global coupling. For a broad range of parameters, these coupled-oscillator models exhibit a dynamical phase transition from a decoherent into a synchronised phase. We derive the normal form of the high-dimensional Hopf-Bifurcation that underlies the phase transition, for arbitrary dynamics and for all q. The normal-form equations are exact in the thermodynamic limit and close to the bifurcation. Making use of the symmetries, we solve these equations exactly and thus uncover the intricate long-time behaviour of driven Potts models, characterised by a rich phase diagram. Connecting with the macroscopic thermodynamics, we show that synchronisation always reduces dissipation. Remarkably, we find that the most stable synchronised states dissipate the least entropy. Close to the phase transition, we discover a linear dissipation-stability relation that connects dissipation with phase-space contraction, a widely-used stability measure. Our findings suggest a minimum-dissipation principle for driven Potts models that holds arbitrarily far from equilibrium.

DY 6.3 Mon 10:15 BH-N 334

Fluctuations in nonequilibrium complex systems: conditional entropy and weak correlation — •Yuichi Itto — Aichi Institute of Technology, Aichi, Japan — ICP, Universität Stuttgart, Stuttgart, Germany

Nonequilibrium complex systems are often organized hierarchically by different dynamics on different time scales. The statistical property of spatiotemporal fluctuations concerning the dynamics is known to be essential for treating a wide class of such systems. Maximum entropy principle has played a crucial role for describing the statistical fluctuation distribution in the literature, not limited to characterizing the equilibrium systems.

Here, an entropic approach [1] is discussed for describing the conditional distribution in nonequilibrium complex systems with two different dynamics that exhibit a weak correlation between associated fluctuations. It is shown that the conditional fluctuation distribution is governed by the weak correlation in a unified manner. The result is illustrated in heterogeneous diffusion phenomena observed in living cells: DNA-binding proteins in bacteria [2], as well as membraneless organelles in embryos [3] and beads in cell extracts [4] as further possible examples.

References
[1] Y. Itto, Entropy, 25, 556 (2023).
[2] A.A. Sadoon and Y. Wang, Phys. Rev. E, 98, 042411 (2018).
[3] R. Benelli and M. Weiss, New J. Phys., 23, 063072 (2021).
[4] K. Speckner and M. Weiss, Entropy, 23, 892 (2021).

DY 6.4 Mon 10:30 BH-N 334

Non-equilibrium generalized Langevin equation from a generic time-dependent Hamiltonian — •Benjamin Héry and Roland R. Netz — Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Department of Physics

It has become standard practice to describe non-equilibrium phenomena by heuristic Langevin equations with colored noise and time-dependent friction kernels that do not obey the fluctuation-dissipation theorem. Since these models are not derived from first-principle Hamiltonian dynamics, it is not clear whether they correspond to physically realizable scenarios. By exact Mori projection in phase space, we derive the non-equilibrium generalized Langevin equation (GLE) from a generic many-body Hamiltonian with a time-dependent force h(t) acting on an arbitrary phase-space dependent observable. The GLE is obtained in explicit form to all orders in h(t). We show that if the observable that is described by the GLE is Gaussian and related to the time-dependent Hamiltonian perturbation term, the resultant non-equilibrium GLE has the same form as the equilibrium GLE and obeys a fluctuation-dissipation theorem. This means that the extraction and simulation methods developed for equilibrium GLEs can be used also for non-equilibrium Gaussian variables. This is a non-trivial and very useful result, as many observables that characterize non-equilibrium systems display Gaussian statistics.

DY 6.5 Mon 10:45 BH-N 334

Non-equilibrium thermodynamics of a particle driven by time-delayed feedback — •Robin A. Kopp and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Berlin, Germany

Time-delayed feedback can act as a propulsion mechanism, which has recently been demonstrated and studied both theoretically [1] and experimentally [2]. In two-dimensional systems and for suitable feedback

parameters, persistent motion occurs despite fluctuations, resembling the behavior of self-propelled particles [3]. Using the framework of stochastic energetics [4] we here study the thermodynamic properties of a colloidal particle in two dimensions driven by time-delayed feedback. Focusing on the dissipated heat, we combine analytical and numerical methods to gain insights into the onset of persistent motion, which occurs above a threshold value in parameter space. Above the threshold of persistent motion we furthermore compare to the well-established active Brownian particle model for self-propulsion with corresponding parameters. Finally we show that even below the threshold a non-zero heat dissipation is to be expected and can indeed be found in numerical simulations.

[1] Kopp R. A. and Klapp S. H. L., Phys. Rev. E, **107** (2023) 024611
[2] Bell-Davies M. C. R., Curran A., Liu Y. and Dullens R. P. A., Phys. Rev. E, **107** (2023) 064601
[3] Kopp R. A. and Klapp S. H. L., EPL **143**, 17002 (2023)
[4] Sekimoto K., Prog. Theor. Phys. Supp. **130**, 17 (1998)

DY 6.6 Mon 11:00 BH-N 334

Memory induced Magnus forces in viscoelastic fluid — •Debankur Das[1], Niklas Windbacher[2], Xin Cao[2], Matthias Krueger[1], and Clemens Bechinger[2] — [1]University of Goettingen — [2]University of Konstanz

When a spinning object moves through a fluid, its direction of motion becomes deflected due to the Magnus force that is perpendicular to both the moving direction and the spinning axis. Since the Magnus effect is caused by inertial effects within the surrounding medium, it is expected to vanish at micro scales where viscous forces dominate over inertia. Our recent experiments have observed a surprisingly strong Magnus effect when spinning colloids are driven through a viscoelastic fluid. Here, we discuss a theoretical framework for such motion, which shows that the Magnus force is caused by finite memory of the viscoelastic fluid, which can last of the order of seconds. This causes a deformation of the fluidic network around the moving particle. When the particle additionally spins, the deformation field becomes misaligned relative to the particle's moving direction, leading to a force perpendicular to the direction of travel and the spinning axis. Our theory predicts that the Magnus motion persists for some time even when the spinning stops, successfully verified by our experiments. The presence of strongly enhanced memory-induced Magnus forces at microscales opens novel applications for particle sorting and steering, the creation and visualization of anomalous flows and more.

15 min. break

DY 6.7 Mon 11:30 BH-N 334

Thermal relaxation asymmetry in reversible and driven systems — •Cai Dieball[1], Miguel Ibáñez[2], Gerrit Wellecke[1,3], Antonio Lasanta[2], Raúl A Rica[2], and Aljaz Godec[1] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen — [2]Universidad de Granada, Spain — [3]Present address: Max Planck Institute for Dynamics and Self-Organization, Göttingen

It was theoretically predicted that small systems subject to temperature changes that push the system far from thermodynamic equilibrium feature an asymmetric thermal relaxation. More precisely, heating was predicted to be faster than cooling [1]. Here, by using an optically trapped colloidal particle, we confirm this prediction [2]. Developing a new theoretical framework that we call *thermal kinematics*, we quantify relaxation between arbitrary pairs of temperatures.

To complete the non-equilibrium picture of thermal relaxation, we also prove the relaxation asymmetry for systems inherently driven out of equilibrium [3]. The resulting relaxation highlights the absence of local equilibria and surprisingly features opposing rotational motions during heating and cooling.

References:
[1] Lapolla & Godec, *Phys. Rev. Lett.* **125**, 110602 (2020)
[2] Ibáñez, Dieball, Lasanta, Godec & Rica, accepted in *Nat. Phys.* (2023)
[3] Dieball, Wellecke & Godec, accepted in *Phys. Rev. Research* (2023)

DY 6.8 Mon 11:45 BH-N 334

Powerful ordered collective heat engines — •Fernando Silva Filho[1,2,3], Gustavo Forao[1], Daniel Busiello[4], Bart Cleuren[3], and Carlos Fiore[1] — [1]University of São Paulo, Instituto de Física, Rua do Matão, 1371, 05508-090 São Paulo, SP, Brazil — [2]Institute for Theoretical Physics IV, University of Stuttgart - 70569 Stuttgart, Germany — [3]UHasselt, Faculty of Sciences, Theory Lab, Agoralaan, 3590 Diepenbeek, Belgium — [4]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

In this talk, we present a recently published work (PhysRevResearch.5.043067) about a class of interacting heat engines in which the regime of units operating synchronously (in ordered phase) can boost the performance. Our approach encompasses a minimal setup composed of N interacting units placed in contact with two thermal baths and subjected to a constant driving worksource. The interplay between unit synchronization and interaction leads to an efficiency at maximum power between the Carnot η_C and the Curzon-Ahlborn bound η_{CA}. Moreover, these limits can be respectively saturated maximizing the efficiency, and by simultaneous optimization of power and efficiency. We show that the interplay between Ising-like interactions and a collective ordered regime is crucial to operate as a heat engine. The main system features are investigated developing an effective discrete-state model that captures the effects of the synchronous phase. The robustness of our findings extends beyond the all-to-all interactions and paves the way for the building of promising far from equilibrium thermal engines based on ordered structures.

DY 6.9 Mon 12:00 BH-N 334

Conditioning in equilibrium and nonequilibrium baths — •Ion Santra and Matthias Krüger — University of Goettingen

Generalized linear Langevin equations are a popular way of describing tracer dynamics in viscoelastic baths. In this talk, starting from a microscopic bath model, I will discuss how the usual form of Generalized Langevin equations are no more valid in the case of nonequilibrium baths. We show that the term dependent on the initial conditions, which is usually dropped for equilibrium baths, become important. A simple way to understand the contribution from this term is to look at conditioned displacements of the tracer in stationary state.

DY 6.10 Mon 12:15 BH-N 334

Thermophoresis and the breakdown of local equilibrium in a far-from-equilibrium bath — •Wade Hodson[1] and Aljaz Godec[2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

We investigate the nonequilibrium steady state properties of a far-from-equilibrium bath, consisting of a chain of harmonic oscillators coupled at the ends to stochastic heat reservoirs at different temperatures. This system, if coupled to a tracer particle, can serve as a medium in which the tracer diffuses in response to the applied thermal gradient, a phenomenon known as thermophoresis. We evaluate interparticle correlations, time-integrated heat current statistics, and other diagnostic properties of the harmonic bath to study how local thermal equilibrium breaks down for large temperature gradients, a regime where thermophoresis still lacks a general theoretical description. These analytical results are supplemented by numerical computations. We also present a preliminary analysis of the effect of the bath on a tracer using the Kac-Zwanzig formalism, which produces an effective equation of motion for the tracer alone.

DY 6.11 Mon 12:30 BH-N 334

Mean Back Relaxation for Position and Densities — •Gabriel Knotz and Matthias Krüger — Institute for Theoretical Physics, Göttingen, Germany

Quantifying detailed balance breakage from particle trajectories is an important problem in simulation and experiment. Recently, it was shown that the mean back relaxation (MBR) of displacements along a particle trajectory can serve as a non-equilibrium marker in confinement. To extend the validity to unconfined systems, we propose a new version of the MBR that is defined on the microscopic particle density function which marks the breakage of detailed balance even in bulk, and discuss general properties of the MBR. [1][2]

[1] Till M. Muenker, Gabriel Knotz, Matthias Krüger and Timo Betz. *Onsager regression characterizes living systems in passive measurements.* bioRxiv:2022.05.15.491928
[2] Gabriel Knotz, Matthias Krüger. *Mean Back Relaxation for Position and Densities.* arXiv:2311.17477

DY 6.12 Mon 12:45 BH-N 334

Selfconsistent diagrammatic transport for light including

time reversal symmetric entropy production — •Regine Frank[1,2] and Bart A. van Tiggelen[3] — [1]College of Biomedical Sciences, Larkin University, Miami, Florida, USA — [2]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain — [3]University Grenoble Alpes, Centre National de la Recherche Scientifique, LPMMC, Grenoble, France

We present novel theory and numerics for transport of light in random complex media, where the production of entropy is positive under time reversal, an Onsager scenario. Numerical solutions based on weighted essentially non-oscillatory solvers (WENO) are introduced. Anderson localization is quantitatively discussed.

[1] R. Frank, A. Lubatsch, Phys. Rev. Research 2, 013324 (2020). [2] D. Vollhardt and P. Wölfle, Phys. Rev. B 22, 4666 (1980). [3] P. D. Lax and R. D. Richtmyer, Commun. Pure Appl. Math. 9, 267 (1956). [4] A. Lubatsch, J. Kroha, K. Busch, Phys. Rev. B.71, 184201 (2005) [5] R. Frank, A. Lubatsch, J. Kroha, Phys. Rev. B 73, 245107 (2006). [6] B. A. van Tiggelen, A. Lagendijk, and A. Tip, Phys. Rev. Lett. 71, 1284 (1993). [7] B. A. Van Tiggelen, Diffuse Waves in Complex Media, 1-60 (1999).

DY 7: Critical Phenomena and Phase Transitions

Time: Monday 11:30–13:00 Location: BH-N 128

Invited Talk DY 7.1 Mon 11:30 BH-N 128

Critical transitions in non-autonomous complex dynamical systems: theory and applications to ecosystems and climate — •Ulrike Feudel — ICBM, Carl von Ossietzky Universität Oldenburg, Germany

Many systems in nature are characterized by the coexistence of different stable states for a given set of environmental parameters and external forcing. Examples for such behavior can be found in different fields of science ranging from mechanical or chemical systems to ecosystem and climate dynamics. Perturbations, applied to those natural systems can lead to a critical transition from one stable state to another. Such critical transitions – also called tipping phenomena – can happen in various ways: (1) due to bifurcations, i.e. changes in the dynamics when external forcing or parameters are varied extremely slow (2) due to fluctuations which are always inevitable in natural systems, (3) due to shocks or extreme events, and (4) due to rate-induced transitions, i.e. when external forcing changes too fast compared to the ability of the forced system to follow the changes. We discuss these critical transitions and their characteristics and illustrate them with examples from mechanical and natural systems. Special emphasis is given to non-autonomous systems, in which we highlight the interplay between different time scales, like the dissipative time scale and the time scale of the variation of parameters or forcing. Moreover, we discuss the role of unstable states, that are not directly observable in nature, but nevertheless act as the organizing centers of the dynamics.

DY 7.2 Mon 12:00 BH-N 128

Critical fluctuations at finite-time dynamical phase transition — •Nalina Vadakkayil[1], Massimiliano Esposito[1], and Jan Meibohm[2] — [1]Complex Systems and Statistical Mechanics, Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [2]Department of Mathematics, King's College London, London WC2R 2LS, United Kingdom and Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

We explore the critical properties of the recently discovered finite-time dynamical phase transition in the non-equilibrium relaxation of Ising magnets. The transition is characterized by a sudden switch in the relaxation dynamics and it occurs at a sharp critical time. While previous works have focused either on mean-field interactions or on investigating the properties of the critical time, we analyse the critical fluctuations at the phase transition in the nearest-neighbor Ising model using Monte Carlo simulations. By means of a finite-size scaling analysis, we extract the critical exponents for the finite-time dynamical phase transition. In two spatial dimensions, these exponents turn out to be neither mean-field nor the same as at equilibrium. Instead, they seem to lie outside of the known universality classes, potentially representing a novel, non-equilibrium critical phenomenon.

DY 7.3 Mon 12:15 BH-N 128

Critical phase transitions through fractal-induced dynamics — •Fabio Salvati — Institute for Molecules and Materials, Radboud University, Heijendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

In our study, we explore the dynamic characteristics of a single-particle system characterized by a non-trivial energy potential landscape, leading to a singular continuous energy spectrum. Typically, such a phase transition is achieved by introducing a periodic potential in the presence of a magnetic field, as described through the analysis of Almost Mathieu Operators. However, in our investigation, this unique phase transition emerges solely through geometric manipulations.

The geometric transformations we implement are tied to lattices of elementary shapes, such as squares and triangles, evolving into intricate fractal geometries like the Sierpinski carpet and gasket. Notably, these transformations manifest by projecting into the system's on-site potential, corresponding to the voids within the considered fractal structures.

Furthermore, we propose the possibility of experimentally validating our numerical findings, especially through the use of an ultracold gas setup.

DY 7.4 Mon 12:30 BH-N 128

Cubic fixed point in three dimensions: Monte Carlo simulations of the ϕ^4 model on the simple cubic lattice — •Martin Hasenbusch — Universität Heidelberg, Heidelberg, Deutschland

We study the cubic fixed point for $N = 3$ and 4 by using finite-size scaling applied to data obtained from Monte Carlo simulations of the N-component ϕ^4 model on the simple cubic lattice. We generalize the idea of improved models to a two-parameter family of models. The two-parameter space is scanned for the point, where the amplitudes of the two leading corrections to scaling vanish. To this end, a dimensionless quantity is introduced that monitors the breaking of the $O(N)$ invariance. For $N = 4$, we determine the correction exponents $\omega_1 = 0.763(24)$ and $\omega_2 = 0.082(5)$. In the case of $N = 3$, we obtain $Y_4 = 0.0142(6)$ for the renormalization group exponent of the cubic perturbation at the $O(3)$-invariant fixed point, while the correction exponent $\omega_2 = 0.0133(8)$ at the cubic fixed point. Simulations close to the improved point result in the estimates $\nu = 0.7202(7)$ and $\eta = 0.0371(2)$ of the critical exponents of the cubic fixed point for $N = 4$. For $N = 3$, at the cubic fixed point, the $O(3)$ symmetry is only mildly broken and the critical exponents differ only by little from those of the $O(3)$-invariant fixed point. We find $-0.00001 \leq \eta_{cubic} - \eta_{O(3)} \leq 0.00007$ and $\nu_{cubic} - \nu_{O(3)} = -0.00061(10)$.

DY 7.5 Mon 12:45 BH-N 128

Universal Approach to Critical Percolation — •Fabian Coupette and Tanja Schilling — Institute of Physics, University of Freiburg, Freiburg, Germany

Percolation is an archetypal critical phenomenon that occurs across a diverse range of contexts, such as the design of composite materials or vaccination strategies on community networks. In contrast to the critical exponents, the critical parameters (percolation threshold) characterizing the emergence of a system-spanning connected cluster, depend sensitively on the system properties. As a consequence, theoretical approaches predicting percolation thresholds are rare, often heuristic in nature, and tailored to specific applications.

We propose a general mapping of any kind of percolation problem onto a branching process which provides rigorous lower bounds for the percolation threshold. These bounds progressively tighten as we incorporate more local information into the description. We demonstrate our approach for different lattice and continuum problems obtaining accurate predictions with minimal effort. Our method is based on first principles, reproduces all exact solutions to percolation problems, and does not require fitting parameters. As such it offers an important theoretical reference in a field that is dominated by simulation studies and heuristic descriptions.

DY 8: Artificial Intelligence in Condensed Matter Physics II (joint session TT/DY)

While artificial intelligence leaves an ever growing footprint in our everyday lives, it has as well inspired various new approaches in the physical sciences; for instance, one of the outstanding success stories is the prediction of protein folding with unprecedented accuracy. But what role can AI play in condensed matter physics? This symposium aims to provide an overview and discussion of recent applications of modern machine learning and its prospects for the advancement of research in this field. The increasingly data-intensive experiments with high-dimensional observations call for the development of new tools for analysis matching known strengths of machine learning algorithms. Reinforcement learning agents can be employed to precisely manipulate many-body systems, which, among other use cases, is a pivotal ingredient for quantum technologies. On the computational side, ideas from deep learning and generative modeling inspire new building blocks to boost numerical simulations. One may even ask the question whether a machine can autonomously discover physical concepts such as effective degrees of freedom or equations of motion, and reveal them in an interpretable manner to human researchers.

Prof. Dr. Simon Trebst, Universität Köln
Prof. Dr. Florian Marquardt, Max-Planck-Institut Erlangen
Dr. Markus Schmitt, FZ Jülich

Time: Monday 15:00–16:00 Location: H 3025

DY 8.1 Mon 15:00 H 3025

Uncertainty-aware active learning for interatomic potentials generation and its applications for spin dynamics — •Valerio Briganti and Alessandro Lunghi — School of Physics, AMBER and CRANN Institute, Trinity College, Dublin 2, Ireland

In the last decade, the materials science community has increasingly exploited the potential of AI for various applications, ranging from the discovery of new materials to the generation of interatomic potentials (IP). Developments in the latter have enabled to perform molecular dynamics simulations with unprecedented timescales, with the promise of successfully overcoming the computational costs required by ab initio methods keeping a sufficiently high accuracy. Two of the main challenges in this field are the design of models to allow greater transferability and the optimal selection of data to be included in the training set. In this contribution, I will show how a linear regression model based on SNAP [1] augmented with an uncertainty aware active learning procedure [2] can efficiently lead to the generation of accurate IPs able to simulate the dynamics of organic and open-shell compounds at room temperature. In addition to this, I will also present the performance of machine learning IPs for prediction of phonons and spin-phonon relaxation time.
[1] A.P. Thompson et al., J. of Comp. Phys., 285 (2015) 316.
[2] V. Briganti, A. Lunghi, Mach. Learn.: Sci. Technol. 4 (2023) 035005.

DY 8.2 Mon 15:15 H 3025

Transverse barrier and filament formation by electrical triggering of a metal-to-insulator or insulator-to-metal transition — •Lorenzo Fratino[1], Marcelo Rozenberg[2], Pavel Salev[3], Javier Del Valle[4], and Ivan K. Schuller[5] — [1]LPTM, CY Cergy Paris Université, Cergy-Pontoise — [2]LPS, Université Paris Saclay, Orsay — [3]University of Denver, USA — [4]University of Geneva, Switzerland — [5]University of California, San Diego, USA

By doing numerical simulations on Mott resistors network model, we were able to give a theoretical background to experimental observations on magnetotransport in ferromagnetic oxide (La,Sr)MnO_3 (LSMO) during electrical triggering of the intrinsic metal-insulator transition (MIT), which produces volatile resistive switching. This switching occurs in a characteristic spatial pattern, the formation of a paramagnetic insulating barrier perpendicular to the current flow, in contrast to the conventional filamentary percolation parallel to the current. This formation was also simulated in order to demonstrate that this process is triggered by nucleation at hotspots, with a subsequent expansion over several decades in time. By comparing three case studies (VO_2, V_3O_5, and V_2O_3), we identified the resistivity change across the transition as the crucial parameter governing this process. Our results provide a spatio-temporal characterisation of volatile resistive switching in Mott insulators, which is important for emerging technologies, such as optoelectronics and neuromorphic computing.
[1] Phys. Rev. B 108 (2023) 174434.
[2] Nat. Comm. 12 (2021) 1.
[3] Science 373 (2021) 907.

DY 8.3 Mon 15:30 H 3025

Autonomous bromine removal in scanning tunneling microscope — •Nian Wu[1], Markus Aapro[1], Alexander Ilin[2], Robert Drost[1], Joakim Jestilä[1], Zhijie He[2], Peter Liljeroth[1], and Adam S. Foster[1,3] — [1]Applied Physics, Aalto University, Helsinki, Finland — [2]Computer Science, Aalto University, Helsinki, Finland — [3]WPI Nano Life Science Institute, Kanazawa University, Kanazawa, Japan

More recent studies have even harnessed scanning probe microscopy (SPM) to control chemical reactions in on-surface molecular synthesis. In general, the SPM manipulations are predominantly controlled via parameters of the tip position, pulse voltages and tunneling conductance in scanning tunneling microscope (STM). However, the selection of proper parameters requires extensive domain knowledge, which is time-consuming and not necessarily transferable to new systems. Recent research has allowed the automation of a wide range of challenges, including lateral and vertical manipulation. However, the automation for breaking or forming covalent bonds, which is an indispensable step in chemical synthesis, is unexplored yet. To address this problem, we build on our deep reinforcement learning approach to automate the bromine removal from 5,15-bis(4-bromo-2,6-methyl-phenyl)porphyrin (Br_2Me_4DPP) through learning manipulation parameters in STM.

DY 8.4 Mon 15:45 H 3025

Neural quantum states for a two-leg Bose-Hubbard ladder under a magnetic field — •Kadir Çeven[1,2], Mehmet Özgür Oktel[2], and Ahmet Keleş[3] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Department of Physics, Bilkent University, Ankara, Turkey — [3]Department of Physics, Middle East Technical University, Ankara, Turkey

This work explores novel quantum phases in a two-leg Bose-Hubbard ladder, achieved using neural quantum states. The remarkable potential of quantum gas systems for analog quantum simulation of strongly correlated quantum matter is well-known; however, it is equally evident that new theoretical bases are urgently required to comprehend their intricacies fully. While simple one-dimensional models have served as valuable test cases, ladder models naturally emerge as the next step, enabling studying higher dimensional effects, including gauge fields. Using [Çeven et al., PRA 106, 063320 (2022)], this work investigates the application of neural quantum states to a two-leg Bose-Hubbard ladder in the presence of strong synthetic magnetic fields. This paper showcased the reliability of variational neural networks, such as restricted Boltzmann machines and feedforward neural networks, in accurately predicting the phase diagram exhibiting superfluid-Mott insulator phase transition under strong interaction. Moreover, the neural networks successfully identified other intriguing many-body phases in the weakly interacting regime. These exciting findings firmly designate a two-leg Bose-Hubbard ladder with magnetic flux as an ideal testbed for advancing the field of neural quantum states.

DY 9: Focus Session: Quantum Interactive Dynamics II (joint session DY/TT)

Quantum many-body systems out of equilibrium represent a challenging frontier and have been shown to exhibit extremely rich phenomena. Recent experimental advances in building Noisy Intermediate-Scale Quantum (NISQ) devices have opened up a completely new territory in this context. The natural evolution implemented by NISQ devices is a quantum interactive dynamics generated by a combination of unitary gates and measurements. These platforms provide an opportunity to explore vastly larger parts of the Hilbert space and go beyond what can be realized in purely unitary systems. In pioneering works, an entanglement phase transition was identified in the dynamics of circuits of random unitary gates interleaved with local projective measurements. This phase transition separates a disentangling phase, obeying an area law, and an entangling phase obeying a volume law. Successively, it has been shown that additional phase transitions between different area phases can occur and new kinds of quantum phase transitions have been discovered. This session aims to give an overview of recent theoretical and experimental developments within this very active field and point towards the open questions.

Organized by Roderich Moesser (Dresden) and Frank Pollmann (München)

Time: Monday 15:00–18:00 Location: A 151

Invited Talk DY 9.1 Mon 15:00 A 151

Quantum Mechanics and Many Body Games — •Shivaji Sondhi — University of Oxford, UK

I will describe some work on the theme of exploring many body quantum mechanics by playing games with its help. I will primarily discuss a set of results that raise the possibility of classifying quantum states by asking whether they confer a quantum advantage in winning a particular game. I will comment briefly on other interesting directions encompassed by this general theme.

Invited Talk DY 9.2 Mon 15:30 A 151

Measurement induced phase transitions of fermions: from theory to observability — •Sebastian Diehl — University of Cologne

The quest for phases and phase transitions in general non-unitary quantum dynamics has been spotlighted by the recent discovery of measurement-induced phase transitions. They result from the competition of deterministic Schrödinger and random measurement dynamics, and surface in a qualitative change of the entanglement structure.

Here we first introduce instances of entanglement transitions in fermion systems, between a regime of logarithmic entanglement growth, and a quantum Zeno regime obeying an area law. We identify the relevant degrees of freedom driving the phase transition in terms of an effective field theory. This yields a physical picture in terms of a depinning from the measurement operator eigenstates induced by unitary dynamics, and places it into the BKT universality class.

In standard quantum mechanical observables however, these transitions are masked due to the degeneracy of measurement outcomes. We then point out a general route of gently breaking this degeneracy – preselection – which makes such transitions observable in state-of-the-art quantum platforms without modifying any of the universal properties. It reveals an intriguing connection to quantum absorbing state transitions.

Invited Talk DY 9.3 Mon 16:00 A 151

Novel quantum dynamics with superconducting qubits — •Pedram Roushan — Google Quantum, Santa Barbara, CA, USA

In recent years superconducting qubits have become one of the leading platforms for quantum computation and simulation. We utilize these Noisy Intermediate Scale Quantum (NISQ) processors to study nonequilibrium quantum dynamics and simulate quantum phases of matter. I will present some of our recent works in studying robustness of bound states of photons [1], measurement-induced quantum information phases [2], braiding of non-Abelian anyons [3], and the universality classes of dynamics in the 1D Heisenberg chain [4]. Time permitting, I will talk about our effort on analog simulation, using the native Hamiltonian of the device. A goal of this talk is to provide a sense of what NISQ discoveries to anticipate and a time scale for them.

[1] Morvan et al., Nature 612, 240*245 (2022) [2] Hoke et al., Nature 622, 481*486 (2023) [3] Andersen et al., Nature 618, 264*269 (2023) [4] Rosenberg et al., Arxiv.org/abs/2306.09333

DY 9.4 Mon 16:30 A 151

Programmable adiabatic demagnetization on noisy quantum devices — •Anne Matthies[1,2], Mark Rudner[3], Achim Rosch[1], and Erez Berg[2] — [1]University of Cologne, Cologne, Germany — [2]Weizmann Insitute of Science, Rehovot, Israel — [3]University of Washington, Seattle, USA

We propose a simple, robust protocol to prepare a low-energy state of an arbitrary Hamiltonian on a quantum computer. The protocol is inspired by the "adiabatic demagnetization" technique, which can cool solid-state systems to extremely low temperatures. The adiabatic cooling protocol is demonstrated via an application to the transverse field Ising model. We use fraction of the qubits to model a bath that is coupled to the system. The bath spins are prepared in the polarized ground state subject to a strong simulated Zeeman field. By an adiabatic downward sweep of the magnetic field, we transfer energy and entropy from the system to the bath qubits. A measurement and reset of the bath qubits allow the restart of the protocol cycle. We find that the algorithm's performance at a finite error rate depends on the nature of the excitations; systems with non-local (topological) excitations are more challenging to cool. Finally, we explore ways to mitigate this problem partially.

DY 9.5 Mon 16:45 A 151

Topological quantum phase transitions in exact two-dimensional isometric tensor networks — •Yu-Jie Liu[1], Kirill Shtengel[2], and Frank Pollmann[1] — [1]Technical University of Munich — [2]University of California, Riverside

Isometric tensor networks (isoTNS) form a subclass of tensor network states that have an additional isometric condition, which implies that they can be efficiently prepared with a linear-depth quantum circuit. In this work, we introduce a procedure to construct isoTNS encoding of certain 2D classical partition functions. By continuously tuning a parameter in the isoTNS, the many-body ground state undergoes quantum phase transitions, exhibiting distinct 2D topological order. We illustrate this by constructing an isoTNS path with bond dimension D = 2 interpolating between distinct symmetry-enriched topological (SET) phases. At the transition point, the isoTNS wavefunction is related to a gapless point in the classical six-vertex model and can be interpreted as a superposition of world lines of random walking particles. The critical wavefunction supports a power-law correlation along one spatial direction while remains long-range ordered in the other spatial direction. We provide an exact linear-depth parametrized local quantum circuit that realizes the path. The above features can therefore be efficiently realized on a programmable quantum device. At the end, we briefly discuss the possibility of isoTNS paths interpolating between other 2D topological phases.

DY 9.6 Mon 17:00 A 151

Quantum simulation of the 1D Fermi-Hubbard model as a Z2 lattice-gauge theory — •Uliana Khodaeva[1], Dmitry Kovrizhin[2], and Johannes Knolle[1,3,4] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]LPTM, CY Cergy Paris Universite, UMR CNRS 8089, Pontoise 95032 Cergy-Pontoise Cedex, France — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [4]Blackett Laboratory, Imperial College of London, London SW7 2AZ, United Kingdom

The Fermi-Hubbard model is one of the central paradigms in the

physics of strongly-correlated quantum many-body systems. Here we propose a quantum circuit algorithm based on the Z2 lattice gauge theory (LGT) representation of the one-dimensional Fermi-Hubbard model, which is suitable for implementation on current NISQ quantum computers. Within the LGT description there is an extensive number of local conserved quantities commuting with the Hamiltonian. We show how these conservation laws can be used to implement an efficient error-mitigation scheme. The latter is based on a post-selection of states for noisy quantum simulators. While the LGT description requires a deeper quantum-circuit compared to a Jordan-Wigner (JW) based approach, remarkably, we find that our error-correction protocol leads to results being on-par with a standard JW implementation on noisy quantum simulators.

DY 9.7 Mon 17:15 A 151

Quantum control on MPS manifolds — Marko Ljubotina, •Elena Petrova, and Maksym Serbyn — IST Austria, Am Campus 1, 3400 Klosterneuburg, Austria

The progress of quantum devices necessitates the development of methods for determining the optimal steering operators, that can efficiently drive quantum systems along desired trajectories of states. In my talk, I will introduce a method for constructing such operators using matrix product states (MPS). Our technique is able to build operators with different supports. To evaluate the effectiveness of our approach, we test it on a specific trajectory. Our analysis involves a comparison of operators with various supports and different free parameter choices. We identify the optimal set of parameters and demonstrate converging behaviour as the support size is increased. The resulting Floquet systems for the closed trajectory of our choice violate the Eigenstate Thermalization Hypothesis (ETH).

DY 9.8 Mon 17:30 A 151

Non-interacting limit of the many-body mean level density as an indicator of integrable vs. chaotic single particle dynamics — •Georg Maier[1], Carolyn Echter[1], Juan-Diego Urbina[1], Caio Lewenkopf[2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Instituto de Física, Universidade Federal Fluminense

A celebrated result of semiclassical analysis states that two definitorial aspects of a system's classical dynamics, integrability and chaos, are universally reflected in the spectral fluctuations of its quantized version. According to this picture, therefore, the mean level density (that encodes the smooth, mean features of the spectrum) provides just a system-dependent background that is routinely removed to focus on fluctuations. I will present that, contrary to a naive application of this paradigm, the smooth part of the many-body level density is extremely sensitive to the nature of the single-particle phase space. Specifically, while the spectral fluctuations of many body systems in the mean field limit can be shown to be Poissonian for both chaotic and integrable single-particle dynamics, it is the average level density the one that reflects such distinction. Our results are based on the study of the mean level density obtained from averaging over ensembles of single-particle spectra with the characteristic fluctuations representing the integrable and chaotic dynamics of the weakly interacting (mean field) limit. We are then able to obtain closed analytical expressions for systems with N=2,3 bosons/fermions, while extensive numerical simulations support our claims for larger values.

DY 9.9 Mon 17:45 A 151

Theory of Two-Dimensional Nonlinear Spectroscopy for Correlated Magnons in Three-Dimensional Canted Antiferromagnets — •Wonjune Choi[1,2], Daniel Schultz[3], Jonas Habel[1,2], Johannes Knolle[1,2], and Yong Baek Kim[3] — [1]Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany — [3]University of Toronto, Toronto, Canada

We investigate how nonlinear response functions can capture the correlated dynamics of magnons, a phenomenon beyond the reach of linear spin wave theory. A recent experiment on the S=5/2 canted antiferromagnet YFeO3 [Zhang et al., arXiv:2301.12555] observed puzzling second-order dynamical responses that cannot be explained by the Landau-Lifshitz-Gilbert simulation. Our key finding addresses this puzzle by revealing that the experimentally observed new signals result from the quantum correction of the ground state and the mode-mode couplings between the distinct magnon modes at the reduced Brillouin zone center. These many-body quantum effects, dynamically generated by three magnon interactions, originate from the Dzyaloshinskii-Moriya interaction responsible for the noncollinear antiferromagnetic order. Our work highlights the potential application of nonlinear spectroscopy as a promising experimental route to understanding intertwined dynamics among correlated magnons.

DY 10: Nonlinear Dynamics, Synchronization and Chaos

Time: Monday 15:00–18:30 Location: BH-N 128

DY 10.1 Mon 15:00 BH-N 128

Biochemical pH oscillators in giant lipid vesicles — Arthur Straube[1,2], •Guillermo Olicón-Méndez[2], Maximilian Engel[3,2], Felix Höfling[2,1], and Stefanie Winkelmann[1] — [1]Zuse Institute Berlin — [2]Fachbereich Mathematik und Informatik, Freie Universität Berlin — [3]Korteweg-de Vries Institute, University of Amsterdam

We study pH oscillators confined to giant lipid vesicles serving as an open reactor [1]. In contrast to conventional pH oscillators in closed reactors, the exchange with the vesicle exterior periodically resets the pH clock that switches the system from acid to basic, resulting in self-sustained oscillations. We analyze the structure of the limit cycle, which controls the dynamics for giant vesicles and dominates the strongly stochastic oscillations in small vesicles of submicrometer size [2]. Based on an accurate reduced two-variable model [1], we further apply geometric singular perturbation theory [3] to rigorously analyze the structure underlying the limit cycle. Insights into the mechanism of pH oscillations for a single oscillator is crucial for rationalizing experiments and understanding communication of vesicles and synchronization of rhythms.

[1] A.V. Straube, S. Winkelmann, F. Höfling, J. Phys. Chem. B. 127, 2955 (2023). [2] A.V. Straube, S. Winkelmann, C. Schütte, F. Höfling, J. Phys. Chem. Lett. 12, 9888 (2021). [3] M. Engel, G. Olicón-Méndez, accepted by Contemp. Math. (preprint arXiv:2305.18021).

DY 10.2 Mon 15:15 BH-N 128

Artificial homeostatic temperature regulation via bio-inspired feedback mechanisms — Petro Feketa[1], Tom Birkoben[2], •Maximiliane Noll[2], Alexander Schaum[3], Thomas Meurer[4], and Hermann Kohlstedt[2,5] — [1]School of Mathematics and Statistics, Victoria University of Wellington, New Zealand — [2]Chair for Nanoelectronics, Kiel University, Germany — [3]Chair for Process Analytics, University Hohenheim, Stuttgart, Germany — [4]Digital Process Engineering Group, Institute for Mechanical Process Eng. and Mechanics, Karlsruhe Institute of Technology, Germany — [5]Kiel NanoSurface and Interface Science KiNSIS, Kiel University, Germany

Homeostasis enables living organisms to maintain robust functioning by adapting to a changing environment. An instance of homeostatic behavior is the thermoregulation in mammals where a stable internal temperature is kept. In this work we present an electronic realization of a temperature regulation based on a single-effector regulation system. The electronic system contains two thermosensitive neurons, a summation unit processing the spikes and a feedback loop which leads to heating or cooling of the neurons via a Peltier element. The spiking trains of thermosensitive neurons can be processed to stabilize an a priori unknown system-inherent set-point. As important parameters for the set-point the feedback control gain and the activity patterns of the thermosensitive artificial neurons are investigated.

DY 10.3 Mon 15:30 BH-N 128

A Sufficient Synchronization Criterion for Memristively Coupled FitzHugh-Nagumo Oscillators — •Jonas Röhrig[1], Robin Lautenbacher[2], Bakr Al Beattie[1], Karlheinz Ochs[1], and Ralf Köhl[2] — [1]Ruhr-University, Bochum, Germany — [2]Christian-Albrechts-University, Kiel, Germany

Moving towards computational hardware that mimics efficient computation schemes from biological nervous systems, oscillator networks are

an abstraction level of biological neuronal nets that is of great interest to study. A key question in that regard is to understand the occurrence of synchronization in oscillator networks whose topology adapts over time. We study electrical implementations of such networks, consisting of FitzHugh-Nagumo oscillators (FNOs) and memristive couplings between them. The latter implement growth and learning of the network. For such networks, we propose a sufficient synchronization criterion. This criterion is formulated in terms of the connectivity of the coupling graph and the maximal absolute negative differential resistance of the FNOs nonlinearity such that it is readily applicable for practitioners. Wave digital emulations of memristively coupled FNO networks demonstrate the application of the criterion.

DY 10.4 Mon 15:45 BH-N 128

A Sensory Driven Adaptive Central Pattern Generator — •Jonas Röhrig, Sebastian Jenderny, Bakr Al Beattie, and Karlheinz Ochs — Ruhr-University, Bochum, Germany

Contributing to the ongoing effort to integrate our understanding of biological neuronal systems into the next generation of computational hardware, we propose an ideal electrical circuit to model a central pattern generator (CPG). A CPG is a fundamental neuronal circuit that can autonomously generate rhythmic muscle contractions that may be modulated by external inputs. Concretely, we consider a CPG that consists of inhibitorily coupled, alternatingly firing pacemaker neurons that are excitatorily coupled with motor neurons. As a technologically and biologically plausible neuron model we use the FitzHugh-Nagumo oscillator. We let some sources and components depend on a sensory signal to achieve varying oscillation frequencies and synchronization patterns. Moreover, we present a wave digital model of the proposed circuit that can be used to emulate the CPGs behavior, demonstrating switching between synchronization patterns and frequency changes.

DY 10.5 Mon 16:00 BH-N 128

Complex state space in high dimension - Impact on chimera dynamics? — •Seungjae Lee[1,2] and Katharina Krischer[2] — [1]Chair for Network Dynamics (cfaed) and Institute of Theoretical Physics, Technische Universität Dresden, Dresden, Germany — [2]Department of Physics, Technische Universität München, Garching bei München, Germany

Chimeras, states of coexisting coherence and incoherence, constitute intriguing collective dynamics of coupled oscillators and arise from symmetry-breaking. Past research focussed on systems of (Abelian) Kuramoto-Sakaguchi (KS) phase oscillators. Recent generalizations studied ensembles of higher-dimensional non-Abelian Kuramoto oscillators moving on the surface of a D-dimensional unit sphere, rather than being confined to a unit circle. Here, we discuss observable chimera dynamics in a system of higher-dimensional KS oscillators in two-population networks. Exploiting a generalized Watanabe-Strogatz transformation and the higher-dimensional Ott-Antonsen ansatz, we explore the macroscopic collective dynamics. For 2-dimensional complex spaces, we find diverse dynamics of the order parameter vectors, depending on the strength of intra-population coupling. We in particular observe both stationary and breathing chimeras. We furthermore show the transition of the chimera state into a component-wise aperiodic dynamics as the coupling strength weakens sufficiently. The emergence of aperiodic chimera dynamics is attributed to the breaking of conserved quantities that are preserved in trajectories of stationary, breathing, and alternating chimera states.

DY 10.6 Mon 16:15 BH-N 128

Emergence of limit cycle in Lindblad dynamics — •Shu Zhang[1], Shovan Dutta[1,2], and Masudul Haque[1,3] — [1]Max-Planck-Institut für Physik Komplexer Systeme, Dresden, Germany — [2]Raman Research Institute, Bangalore, India — [3]Technische Universität Dresden, Dresden, Germany

Among the most iconic features of classical nonlinear dynamics are persistent limit-cycle oscillations and critical slowing down at the onset of such oscillations, where the system relaxes purely algebraically in time. On the other hand, quantum systems subject to generic Markovian dissipation decohere exponentially in time, approaching a unique steady state. Here we show how coherent limit-cycle oscillations and algebraic decay can emerge in a quantum system governed by a Markovian master equation as one approaches the classical limit. We illustrate these general mechanisms using a single-spin model and a two-site lossy Bose-Hubbard model, contrasting with the scenario of a classical fixed point. In particular, we demonstrate that the fingerprint of a limit cycle is a slow-decaying branch with vanishing decoherence rates in the Liouville spectrum, while a power-law decay is realized by a spectral collapse at the bifurcation point.

DY 10.7 Mon 16:30 BH-N 128

The Dynamics of Future Power Grids - Bridging Theory and Application — •Anna Büttner and Jakob Niehues — Potsdam Institute for Climate Impact Research (PIK), 14412 Potsdam, Germany

Renewable energy sources such as wind turbines and solar cells are connected to the power grid via inverters. As we move towards a fully renewable grid, there is a growing need for so-called grid-forming inverters (GFIs) that can contribute to grid stability and synchronization. This shift presents a significant challenge as GFIs are a relatively new and complex technology, of which there is a limited practical and theoretical understanding. The so-called normal form of GFIs is a formulation that does not depend on the technology of the grid-forming actors and can be estimated from data.

In this talk, we show recent results from the validation of the normal form via system identification. The normal form can accurately model the dynamic behavior of a large class of GFIs. We present these results for lab measurements as well as complex simulation data.

We also show novel analytical results on the linear stability of the synchronous state of general power grid dynamics. Using the novel small-phase theorem we have shown that the stability can be analyzed in terms of a network component and the local dynamics, given by the normal form.

We are thus for the first time able to show stability results for validated power grids thereby bridging the gap between theoretical calculations and real-world application.

15 min. break

DY 10.8 Mon 17:00 BH-N 128

Chaos Control in Cardiac Dynamics: A novel approach to low-energy defibrillation — •Daniel Suth and Thomas Lilienkamp — Computational Physics for Life Science, Nuremberg Institute of Technology Georg Simon Ohm, Nuremberg, Germany

Various dynamical systems exhibit chaotic states with spiral wave-like patterns. Control schemes for chaotic patterns aim to terminate or synchronize such states, by applying a single or multiple stimuli to the system. One possible application is the use of multiple low-energy pulses to terminate ventricular and atrial fibrillation, with the advantage of avoiding negative side effects associated with singular high-energy defibrillation shocks.

This study demonstrates that sequences of well-timed stimuli provide high success rates at low amplitudes to terminate chaotic dynamics in numerical simulations of cardiac tissue. Therefore, we propose a simple and robust approach to calculate the pulse timings derived directly from simple characteristic features of the associated state variables.

We demonstrate this method using numerical simulations with four different 2D computational models of cardiac dynamics that vary in complexity and target species. Therefore, a detailed statistical analysis of the proposed approach, the results that can be achieved with it and a comparison with multiple existing methods is provided.

Furthermore, we investigate fundamental mechanisms of cardiac dynamic models that can be utilised to terminate chaotic states in such systems.

DY 10.9 Mon 17:15 BH-N 128

Pulse Optimization for Activation of Virtual Electrodes — •Justine Wolter[1,2], Ulrich Parlitz[1,2], and Stefan Luther[1,2,3] — [1]MPI for Dynamics and Self-Organization, Göttingen — [2]University Medical Center, Göttingen — [3]Deutsches Zentrum für Herz-Kreislauf-Forschung, Partner Site Niedersachsen, Göttingen, Germany

Cardiac arrhythmias represent one of the major causes of mortality worldwide. In case of cardiac arrhythmias, the normal heart beat is disturbed, affecting the heart's pumping function. Life-threatening cases such as ventricular fibrillation are commonly treated with a single high-energetic shock that causes traumatic pain, tissue damage and a worsening prognosis. Low-energy defibrillation techniques that apply a sequence of weak electrical pulses reduce the necessary energy while still being able to control the fibrillation. These methods use virtual electrodes which consist of heterogeneities in cardiac tissue acting as wave emitters in the presence of an external electrical field.

In this study, we present numerical simulations of two dimensional excitable media in a mono- and a bidomain model, showing the impact and dynamics of such virtual electrodes.

For different sizes of heterogeneities we find that by optimizing the pulse duration and form, the necessary energy for activation is significantly reduced. With our work, defibrillation protocols that apply sequences of weak, energetic electrical pulses can be further optimized. Therefore, we provide valuable insights for the further development of improved defibrillation techniques.

DY 10.10 Mon 17:30 BH-N 128

Toward Better Defibrillation through Genetic Optimisation — •Marcel Aron[1,2,3,4], Ulrich Parlitz[1,3,4], and Stefan Luther[2,1,3,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Germany — [3]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Germany — [4]German Center for Cardiovascular Research (DZHK e.V., partner site Niedersachsen), Göttingen, Germany

Cardiac fibrillation results in the lethal, chaotic disruption of the heart's electricity-coordinated contraction mechanism. Its current standard treatment, defibrillation, may damage tissue and even lead to (e.g.) elevated fibrillation susceptibility long-term. This has motivated research into alternative, less intrusive (i.e. low-energy) defibrillation schemes beyond the usual singular, potent shock.

The search for better defibrillation schemes has proven difficult largely due to the sheer amount of possible shock sequences to consider. We sought to reduce the number of candidate low-energy shock sequences through the design and application of an optimisation heuristic inspired by evolutionary biology. To guide this heuristic, we consulted simplified defibrillation simulations.

This talk covers our quantification of "better" in the context of defibrillation schemes and an outline of our optimisation heuristic. We also show our findings in its application to optimising multi-shock defibrillation, including the discovery of a potentially global optimum.

DY 10.11 Mon 17:45 BH-N 128

Dynamics of transient chaos in excitable media — Melvin Dix[1,2], Paula Luttermann[1,2], Thomas Lilienkamp[3], Stefan Luther[1,2,4,5], and •Ulrich Parlitz[1,2,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Germany — [3]Computational Physics for Life Science, Nuremberg Institute of Technology Georg Simon Ohm, Nuremberg, Germany — [4]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Göttingen, Germany — [5]German Center for Cardiovascular Research (DZHK e.V., partner site Niedersachsen), Göttingen, Germany

Chaotic spatio-temporal dynamics in excitable media such as cardiac tissue is often not permanent but limited in time. In this contribution, we discuss the influence of heterogeneities and stochastic perturbations on the mean lifetime of such chaotic transients. Using simulations with the Aliev-Panfilov and the Fenton-Karma model, we show that both forms of perturbationss can (significantly) prolong the duration of chaotic transients.

DY 10.12 Mon 18:00 BH-N 128

Patched patterns and emergence of chaotic interfaces: a new paradigm in coupled excitable systems — •Igor Franovic[1] and Sebastian Eydam[2] — [1]Institute of Physics Belgrade, Serbia — [2]RIKEN Center for Brain Science, Wako, Japan

While coherence-incoherence patterns have been extensively explored for coupled oscillators, much less is known about onset mechanisms and finite-size effects associated with such patterns in coupled excitable systems. Here we present a new class of patterns, called patched patterns, in non-locally coupled arrays of excitable units with attractive and repulsive interactions. Their self-organization involves the formation of patches, the spatial domains of units locked by their average spiking frequencies. Depending on the prevalence of attraction vs repulsion, patched patterns can be temporally periodic, quasiperiodic or chaotic, whereby in contrast to chimeras, chaos is not spatially localized. Chaotic patterns may develop interfaces where the units display a slow alternation between epochs of locking to adjacent patches and epochs of increased variability. We demonstrate typical bifurcation scenarios giving rise to chaos, showing that adapting the coupling range may change the character of the transition to chaos. Unlike chimeras, the maximal Lyapunov exponent for chaotic patched patterns converges to a finite value with system size. Nevertheless, interfaces may undergo an unpinning transition, which leads to diffusive motion similar to that of the incoherent part of chimeras.

Reference: I. Franović and S. R. Eydam, Chaos 32, 091102 (2022), https://doi.org/10.1063/5.0111507

DY 10.13 Mon 18:15 BH-N 128

Self-similar growth patterns in 2-dimensional von Neumann elementary cellular automata: a complete exploration of all outer-totalistic rules — •Kian Siadat and Jens Christian Claussen — School of Computer Science, University of Birmingham, UK

Growth patterns of cellular automata emerging from a localized single seed initial condition have intrigued the nonlinear dynamics community through the identification of two universality (sub)classes within the Wolfram class IV cellular automata [1], where rule 90 (Sierpinski) and rule 150 are representatives of these classes. In this work, we perform an exhaustive exploration of all 2-dimensional cellular automata rules which in addition obey the criterion of outer-totalistic, i.e., the output depends on the number of active neighbour cells, but not about their spatial pattern. While being a subset of all possible 2-dim CA rules, this is the most central class of CA rules as they retain a maximum of symmetries. We identify several distinct time series related to the growth patterns, and beside the 1-dim and 2-dim versions of rule 90, we also identify a rule providing a triple replication, and generating a 2-dim spatial Sierpinski pattern.

Our findings indicate that despite the large number of possible cellular automata rules, we observe only a few self-similar growth patterns and associated time series.

[1] Nagler, J. Claussen, J. (2005) $1/f^{\alpha}$ spectra in elementary cellular automata and fractal signals, Phys. Rev. E 71, 067103 (2005)

DY 11: Active Fluids and Microswimmers (joint session DY/BP/CPP)

Time: Monday 15:00–18:30 Location: BH-N 243

Invited Talk DY 11.1 Mon 15:00 BH-N 243

Control of active turbulence — •Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Active turbulence is one of the prominent features of active matter and occurs in diverse systems such as bacterial suspensions, biopolymeric assemblies, and tissues. One of the current challenges is to control these turbulent flow patterns for powering processes at small scales.

In the first part of the talk we rely on a continuum description of active paranematics, the Doi-Edwards theory supplemented by an active stress tensor [1]. We characterize the occuring turbulent flow for extensile active stresses. Then, motivated by the possibility to control the activity of bacteria by light, we consider a square lattice of spots, where activity drops to zero. Depending on the lattice constant and the size of the spots, we identify a trapped-vortex and, most interestingly, a multi-lane flow state. The latter consists of lanes with opposite flow directions separated by a street of vortices. It displays multistability and can also appear transiently.

Second, we perform hydrodynamic simulations of a collection of active or squirmer rods moving in their fluid environment [2]. We classify their dynamic states for the pusher/puller type as a function of density and aspect ratio of the rods and observe clustering and swarming. In particular, pusher rods show active turbulence as a compromise of disordering hydrodynamic and aligning steric interactions.

[1] A. Partovifard and H. Stark, submitted.

[2] A.W. Zantop and H. Stark, Soft Matter **18**, 6179 (2022).

DY 11.2 Mon 15:30 BH-N 243

Entropy production in active turbulence — •Byjesh N. Radhakrishnan, Thomas L. Schmidt, and Etienne Fodor — Department of Physics and Material science, University of Luxembourg

Active particles like bacteria and sperm cells sustain a continuous intake and dissipation of energy. Consequently, they are intrinsically out of equilibrium which leads to a non-vanishing entropy production rate (EPR) even in steady states. Quantifying how the EPR varies in different collective phases is crucial in developing a thermodynamic framework for active matter. In this work, we look at the EPR in active turbulence. We use Active Model H, a continuum model for active particles in a momentum-conserving fluid, to study turbulence in contractile scalar active systems. We measure the local EPR in numerical simulations, which unveils the relation between the magnitude of entropy production and $+1/2$ topological defects in the system. Also, we study how EPR and the properties of defects such as mean square displacement and defect lifetime vary with the activity parameter.

DY 11.3 Mon 15:45 BH-N 243

Active turbulent mixing — •Till Welker[1], Malcolm Hillebrand[2], Ricard Alert[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, TU Berlin, Germany — [2]MPI for the Physics of Complex Systems, Dresden, Germany

Mixing on the mesoscale is crucial for both microfluidic devices and living cells. Experiments backed by simulations show a significant increase in mixing efficiency caused by active turbulence.

Our goal is to enhance the theoretical understanding of active turbulent mixing by transferring theories and concepts originally developed for inertial turbulent mixing. We therefore study a defect-free active nematic model known to show universal scaling of the energy spectrum with a passive chemical diffusing and advecting in the flow.

The efficiency of mixing χ rises with both activity of the nematic A and diffusion coefficient of the chemical D. Intriguingly, as D approaches zero, mixing efficiency converges to a non-zero value $\chi_0(A)$ because smaller D are compensated by larger concentration gradients. This presents an attractive mechanism to mix poorly diffusive substances, and is also observed in inertial turbulent mixing.

The scaling of the concentration spectrum $E_c(q)$ is of great interest and has been extensively studied in the context of inertial turbulence. We demonstrate that Batchelor-Howells-Townsend theory and Batchelor theory for strongly and poorly diffusive substances can be transferred to active turbulence. As a consequence of the universal energy scaling of our active nematic, we predict universal scaling regimes for $E_c(q)$ which we validate in simulations.

DY 11.4 Mon 16:00 BH-N 243

Simultaneous emergence of active turbulence and odd viscosity in a colloidal chiral active system — •Joscha Mecke[1,2], Yongxiang Gao[1], Gerhard Gompper[2], and Marisol Ripoll[2] — [1]Institute for Advanced Study, Shenzhen University, China — [2]Institute of Biological Information Processing and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

Active fluids display collective phenomena such as active turbulence or odd viscosity, which refer to spontaneous complex and transverse flow. We report the simultaneous emergence of these seemingly separate phenomena in experiment for a chiral active fluid composed of a carpet of standing and spinning colloidal rods, and in simulations for synchronously rotating hard discs in a hydrodynamic explicit solvent (see also Commun. Phys. 6, 324 (2023), https://doi.org/10.1038/s42005-023-01442-3). Stresses among the colloids encompass rotational and odd shear contributions absent in usual fluids. Rotational viscosity couples the colloids' rotation to translation, causing active turbulence. Odd viscosity involves a perpendicular coupling of shear stresses, leading to an effective pressure pointing into or out of the emergent vortices. We quantify the two phenomena in experiments and simulation using the same setup. Both rotational and odd viscosity originate from the same source and the system behaviour hinges on the propagation of odd stresses via long-ranged hydrodynamics. Our findings are relevant for the understanding of biological systems and for the design of microrobots with collective self-organised behaviour.

DY 11.5 Mon 16:15 BH-N 243

Hydrodynamic synchronization of elastic cilia: How flow confinement and boundary conditions determine the characteristics of metachronal waves — Albert von Kenne, •Markus Bär, and Thomas Niedermayer — Physikalisch-Technische Bundesanstalt, Berlin, Germany

We model hydrodynamically interacting cilia by a coupled phase oscillator description by reducing the dynamics of hydrodynamically interacting elastic cilia to the slow time scale of synchronization [1]. In this framework, we determine analytical metachronal wave solutions as well as their stability and perform simulations in a periodic chain setting. The flow confinement at the wall stabilizes metachronal waves with long wavelengths propagating in the direction of the power stroke and, moreover, metachronal waves with short wave lengths propagating perpendicularly to the power stroke. In open chains of phase oscillators, the dynamics of metachronal waves is fundamentally different. Here, the elasticity of the model cilia controls the wave direction and selects a particular wave number: At large elasticity, waves traveling in the direction of the power stroke are stable, whereas at smaller elasticity waves in the opposite direction are stable. In addition, coexistence of waves traveling in opposite directions and irregular, chaotic dynamics are observed. [1] A. von Kenne, M. Bär and T. Niedermayer. Preprint, https://www.biorxiv.org/content/10.1101/2023.10.20.563276v1.full.pdf.

DY 11.6 Mon 16:30 BH-N 243

Pattern formation in non-Newtonian active suspensions — •Henning Reinken and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Controlling spatiotemporal patterns in active matter is of essential importance in view of prospective applications. In contrast to previous studies utilizing external control such as geometrical constraints [1], we here explore the possibility of controlling suspensions of microswimmers via the internal rheological properties of the suspension. Recent work has focused on the impact of viscoelastic and non-Newtonian behavior on the dynamics of single swimmers [3], but only a limited number of studies explores the consequences for collective motion and emergent patterns. Here, employing a recent continuum model for mesoscale turbulence in microswimmer suspensions [4], we investigate the impact of non-Newtonian behavior on the pattern formation. In particular, we focus on the stabilization of regular vortex structures in otherwise turbulent suspensions without the need for external intervention.

[1] H. Reinken, D. Nishiguchi, S. Heidenreich, A. Sokolov, M. Bär, S. H. L. Klapp, and I. S. Aranson, Commun. Phys. **3**, 76 (2020)

[3] G. Li, E. Lauga, and A. M. Ardekani, J. Non-Newton. Fluid Mech.

297, 104655 (2021)
[4] J. Słomka and J. Dunkel, Eur. Phys. J. ST **224**, 1349 (2015), Phys. Rev. Fluids **2**, 043102 (2017), Proc. Natl. Acad. Sci. U.S.A. **114**, 2119 (2017)

15 min. break

DY 11.7 Mon 17:00 BH-N 243

Bacterial swimming strategies in a shear flow — •Valeriia Muraveva, Agniva Datta, and Carsten Beta — Potsdam University, Potsdam, Germany

By changing the configuration of their flagella, bacterial swimmers can control their direction and speed of locomotion. The soil bacterium Pseudomonas putida pushes itself forward by counterclockwise (CCW) rotation of its flagellar bundle, while clockwise (CW) rotation pulls the cell body in the opposite direction. Additionally, P. putida can wrap its bundle of flagella around the cell body to move in a screw thread fashion. However, the benefits of having different modes of swimming still remain unclear. Here, we used microfluidics in combination with fluorescence microscopy to show how the swimming behavior changes under laminar shear flow conditions. Compared to a fluid at rest, we found that in flow, swimmers prefer the pull configuration over the wrapped one (both emerging under CW flagellar rotation). Moreover, we investigated flow-induced alignment effects and compared the distributions of swimming modes and velocities in the bulk fluid and close to the fluid-substrate interface. Our results provide first insights into how bacteria adapt their swimming strategy under different flow conditions at the single-cell level.

DY 11.8 Mon 17:15 BH-N 243

Artificial Microswimmers in locally-tuneable hydrodynamic flow fields — •Lisa Rohde and Frank Cichos — Molecular Nanophotonics Group, Peter-Debye-Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Biological components on the microscale, which constantly consume energy can organize themselves into functional structures through interaction with their environment. Interaction potentials, temperature or composition gradients as well as flow fields play an important role in this structure formation. We would like to transfer such self-organization principles to synthetic active particles, which are a model system to mimic the function of motors in biology, but yet have only limited functionality. Here, we expose thermo-phoretic Janus particles to an environment with tuneable hydrodynamic flow fields generated by local temperature gradients. A heated paramagnetic silica particle acts as a heat source and generates a thermo-osmotic flow field due to a temperature gradient on the substrate. By controlling the temperature of the heat source, we are able to locally change the generated hydrodynamic flow field. We study the orientational dynamics and the distance of the Janus particles relative to the heat source in dependence of temperature and laser intensities. The interplay of the local flow fields with the activity of the Janus particles results in a potential that traps the Janus particles in a configuration around the heat source. We find a polarisation of the Janus particles that align with the flow field having a stable orientation relative to the heat source.

DY 11.9 Mon 17:30 BH-N 243

Run-and-tumble motion of ellipsoidal swimmers — •Gordei Anchutkin[1], Viktor Holubec[2], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, CZ-180 00 Praha, Czech Republic

The characteristic motion of bacteria, the so-called "run-and-tumble" motion, is a hallmark of living active particles. It consists of a sequence of linear directional movements and random rotations that constantly alternate based on a biochemical feedback process. In contrast to bacteria, synthetic active particles do not exhibit run-and-tumble motion, except they are forced to do so by sophisticated optical control feedback loops.

In this study, we show that self-thermophoretic Janus ellipsoids can carry out run-and-tumble-like dynamics under strong confinement. Our Janus ellipsoids are propelled along the short axis and exhibit long periods of directed motion before reversing the propulsion direction. We show that a bimodal out-of-plane angular distribution arises at high propulsion velocities, which is mainly the result of hydrodynamic wall interactions. We evaluate hydrodynamic interactions, and gravitational and optical forces to give a quantitative model of the observed dynamics. These interactions together with the slow rotational diffusional dynamics around the short ellipsoid axis provide the basis of the run-and-tumble dynamics.

DY 11.10 Mon 17:45 BH-N 243

Microswimming under a wedge-shaped confinement — •Alexander R. Sprenger and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Microswimmers, both living and artificial, frequently navigate through diverse and often confined environments. Their out-of-equilibrium nature of self-propulsion and associated fluid flows lead to complex hydrodynamic interactions with their surroundings. Understanding the impact of various confinements on the behavior of self-propelled particles is crucial for gaining insights into biological phenomena and motivating advancements in microtechnologies.

In this contribution, we study the low-Reynolds-number dynamics of microswimmers confined within a wedge-shaped free-slip boundary [1]. Such scenarios naturally occur in experiments on inhomogeneously evaporating fluid flows, which form a free-standing confinement between two converging interfaces. Additionally, wedge-shaped environments possess distinctive geometric trapping and guiding properties relevant to various microfluidic applications.

Here, we present an exact solution for the resulting flow fields for various opening angles of the wedge employing the method of images. In this manner, we investigate the hydrodynamic interactions between each swimmer and the confining interfaces. We find either attraction or repulsion towards the tip of the wedge, depending on the propulsion mechanism (pusher or puller) and the opening angle of the wedge.

[1] A. R. Sprenger, A. M. Menzel (submitted).

DY 11.11 Mon 18:00 BH-N 243

AcoDyn: Efficient computer simulations of acoustically propelled microparticles — •Adrian Paskert and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Universität Münster, 48149 Münster, Germany

For future applications in science and engineering, active microparticles have great potential. Acoustically propelled microparticles are particularly advantageous for medical applications because they operate well within medically safe intensity ranges and are generally considered biocompatible. However, due to the complexity of the flow fields generated around these particles and the high computational cost of direct computer simulations even for simple 2D particle geometries, the theoretical understanding of the particles' propulsion and dynamics is still very limited. In this talk, we will give an overview of how these particles can be simulated efficiently to enable the numerical study of complex 3D particles. Moreover, our novel software solution `AcoDyn` will be presented, along with key results we have obtained through its application.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 283183152

DY 11.12 Mon 18:15 BH-N 243

Opto-fluidic dynamic patterning of microparticles — •Elena Erben[1], Weida Liao[2], Antonio Minopoli[3], Nicola Maghelli[4], Eric Lauga[2], and Moritz Kreysing[1] — [1]IBCS-BIP, KIT, Karlsruhe, Germany — [2]DAMTP, University of Cambridge, UK — [3]University of Pisa, Pisa, Itlay — [4]Fondazione Human Technopole, Milano, Italy

Techniques for the precise manipulation of microscopic objects bear great potential for application in a wide range of fields, from basic biological research to microfabrication. Our method uses rapid scanning of an infrared laser beam to optically generate thermoviscous flows [1] within a sample. Combined with closed-loop control this enables the automatic positioning of a single microparticle, with a precision of up to 24 nm [2]. Our approach can be multiplexed to manipulate up to 15 particles in a parallel and dynamic fashion. Furthermore, we have found that the positioning of multiple particles can be greatly accelerated by exploiting the complex flow patterns that result from the time-sharing of different laser scan paths. We plan to combine our approach with a full analytical model of the flows [3], which we expect will further increase the precision and speed of this manipulation method, facilitating its translation to applications in the life sciences and beyond.

[1] Weinert et al. Phys. Rev. Lett. 2008; [2] Erben et al. Opt. Express 2021; [3] Liao et al. Phys. Rev. Fluids 2023.

DY 12: Statistical Physics far from Thermal Equilibrium II

Time: Monday 15:00–17:00 Location: BH-N 334

DY 12.1 Mon 15:00 BH-N 334

Dynamic renormalization of active field theories — •Nikos Papanikolaou and Thomas Speck — Institute of Theoretical Physics 4, University of Stuttgart, Stuttgart, Germany

Conservative scalar field theories function as coarse-grained models that describe systems with conserved dynamics featuring a single order parameter, such as density, magnetization, or height. Notable examples include Model B (for liquid-gas separation), cKPZ (for surface growth with conserved dynamics), and Active Model B+ (AMB+) (for self-propelled particles with density-dependent speed). Dynamical renormalization is a powerful tool to study the critical behavior of these theories and to determine the relevant parameters dictating their large-scale dynamics. Here, we apply this technique to AMB+, a recent generalization of Model B involving non-potential terms. Analyzing such complex field theories poses a challenge due to its cumbersome calculations. To facilitate the analysis, we developed a symbolic computer algebra code to obtain the graphical corrections of the model parameters. Applying this framework to AMB+, we find that potentially relevant higher-order non-linear terms are generated, limiting the regime of the perturbative renormalization. We explore strategies to ameliorate this problem and provide evidence that no perturbative fixed points other than the Wilson-Fisher fixed point exist.

DY 12.2 Mon 15:15 BH-N 334

Time-reversal and PT symmetry breaking in non-Hermitian field theories — •Thomas Suchanek[1], Sarah Loos[2], and Klaus Kroy[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany — [2]DAMTP, University of Cambridge, Cambridge, United Kingdom

We study time-reversal symmetry breaking in non-Hermitian fluctuating field theories with conserved dynamics, comprising the mesoscopic descriptions of a wide range of nonequilibrium phenomena [1]. They exhibit continuous parity-time (PT)-symmetry breaking phase transitions to dynamical phases. We introduce the (informatic) entropy rate as a method to quantify non-equilibrium dynamics emerging on the mesoscale. For two concrete transition scenarios, exclusive to non-Hermitian dynamics, namely oscillatory instabilities and critical exceptional points, a low-noise expansion exposes a pre-transitional surge of the entropy production, inside the static phases. For critical exceptional points, we identify the coupling of eigenmodes as the entropy-generating mechanism, causing a drastic noise amplification in the Goldstone mode. We illustrate our findings with a model of nonreciprocally coupled Cahn-Hilliard fields and an assembly of Brownian particles, interacting asymmetrically through chemotactic interactions.

[1] Suchanek, T., Kroy, K., & Loos, S. A. (2023). Irreversible mesoscale fluctuations herald the emergence of dynamical phases. arXiv preprint arXiv:2303.16701.

DY 12.3 Mon 15:30 BH-N 334

Pulsating with discrete symmetries: from microscopic dynamics to field theory — Massimiliano Esposito[1], Étienne Fodor[1], •Alessandro Manacorda[1], and Jan Meibohm[2] — [1]Department of Physics and Materials Science, University of Luxembourg — [2]Institute for Theoretical Physics, Technische Universität Berlin

Deformable active matter is a growing research field: it enables to model and analyze collective dynamics in dense systems where units have the ability to change their shape, such as epithelial or cardiac tissues.

Collective behavior emerges through the propagation of waves with intriguing patterns. The latter are intimately related with the symmetries of the system: the transition between arrest and wave propagation requires a symmetry breaking mechanism. Coarse-graining the microscopic dynamics in the complex Ginzburg-Landau approach (CGLE) leads to fluctuating hydrodynamics with predictive power.

Surprisingly, the presence of a discrete symmetry makes the CGLE approach unsuitable to describe the dynamics. We will show how one can build an active field theory with the prescribed symmetries, and how these affect the active phases and pattern formation at hydrodynamic level, opening the door to field theories of pulsating active matter.

DY 12.4 Mon 15:45 BH-N 334

Hydrodynamics of dense pulsating matter — •Tirthankar Banerjee[1], Jonas Ranft[2], Thibault Desaleux[3], and Etienne Fodor[1] — [1]Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Ecole Normale Superieure, Paris, France — [3]French Alternative Energies and Atomic Energy Commission (CEA), St-Paul-lez-Durance, France

Dense assemblies of deforming cells, e.g., in the heart, show rich behaviours from synchronized collective oscillation to various types of wave propagation. We propose a generic minimal hydrodynamic model of out-of-equilibrium pulsating (due to a global drive) particles in the presence of thermal fluctuations. Derived through a mechanistic approach, our model equations encode the coupled dynamics of two fields: a conserved density and a non-conserved phase variable that carries information on the size of deforming particles. We show that homogeneous arrested and cycling states can be separated by a sector of instabilities in the space of control parameters. Using a perturbative method, we show analytically how thermal fluctuations can modify these phase boundaries. Extensive numerical simulations on a two-dimensional lattice strongly corroborate the analytical phase diagrams and reveal that the instabilities grow into target wave patterns both in density and phase.

DY 12.5 Mon 16:00 BH-N 334

Hard sphere nucleation revisited: bringing simulation and experiment together — Sahana Kale and •Hans Joachim Schöpe — Universität Tübingen, Institut für angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Crystallization of a metastable melt is one of the most important non-equilibrium phenomena in classical physics. A milestone in crystal nucleation studies was the first prediction of absolute nucleation rate densities (NRDs) in hard sphere (HS) systems using the combination of computer simulations and classical nucleation theory (CNT), published in Nature in 2001. This work has been complemented in recent years by more advanced simulation work. However, a direct comparison of the experimental NRDs with those from the simulations shows a highly unsatisfactory result: the shape of the curves are qualitatively different and experimental and theoretical data diverge by up to 18 orders of magnitude!

Using laser-scanning confocal microscopy we study crystal nucleation in colloidal HS. We follow and characterise the formation of individual crystallites. Furthermore, we determine NRDs and critical radii in two different ways: 1) directly from the data without recourse to any model and 2) within the framework of CNT. The direct data analysis reproduces the existing experimental data sets from Bragg and small angle scattering, while the CNT-based analysis reproduces the simulation data. However, as mentioned above, the two data sets are incompatible. Accordingly, the cause of the huge discrepancy is due to shortcomings of the CNT and simulation techniques.

DY 12.6 Mon 16:15 BH-N 334

Sharp and soft metastable transitions under driving: A study with hard rods — •Miriam Klopotek[1], Martin Oettel[2], and Hans Joachim Schöpe[2] — [1]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [2]University of Tübingen, Institute for Applied Physics, Tübingen, Germany

When external forces drive systems, states that are otherwise ephemeral in equilibrium can unfold. Metastability can imply a characteristic change in the dynamics for long periods and a blanketing of the whole system with new structures. The degree of (non-)stability depends on the time scale of the driving. In a model system of sticky hard rods on lattices confined to quasi-2D [1], we observe a crossover from "sharp" to "soft" metastable transitions in the evolution of order parameters. Static external potentials can "sharpen" and even potentially stabilize them thermodynamically. Their underlying nature is thus challenging to discern when observing the dynamical evolution alone. Implications include critically examining data from thin film growth experiments.

[1] M. Klopotek, H. J. Schöpe, and M. Oettel (2024), in preparation.

DY 12.7 Mon 16:30 BH-N 334

Phase behavior of particles with different temperatures — •Amir Abbasi and Roland R. Netz — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

A well-known phenomenon in nonequilibrium thermodynamics is the phase separation in mixtures of hot and cold particles with purely repulsive interactions, coupled to heat baths at different temperatures [1-2]. Theoretical studies have explored this separation, often using the concept of an *effective* free energy, though its application is debatable due to the undefined temperature in such mixtures [3-4]. Our study aims to delineate the steady state of these particle mixtures using simulations and theoretical analysis of the extremal properties of the free entropy functional [5].

[1] S. N. Weber, C. A. Weber, and E. Frey, Phys. Rev. Lett. 116, 058301 (2016).

[2] S. S. N. Chari, C. Dasgupta, and P. K. Maiti, Soft Matter 15, 7275-7285 (2019).

[3] C. A. Weber, D. Zwicker, F. Jülicher, and C. F. Lee, Rep. Prog. Phys. 82, 064601 (2019).

[4] E. Ilker and J.-F. Joanny, Phys. Rev. Res. 2, 023200 (2020).

[5] R. R. Netz, Phys. Rev. E 101, 022120 (2020).

DY 12.8 Mon 16:45 BH-N 334

The spectral boundary of the Asymmetric Simple Exclusion Process (ASEP) - free fermions, Bethe ansatz and random matrix theory — •Goran Nakerst[1], Tomaz Prosen[2], and Masud Haque[1,3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]University of Ljubljana, Faculty for Mathematics and Physics, Jadranska 19, Ljubljana, Slovenia — [3]Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany

The dynamical timescales of Markov processes are determined by the spectrum of their generator matrices. In this talk, we explore the spectral boundary characteristics of the generator matrix in a paradigmatic model: the 1D Asymmetric Simple Exclusion Process (ASEP) with both periodic and open boundary conditions. Our focus centers on the emergence of a distinctive spiky spectral boundary (SSB). We will illustrate how the ASEP generator is represented by an interacting fermion model, which, in its non-interacting variant, exhibits a pronounced SSB. Notably, the SSB persists upon the reintroduction of interactions, which revert to the conventional generator of ASEP. Furthermore, we will establish the universality of the SSB, illustrating its prevalence in random matrix ensembles characterized by particular trace correlations and, equivalently, in random graphs with specific cycle structures. This presentation aims to meld concepts from stochastic processes, quantum mechanics, and random matrix theory.

DY 13: Glasses and Glass Transition (joint session CPP/DY)

Time: Monday 16:15–17:45 Location: H 0107

Invited Talk DY 13.1 Mon 16:15 H 0107

The boson peak in the vibrational spectra of glasses — •Edan Lerner — Institute for Theoretical Physics, University of Amsterdam, Science Park 904, Amsterdam, Netherlands

A hallmark of glasses is an excess of low-frequency, nonphononic vibrations, in addition to phonons. It is associated with the intrinsically nonequilibrium and disordered nature of glasses, and is generically manifested as a THz peak — the boson peak — in the ratio of the vibrational density of state (VDoS) and Debye's VDoS of phonons. Yet, the excess vibrations and the boson peak are not fully understood. In my contribution I will provide direct numerical evidence that vibrations near the boson peak consist of hybridizations of phonons with many quasilocalized excitations; the latter have recently been shown to generically populate the low-frequency tail of the vibrational spectra of structural glasses quenched from a melt and of disordered crystals. I will next use a reanalysis of experimental data, extensive computer simulations and a mean-field model, to show that the nonphononic part of the VDoS itself features both a universal power-law tail and a peak, entirely accounted for by quasi-localized nonphononic vibrations. Our results provide a unified physical picture of the low-frequency vibrational spectra of glasses, and in particular shed basic light on the origin, nature and properties of the boson peak.

DY 13.2 Mon 16:45 H 0107

Dynamics and Timescales of Higher Order Correlations in Supercooled Colloidal Systems — •Nele N. Striker[1], Irina Lokteva[1,2], Michael Dartsch[1,2], Francesco Dallari[1], Claudia Goy[1], Fabian Westermeier[1], Verena Markmann[1], Svenja C. Hövelmann[1], Gerhard Grübel[1,2], and Felix Lehmkühler[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

There has been extensive research into the nature of the glass transition, however its mechanisms remain mostly unclear. Recent works show that long-living locally favored structures (LFS), such as icosahedral structures forming upon supercooling, may play a key role. We show results from a combined X-ray Photon Correlation Spectroscopy (XPCS) and X-ray Cross Correlation Analysis (XCCA) experiment on colloidal hard spheres in the vicinity of the glass transition [1]. We defined a new correlation function g_c probing the timescales of higher-order correlations by tracking the time evolution of the structural higher-order correlations within the sample. We observed an increase in the ratio of the relaxation times of g_c and the standard individual particle relaxation time from about 0.4 to 0.9. The increasing values suggest that the local orders within the sample are becoming more long-lived approaching the glass transition. These results indicate that not only the presence but also the lifetime of LFS grows close to the glass transition.

[1] N. Striker et al., J. Phys. Chem. Lett., 2023, 14(20), 4719-4725

DY 13.3 Mon 17:00 H 0107

What can MD simulations tell us about the micromechanics of deformation of glassy amorphous polymers? — •Pramod Kumar Patel[1] and Sumit Basu[2] — [1]Department of Mechanical Engineering, Indian Institute of Technology, Kanpur, India — [2]Department of Mechanical Engineering, Indian Institute of Technology, Kanpur, India

Under uniaxial compression, the stress-strain responses of glassy amorphous polymers exhibit a yield drop followed by hardening at large strains. The extent of the yield drop and the steepness of the hardening response seem connected to the polymer's molecular architecture. Moreover, these materials exhibit strain rate sensitivity, pressure-dependent yielding, and somewhat peculiar unloading behaviour. The connections between the molecular architecture of the glassy amorphous polymer and its uniaxial compressive response are not well understood.

Micromechanically motivated constitutive models proposed by various authors are often able to negotiate many of the subtle aspects of the stress-strain behaviour but need to incorporate several fitting parameters to do so. We attempt to probe the physical processes and the effect of the underlying macromolecular force fields that lead to the typical stress-strain response through well-designed molecular dynamics (MD) simulations. Moreover, using a recently developed probe for quantifying the entanglement structure of the polymer, we show that the large strain uniaxial behaviour is governed by disentanglements and entanglement slips that invariably accompany deformation.

DY 13.4 Mon 17:15 H 0107

Sampling energy landscapes through resistance fluctuations in germanium telluride glass — •Sebastian Walfort, Jakob Ballmaier, Nils Holle, and Martin Salinga — University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Str. 10, 48149 Münster

Germanium telluride (GeTe) is a fragile glass former with a large electrical property contrast between a conductive crystalline phase and highly resistive glass states. It is further possible to repeatedly amorphize and crystallize a nanoscopic, confined volume by applying short voltage pulses, which makes GeTe an interesting model system for observing glassy dynamics. For instance, physical aging following melt-quenching of GeTe glass seems to manifest in a continued evolution of the electronic properties, e.g. in a power-law-like increase of the resistivity. In this experimental study, resistance serves as the observable to probe the structural dynamics of the glass. We demonstrate

that, as a consequence of reducing the nanoscopic amorphous volume, individual resistance states can be resolved in time. The fluctuations between these states are measured over a wide temperature range, six orders of magnitude in time and modeled as a (hidden) Markov process. The resulting attempt frequencies and activation energies reveal a complex free energy landscape, where transitions between states are governed by both energetic and entropic contributions to energy barriers. Beyond their relevance for electronic memory applications, these results illustrate the feasibility of the experimental approach to probe the energy landscape of a glass through a fluctuating resistance

DY 13.5 Mon 17:30 H 0107

A self-consistent current response theory of jamming and vibrational modes in low-temperature amorphous solids — •Florian Vogel, Philipp Baumgärtel, and Matthias Fuchs — University of Konstanz, Konstanz 78464, Germany

Topologically disordered solids exhibit characterisitc anomalies like sound attenuation in the absence of thermal fluctuation and deviations from Debye*s law in the density of states. We present a novel mode-coupling approach to the understanding of athermal amorphous solids, which goes beyond the usual self-consistent Born approximation. To successfully predict the correct sound attenuation, we had to take correlated fluctuations into account. The resulting first principle theory successfully describes the jammed phase. It can also be mapped to the schematic theory [1] of the Euclidean-random-matrix model introduced by Parisi and co-workers [2] and provides a sound description of the unjammed athermal phase and our predictions for the critical dynamics agree with simulations. Most importantly, we manage to describe the unjamming transition without having to rely on negative eigenvalues of the Hessian. The softness of our systems expresses itself as a vanishing dispersion relation, which always stays non-negative. Our theory is in qualitative and semi-quantitative agreement with the numerical solutions of the ERM-model.

References

[1] F. Vogel and M. Fuchs. Phys. Rev. Lett., 130:236101, 2023.

[2] M. Mézard, G. Parisi, and A. Zee. Nuclear Physics B, 559(3):689*701, 1999.

DY 14: Quantum Coherence (joint session TT/DY)

Time: Monday 16:15–18:00 Location: H 3025

Invited Talk DY 14.1 Mon 16:15 H 3025

Quantum thermodynamics and its statistical mechanics: Facts, debatable issues and still unsolved problems — •Peter Hänggi — 1 University of Augsburg, Dept. Physics, 86159 Augsburg, Germany

The present state of the art of this topic contains several subtleties, pitfalls, inconsistencies as well as still open issues. Those are present in both, classical and quantum settings. Even at manifest thermal equilibrium, these thermodynamic notions become surprisingly tricky when strong system-bath interactions matter. A particular intriguing difficulty comprises the notorious invasive character of quantum measurements; i.e., the role of quantum back-action. Fact is: If anything can be said at all, - it preferably should be stated most clearly (Ludwig Wittgenstein, 1889-1951).

[1] D. Castelvecchi, Nature 543 (2017) 597 ; Z. Merali, Nature 551 (2017) 20

[2] P. Hänggi and P. Talkner, Nature Physics 11 (2015) 108

[3] P. Talkner and P. Hänggi, Phys. Rev. E 93 (2016) 022131

[4] P. Talkner and P. Hänggi, Rev. Mod. Phys. 92 (2020) 041002.

DY 14.2 Mon 16:45 H 3025

Efficiency of pulsed electron spin resonance protocols for quantum state storage with phosphorus donors in silicon — •Patricia Oehrl[1,2], Nadezhda Kukharchyk[1,2,3], Kirill G. Fedorov[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Garching, Germany — [3]Munich Center for Quantum Science and Technologies (MCQST), Munich, Germany

The storage of quantum states is considered to be a key element for the successful realization of a multimode quantum network [1]. Solid-state spin ensembles, such as phosphorus donors in silicon, offer exceptional coherence times and resonant transitions in the GHz range [2]. Therefore, they are promising candidates for the realization of quantum memories without frequency conversion techniques. Here, we present a hybrid system consisting of a superconducting lumped-element microwave resonator coupled to a phosphorus donor electron spin ensemble hosted in isotopically engineered silicon. We use continuous-wave spectroscopy complemented by pulsed excitation and time-domain detection techniques. To this end, we operate our hybrid system at millikelvin temperatures and moderate static magnetic fields. We investigate the performance of our hybrid system with regard to quantum memory applications by analyzing the storage efficiency based on various pulse shapes and sequences.

[1] M. Pompili et al., Science 372 (2021) 6539

[2] M. Steger et al., Science 336 (2012) 1280

DY 14.3 Mon 17:00 H 3025

Characterization of hyperfine transitions of rare-earth spin ensembles via broadband ESR spectroscopy at mK temperatures — •Ana Strinic[1,2,3], Patricia Oehrl[1,2,3], Owen Huisman[4], Hans Huebl[1,2,3], Rudolf Gross[1,2,3], and Nadezhda Kukharchyk[1,2,3] — [1]Walther-Meissner-Institute, Bavarian Academy of Sciences and Humanities, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, Munich, Germany — [4]Delft University of Technology, Delft, The Netherlands

Hybrid quantum systems consisting of a superconducting quantum processor coupled to a quantum memory (QM) offer great potential for quantum computing [1]. For interfacing the two components, a microwave (mw) QM is advantageous, since losses due to frequency transduction can be avoided. A potential platform for mw QMs are rare-earth spin ensembles, due to their hyperfine transitions in the GHz regime, which exhibit long coherence times [2]. In this work, we study the hyperfine transitions in ^{167}Er:^{7}LiYF$_4$ using broadband microwave spectroscopy employing a coplanar waveguide. The high resolution ESR spectra obtained at 10 mK allow to quantify the parameters of the spin Hamiltonian, in particular the hyperfine and quadrupole coefficients. Moreover, this technique allows to directly address various hyperfine transitions at their zero first-order Zeeman points, which is key for the implementation of mw QM schemes.

[1] E. Gouzien, N. Sangouard, Phys. Rev. Lett. 127 (2021) 140503

[2] P.Y. Li et al., Phys. Rev. Appl. 13, 024080 (2020)

DY 14.4 Mon 17:15 H 3025

Dichroic cavity mode splitting and lifetimes from interactions with ferromagnetic metal — •Henning G. Hugdal, Eirik Jaccheri Høydalsvik, and Sol H. Jacobsen — Center for Quantum Spintronics, Department of Physics, NTNU, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

We study the effect of ferromagnetic metals (FM) on the circularly polarized modes of an electromagnetic cavity and show that broken time-reversal symmetry leads to a dichroic response of the cavity modes. In the simple model of only one spin split band, the Zeeman coupling between the FM electrons and cavity modes leads to an anticrossing for mode frequencies comparable to the spin splitting. However, this is only the case for one of the circularly polarized modes, while the other is unaffected by the FM. Hence, the cavity photons display a dichroic response to the presence of the FM, allowing for the determination of the spin-splitting of the FM using polarization-dependent transmission experiments. Moreover, using a spin-split two-band model, we show that also the lifetimes of the cavity modes display a polarization dependent response. The reduced lifetime of modes of only one polarization could potentially be used to engineer and control circularly polarized cavities.

DY 14.5 Mon 17:30 H 3025

Diagrammatic approach to quantum heat transport in the quantum Rabi model — •Luca Magazzu[1], Elisabetta Paladino[2,3], and Milena Grifoni[1] — [1]University of Regensburg — [2]Università di Catania, Italy — [3]INFN, Sez. Catania, Italy

A diagrammatic approach to quantum transport in Liouville space, valid for bosonic/fermionic environments, is applied to bosonic heat transport in the quantum Rabi model. Heat transport at weak interaction with the heat baths is controlled by the qubit-oscillator coupling g. Universality of the linear conductance versus the temperature is found below a coupling-dependent Kondo-like temperature.

At low temperature, coherent 4th-order processes dominate transport yielding a T^3 behavior for the thermal conductance κ. In the high-temperature regime, incoherent emission/absorption processes constitute the main transport mechanism, giving resonant peaks, at low g, when the qubit frequency matches the one of the oscillator. In these conditions, the spectrum of the Rabi model displays quasi-degeneracies that produce non-vanishing coherences at the steady state which, in turn, impact κ.

In moving from the weak to the ultrastrong qubit-oscillator coupling regime, the low-T conductance converges to the one of an effective two-level system. At high T, κ makes a transition from a resonant peak to a broad, zero-bias peak regime, a behavior that parallels the one found for the spin-boson model at strong qubit-bath coupling.

DY 14.6 Mon 17:45 H 3025

An on-demand source of energy-entangled electrons using Levitons — Bruno Bertin-Johannet, Laurent Raymond, •Flavio Ronetti, Jérôme Rech, Thibaut Jonckheere, Benoît Grémaud, and Thierry Martin — Aix-Marseille Univ, Université de Toulon, CNRS, CPT, Marseille, France

The on-demand generation of single- and few-electron states in mesoscopic systems has opened the way to the fascinating field of electron quantum optics (EQO), where individual fermionic quantum states are manipulated with methods borrowed from photonic quantum-optical experiments. In this framework, a train of Lorentzian voltage pulses represents one of the most reliable experimental protocol to inject coherent single-electronic states, known as Levitons, into ballistic channels of meso-scale devices. In this talk, we will discuss how the propagation of Levitons is affected by the presence of correlations between electrons and how these effects can be exploited in potential applications for quantum electronics and quantum information. We propose a device where EQO is combined with a BCS superconductor – a reservoir of Cooper pairs. With spin polarized wave guides, this version of the Cooper pair beam splitter is driven by an AC drive, and observables such as period-averaged noise are computed using a Keldysh-Nambu-Floquet formalism. This allows to propose an on-demand source of non-local energy-entangled states. By measuring current fluctuations we propose a way to observe the entangled nature of this state.

DY 15: Active Matter II (joint session BP/CPP/DY)

Time: Tuesday 9:30–13:00 Location: H 1028

DY 15.1 Tue 9:30 H 1028

Disorder-induced cooperative behaviour in aligning self-propelled particle systems — •Eloise Lardet and Thibault Bertrand — Imperial College London, London, UK

In 1995, Vicsek et al. wrote a seminal paper describing a simple model that displays a transition from disorder to collective ordered behaviour. It describes a system of self-propelled point particles that align with their neighbours within a certain radius. This minimal model displays rich nonequilibrium behaviours such as flocking and banding. Inspired by the random couplings of spin glass models, I present numerical findings of introducing Gaussian distributed pairwise couplings into a self-propelled particle system. Through adding further disorder by increasing the standard deviation of the Gaussian distribution that the couplings are drawn from, we are able to observe the emergence of global polar order in systems where the majority of couplings are anti-aligning.

DY 15.2 Tue 9:45 H 1028

Swarming of self-steering and responsive active particles — •Rajendra Singh Negi, Roland G. Winkler, and Gerhard Gompper — Theoretical Physics of Living Matter, Institute of Biological Information Processing (IBI-5), Forschungszentrum Jülich, 52425 Jülich, Germany

The collective behavior of self-propelled agents emerges from the dynamic response of individuals to various input signals [1,2]. In our model of intelligent active Brownian particles (iABPs), information about the position and orientation of neighboring particles, obtained through directed visual and isotropic perception, respectively, is used to adjust the propulsion direction. The maneuverability due to visual signal and polar alignment determines the self-organization. Several non-equilibrium structures like worms, milling, compact, and dispersed clusters are obtained at different parameter sets [2]. As the strength of polar alignment increased compared to visual maneuverability, worm structures dominate over compact structures. Our results help to understand the collective behavior of cognitive self-propelled particles, like animal herds and micro-robotic swarms.

[1]. R. S. Negi, R. G. Winkler, and G. Gompper, Emergent collective behavior of active Brownian particles with visual perception, Soft Matter **18**, 6167 (2022).

[2]. R. S. Negi, R. G. Winkler, and G. Gompper, Collective behavior of self-steering particles with velocity alignment and visual perception, (2023) arXiv:2308.00670 .

DY 15.3 Tue 10:00 H 1028

Effect of cell-cell interactions on the collective behaviour of gliding *Chlamydomonas* populations — •Alexandros Fragkopoulos, Justin Nevells, Timo Völkl, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

Cilia and flagella represent universal tools enabling cells and microbes to propel themselves in diverse environments. In the case of the unicellular biflagellated microbe *Chlamydomonas reinhardtii*, the flagella are used not only to swim in the surrounding medium, but also to adhere to surfaces. In this adhered state, a second flagella-mediated motility mode is observed, during which the cells glide along the surface. This is achieved by means of force transduction through an intraflagellar transport machinery. We recently showed that gliding *C. reinhardtii* cells form weak clusters, most likely assisted by mechanosensing of their flagella [1]. Here we show that *Chlamydomonas noctigama*, a close relative of *C. reinhardtii*, exhibits significantly stronger cell-cell interactions, resulting in pronounced cell clustering even at low densities. In addition, we observe that *C. noctigama* preferentially attach nearby other cells. Finally, we use morphological tools to quantify and compare the clusters to *C. reinhardtii*. By understanding the changes of the cell-cell interactions between the species, we aim to dissect their contribution to the observed cell clustering.

[1] Till et al., *Phys. Rev. Res.* **4**, L042046 (2022).

DY 15.4 Tue 10:15 H 1028

Magnetic colloidal crystals activated by light-driven bacteria — •Helena Massana-Cid[1], Claudio Maggi[1,2], Giacomo Frangipane[1], and Roberto Di Leonardo[1,2] — [1]Department of Physics, Sapienza University of Rome, Rome, Italy — [2]NANOTEC-CNR, Institute of Nanotechnology, Rome, Italy

Active solids, or self-propelling units elastically coupled on a lattice, are recently of growing interest and are predicted to show emerging out-of-equilibrium behaviour, while they can inspire the design of numerous applications. We show for the first time an experimental realisation of a large ordered active solid with activity and confinement tuneable in-situ and on-command. This two-dimensional active solid is composed of repulsive magnetic particles activated by a photokinetic bacterial bath. The bacteria induce active motion into the crystal by pushing its particles and, in a simplified picture, this can be described by an equilibrium state with a higher effective temperature. Nevertheless, this framework breaks down qualitatively because of the active fluctuations time correlations due to the persistent motion of bacteria. We explore the emerging dynamics of this active solid for different values of activity, controlled by the applied light, and repulsion strength, determined by the external magnetic field. Furthermore, we show how we can melt the crystal by increasing activity. Our findings pave the way to unveil the properties of a novel out-of-equilibrium system, an active colloidal solid, which presents questions vastly interesting from a statistical mechanics point of view.

DY 15.5 Tue 10:30 H 1028

Billiards with Spatial Memory — Thijs Albers, Stijn Delnoij, Nico Schramma, and •Mazi Jalaal — Institute of Physics, University of Amsterdam, Amsterdam, The Netherlands

It has been proposed that spatial memory can lead to more efficient navigation and collective behaviour in biological systems. This raises important questions about the fundamental properties of dynamical systems with spatial memory. We present a framework based on mathematical billiards in which particles remember their past trajectories and react to them. Despite the simplicity of its fundamental deterministic rules, such a system is strongly non-ergodic and exhibits highly-intermittent statistics, manifesting in complex pattern formation. We show how these self-memory-induced complexities emerge from the temporal change of topology and the consequent chaos in the system. We study the fundamental properties of these billiards and particularly the long-time behaviour when the particles are self-trapped in an arrested state. We exploit numerical simulations of several millions of particles to explore pattern formation and the corresponding statistics in polygonal billiards of different geometries. Our work illustrates how the dynamics of a single-body system can dramatically change when particles feature spatial memory and provide a scheme to further explore systems with complex memory kernels.

DY 15.6 Tue 10:45 H 1028

Chemical communication in suspensions of active particles — •Nils Göth and Joachim Dzubiella — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany

Chemical communication of bacteria plays an important role in their individual and collective behavior. Here, we study how a simple form of interparticle communication influences a system of colloidal particles. We employ two-dimensional Brownian dynamics simulations of a model of Responsive Colloids, in which the particle size and the internal proton concentration are explicit internal degrees of freedom. The communication between the particles is modeled as a chemical field around each particle to which the other particles respond by changes in their size. We find a rich behavior of structures, including pseudo-regular oscillations and longitudinal waves.

15 min. break

DY 15.7 Tue 11:15 H 1028

Structural Colour from Collective Gliding Bacteria Motion — •Junwei Wang[1], Marina Portoghese[2], Laura Caton[2], Colin Ingham[3], and Silvia Vignolini[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]University of Cambridge, Cambridge, UK — [3]Hoekmine BV, Utrecht, Netherland

We report a type of marine, non-pathogenic, gliding bacteria, Flavobacterium Iridescent 1 (IR1), that grows into a dense active liquid crystal colony, exhibiting structural colour. We demonstrate different crystalline phases arising from collective bacteria motility correlate with varied optical appearances of the colony. We show the hierarchical collective motions of the rod-like bacteria that organize into clusters, monolayer, multi-layers and finally into large scale vortices. We also illustrate how the bacteria colony adapts to confinement of different geometries.

DY 15.8 Tue 11:30 H 1028

Chiral active molecules in traveling activity waves — •Bhavesh Valecha[1] and Abhinav Sharma[1,2] — [1]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [2]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, 01069 Dresden, Germany

Directed motion is crucial for the survival and maintenance of life-supporting functions of numerous biological systems, e.g., motion of sperms towards the egg during fertilisation or movement of immune cells to fight-off an infection. While systematic studies of chiral active molecules simulating crucial aspects of these systems in stationary activity gradients do exist [1-3], the majority of physical scenarios revolve around activity fields that vary with time. So, in this project we study the simplest possible case of an active molecule, the active dimer, in a propagating activity wave. We show that this simple molecule can show very rich emergent tactic behaviour using a cooperative mechanism between the two active chiral particles. In particular, this dimer can, on average, move along with the wave, against the wave motion or not move at all depending on the magnitude of chiral torque and the wave speed. We believe that this study can provide important insights into the design principles of hybrid bio-molecular devices of the future.

[1] P. L. Muzzeddu, H. D. Vuijk, H. Löwen, J.-U. Sommer, and A. Sharma, J. Chem. Phys. **157**, 134902 (2022)

[2] H. D. Vuijk, S. Klempahn, H. Merlitz, J.-U. Sommer, and A. Sharma, Phys. Rev. E **106**, 014617 (2022)

[3] H. Merlitz et al., J. Chem. Phys. **148**, 194116 (2018)

DY 15.9 Tue 11:45 H 1028

Physical principles of space allocation in an active biofluid — •Sebastian W. Krauss, Mithun Thampi, Pierre-Yves Gires, and Matthias Weiss — Experimental Physics I, Bayreuth, Germany

Living matter has the remarkable ability to self-organize into distinct cellular entities that ultimately form the building blocks of organisms. The organisation in multi-cellular systems emerges by replicating a single fertilized oocyte as template structure in multiple division cycles. In contrast, recent studies on Xenopus egg extracts have shown that an active biofluid that is devoid of template structures and genetic material can spontaneously self-organize into compartments in an ATP-driven fashion even when protein synthesis is blocked. The emerging compartments (protocells) are distinct, lack a confining membrane envelope, and vanish after all ATP has been consumed. Here, we show that protocell geometry is determined by a random-packing process with a coarse-graining dynamics that is similar to two-dimensional foams [Development 150, dev200851 (2023)]. Protocell sizes are seen to be tunable by altering the dynamics of microtubules while preserving geometric features of the pattern. Confining the self-organizing fluid in ellipsoidal microfluidic cavities, i.e. mimicking natural confinements like those in embryos, pattern formation is seen to adapt to the confinement, exhibiting a surprising similarity to spatial compartmentalization in early embryos. Further, we observe that an increasing aspect ratio of the chamber results in the formation of smaller protocells. Our results indicate that mechanical cues and simple self-organization principles are key ingredients in many developmental processes.

DY 15.10 Tue 12:00 H 1028

Foams Come to Life — •Ivan Maryshev[1], Filippo De Luca[1,2], and Erwin Frey[1] — [1]Ludwig-Maximilians-Universität München, München, Germany; — [2]University of Cambridge, Cambridge, United Kingdom

Recent experiments on active filament mixtures revealed a new non-equilibrium phase called active foam, consisting of a continuously reconfiguring network of bilayers [1]. The existence of similar structures was previously predicted in phenomenological models [2]. Here we introduce a microscopic model for microtubule-motor mixtures and rigorously derive a hydrodynamic theory that recapitulates the experimental observations. We explain the observed instabilities and associated mechanisms. Finally, we discuss various forms of foam that can be realized in different active matter systems and classify them according to the symmetry and order parameters involved. This research contributes to our understanding of the complex behavior exhibited by active foams and provides insights into their dynamics.

[1] B. Lemma, N. P. Mitchell, R. Subramanian, D. J. Needleman, and Z. Dogic (2022). Active microphase separation in mixtures of microtubules and tip-accumulating molecular motors. Phys. Rev. X 12(3), 031006.

[2] I. Maryshev, A. Morozov, B. Goryachev, and D. Marenduzzo (2020). Pattern formation in active model C with anchoring: bands, aster networks, and foams. Soft Matter 16(38), 8775-8781.

DY 15.11 Tue 12:15 H 1028

Modelling cancer metastasis with active nematics — •Josep-Maria Armengol-Collado[1], Luca Giomi[1], Oleksandr Chepizhko[2], Stephanie Alexander[3], Esther Wagena[3], Bettina Weigelin[3], Peter Friedl[3], Stefano Zapperi[4], and Caterina A.M. La Porta[5] — [1]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [2]Faculty of Physics, University of Viena, Boltzmanngasse 5, Viena, Austria — [3]Department of Medical Biosciences, Sciences, Radboud University Medical Centre, 6525 GA Nijmegen, The Netherlands — [4]Center for Complexity and Biosystems, Department of Physics, University of Milan, via Celoria 16, 20133 Milan, Italy — [5]Center for complexity and Biosystems, Department of Environmental Science and Policy, University of Milan, via Celoria 10, 20133 Milan, Italy

Tumor invasion is characterized by the coordinated movement of cancer cells through complex tissue structures. Here, we focus on recent in vivo experiments where metastasis is observed through the dermis of a living mouse, and low-cohesive modes of collective migration

have been identified. Interestingly, local rotational patterns give rise to antiparallel flow tracks that deform the extracellular matrix and establish a sustained flow of cells. To model this phenomenon, we employ the framework of nematic liquid crystals in the so-called "active turbulence" regime. Analysing the effects of confinement and the role of topological defects we provide significant insights to better understand the underlying mechanisms of cancer cell migration.

DY 15.12 Tue 12:30 H 1028

Flow Localization on Active Ordered Surfaces — •Rushikesh Shinde[1], Raphael Voituriez[2], and Andrew Callan-Jones[1] — [1]Laboratoire de Matière et Systèmes Complexes, Université de Paris Cité and CNRS, Paris, France — [2]Laboratoire de Physique Théorique de la Matière Condensée, Sorbonne Université and CNRS, Paris, France

During morphogenetic processes, active flows occur in the plane of curved tissues. Tissues often exhibit orientational order, and topological defects arise during tissue development. We have studied the behavior of a +1 defect in a film of active ordered fluid on a curved axisymmetric surface. We find strikingly different physics compared with the flat-space variant of the problem, in which extensile activity causes vortex-like or aster-like integer defects to undergo spiral ordering and rotational motion. We focus in particular on the influence of extrinsic curvature in the elastic free energy, usually neglected in theories of ordered fluids on curved surfaces. We consider two biologically-relevant surfaces: a capped-tube-like rigid surface, similar to epithelial tubes; and a bump on an otherwise flat plane. In the first case, we find that the activity threshold for instability becomes independent of system size, and spontaneous rotational flows become localized. In the latter case, we find that an aster can be passively unstable towards a spiral state, and as a result, contractility-driven active flows are thresholdless and localized. High contractility extinguishes the flow and restores the aster. Surprisingly, for high enough saddle curvature, the spiral to aster transition shifts from continuous to discontinuous.

DY 15.13 Tue 12:45 H 1028

Self-Organization in Quorum-Sensing Active Matter: The Interplay between Nonreciprocity and Motility — •Yu Duan[1], Jaime Agudo-Canalejo[1], Ramin Golestanian[1,2], and Benoît Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Over the past years, the generation of interactions breaking action-reaction symmetry has emerged as new paradigm for active matter. The generalization of the Cahn-Hilliard theory of phase separation to nonreciprocal mixtures predicts the emergence of traveling states that break time reversal symmetry when intra-species attraction leads to demixing while chasing inter-species interactions are present. Here, we study a minimal model of active phase separation involving two species of particles regulating their self-propulsion speed via quorum-sensing rules, and identify a mechanism for dynamical pattern formation that does not rely on the standard route of intra-species effective attractive interactions. Instead, our results reveal a highly dynamical phase of chasing bands induced only by the combined effects of self-propulsion and nonreciprocity in the inter-species couplings. Turning on self-attraction, we find that the system may phase separate into a macroscopic domain of such chaotic chasing bands coexisting with a dilute gas. We show that the chaotic dynamics of bands at the interfaces of this phase-separated phase results in anomalously slow coarsening.

DY 16: Nonequilibrium Quantum Systems 1 (joint session TT/DY)

Time: Tuesday 9:30–13:00 Location: H 3005

DY 16.1 Tue 9:30 H 3005

Periodically Driven Heavy-Fermion Systems — •Michael Turaev[1] and Johann Kroha[1,2] — [1]Physikalisches Institut, Universität Bonn, Germany — [2]School of Physics & Astronomy, University of St. Andrews, UK

In this work we study the effects of terahertz (THz) light irradiation on heavy-fermion systems. A typical model for such systems is the periodic Anderson model where strongly repulsive, localized electrons in the 4f shell of rare-earth ions hybridize with a sea of conduction electrons. The Kondo effect induces a new flat band of heavy-fermions, near the Fermi energy. Applying a stationary THz light field induces a time-periodic hybridization between the conduction and the 4f electrons, rather than a modulation of the on-site 4f energy, due to the dipole selection rules. On one hand, the Floquet theorem predicts that the periodic driving produces replicas of the Kondo resonance, centered around multiples of the driving frequency. However, the THz light field could also break up the Kondo singlets, thereby destroying the heavy-fermion state altogether.

To analyze such a scenario we use the non-equilibrium dynamical mean field theory (DMFT), combined with the Floquet-Keldysh Green function method. We obtain that for weak driving compared to the bare hybridization, the Kondo effect is preserved and Floquet replicas of the heavy-fermion bands are observed. However, a strong driving can lead to an efficient suppression of the Kondo effect where the spectral weight of the flat band is reduced.

DY 16.2 Tue 9:45 H 3005

Stabilization of a paramatrically driven BEC: an open quantum system approach — •Larissa Schwarz, Simon B. Jäger, and Sebastian Eggert — Physics Department and Research Center OPTIMAS, University of Kaiserslautern-Landau, Germany

We theoretically analyze the effects of periodically modulated repulsive interactions in a Bose-Einstein condensate (BEC) that features intrinsic damping mechanisms. We derive a master equation describing the dynamics of the momentum modes of the BEC in the parameter regime of weak driving strengths. Above a threshold for the modulation strength we find that the BEC becomes unstable. Below this threshold the combination of damping and periodic driving guides the system into a stationary state that shows an enhancement of fluctuations for specific momentum modes that can be controlled by the driving frequency. We analyze the stationary state of these fluctuations, quantify the condensate depletion and analyze the squeezed and anti-squeezed quadratures generated by the parametric driving, emphasizing the possibility to generate non-classical states of matter.

DY 16.3 Tue 10:00 H 3005

Charge density wave melting in higher dimensional Holstein models — •Eva Paprotzki[1], Alexander Osterkorn[2], Vibhu Mishra[3], and Stefan Kehrein[3] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Institut "Jožef Stefan", Ljubljana, Slovenien — [3]Institut für Theoretische Physik, Georg-August-Universität Göttingen

We study the Holstein model after a quench from the insulating charge density wave (CDW) state. Employing a semiclassical treatment of the phonons ('Truncated Wigner Approximation'), we are able to track the CDW order parameter in two- and three-dimensional systems. The number of dynamical variables increases only quadratically with system size. We pose the question whether the order parameter dynamics in higher-dimensional lattices can be connected to the dynamics of the one-dimensional case via factorization. Next to an analytical estimation for the time scale of such a relation, we provide numerical evidence for the weak and strong coupling regime based on our semiclassical methods. An additional semiclassical description of the electrons ('fermionic Truncated Wigner Approximation') yields better agreement with exact reference data in one spatial dimension for the order parameter and, in particular, for the phonon number than the approach with purely phononic semiclassical dynamics.

DY 16.4 Tue 10:15 H 3005

Quantum geoemtry and dynamics in in-homogeneous fields — •Chen Xu[1,2], Andreas Haller[1], Suraj Hegde[2], Tobias Meng[2], and Thomas L. Schmidt[1] — [1]Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Faculty of Physics, TU Dresden, Germany

We revisit the problem of nonequilibrium semiclassical electron transport in the presence of inhomogeneous external perturbations. For this purpose, we study the quantum geometry of Bloch band structure beyond the Berry connection contribution. We provide a systematic way of obtaining semiclassical equations of motion in an N-band system

and for higher order variations in inhomogeneities, we compute geometric corrections containing for example Berry phase and quantum geometric tensor. We also demonstrate how to derive the dynamics from a generic coupling between Bloch momentum and an inhomogeneous external field, thus generalizing previous studies.

DY 16.5 Tue 10:30 H 3005

Non-equilibrium Eliashberg theory for photon-mediated superconductivity — •Michele Pini[1], Christian H. Johansen[1,2], and Francesco Piazza[3,1] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland — [3]Institute of Physics, Universität Augsburg, 86159 Augsburg, Germany

In the recent years, new mechanisms have been proposed to induce photon-mediated superconductivity in a non-thermal steady-state. Within these settings, the photon-electron interaction which generates the pairing can assume a form analogous to an electron-phonon interaction. This suggests a description of the superconducting phase transition within Eliashberg theory, similarly to phonon-mediated superconductivity. However, as soon as photons and electrons are pulled away from mutual equilibrium, a standard Matsubara formulation of Eliashberg theory becomes impossible. To tackle this issue, we derive a more general non-equilibrium version of Eliashberg theory. We then apply this theory to describe the superconducting phase transition in a generic non-thermal steady-state setting. We present a numerical solution of the non-equilibrium Eliashberg equations and show that bringing the system out of equilibrium can have dramatic effects on the superconducting phase transition.

Note: The authors M. Pini and C. H. Johansen contributed to this work equally.

DY 16.6 Tue 10:45 H 3005

Few-body purity as an arrow of time in the Lanczos picture — •Merlin Füllgraf and Jochen Gemmer — Department of Mathematics/Computer Science/Physics, University of Osnabrück, D-49076 Osnabrück, Germany

The Lanczos method to compute autocorrelation functions in quantum mechanics gives rise to so-called Lanczos coefficients associated with operator growth in the respective systems. These coefficients can be interpreted as hopping amplitudes of a semi-infinite tight-binding model whose first site corresponds to the correlation function itself. In this picture we introduce a few-body purity and study it against the background of an arrow of time. Moreover, we investigate the influence of structures in the Lanczos coefficients on this quantity and propose a qualitative model solely based on these coefficients describing their influence on the systems' dynamics.

[1] D.E. Parker, X. Cao, A. Avdoshkin, T. Scaffidi, E. Altman, Phys. Rev. X 9 (2019) 041017

[2] V.S. Viswanath, G. Müller, The Recursion Method: Applications to Many-Body Dynamics, Springer, New York (2008).

DY 16.7 Tue 11:00 H 3005

Hilbert space fragmentation and slow dynamics in particle-conserving quantum East models — •Pietro Brighi[1], Marko Ljubotina[2], and Maksym Serbyn[2] — [1]University of Vienna, Boltzmanngasse 5, 1090 Vienna Austria — [2]ISTA, am Campus 1, 3400 Klosterneuburg Austria

Quantum kinetically constrained models have recently attracted significant attention due to their anomalous dynamics and thermalization. In this work, we introduce a hitherto unexplored family of kinetically constrained models featuring conserved particle number and strong inversion-symmetry breaking due to facilitated hopping. We demonstrate that these models provide a generic example of so-called quantum Hilbert space fragmentation, that is manifested in disconnected sectors in the Hilbert space that are not apparent in the computational basis. Quantum Hilbert space fragmentation leads to an exponential in system size number of eigenstates with exactly zero entanglement entropy across several bipartite cuts. These eigenstates can be probed dynamically using quenches from simple initial product states. In addition, we study the particle spreading under unitary dynamics, and find faster than diffusive dynamics at high particle densities, crossing over into logarithmically slow relaxation at smaller densities. Our work suggests that particle conserving constrained models with inversion symmetry breaking realize so far unexplored dynamical behavior and invite their further theoretical and experimental studies.

15 min. break

DY 16.8 Tue 11:30 H 3005

Influence of low- and high-energy magnetic excitations on electron dynamics in the vicinity of the Mott transition: a non-equilibrium D-TRILEX study — •Nagamalleswara Rao Dasari[1], Hugo U. R. Strand[2], Martin Eckstein[1], Alexander I. Lichtenstein[1], and Evgeny A. Stepanov[3] — [1]Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9 , 22607 Hamburg, Germany — [2]School of Science and Technology, Orebro University, SE-70182 Obrebo, Sweden — [3]CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

We present a simplified real-time diagrammatic method based on the dual triply irreducible local expansion (D-TRILEX) formalism and apply it to the single-band extended Hubbard model. In the vicinity of Mott-transition, we observed signatures of "water-fall" structures at low-binding energies and sharp dispersive high-energy bands in the momentum-resolved electronic spectrum. In the photo-excitation dynamics, these spectral features melt very slowly on the electronic time scale, allowing us to measure these slow dynamics in the time-resolved photo-emission spectrum. In addition, the electron-magnon interaction in metals manifests through the fast relaxation of electronic kinetic energy due to the rapid thermalization of magnons much earlier than the electron's thermalization time scale. However, in the Mott-insulators, the photo-excited charge carriers transfer their excess kinetic energy to low-energy magnons instead of low-energy electrons (expected for impact ionization), leading to a non-thermal magnon distribution on a typical electronic time scale.

DY 16.9 Tue 11:45 H 3005

Effective time-dependent temperature method for fermionic master-equations — •Lukas Litzba, Eric Kleinherbers, Nikodem Szpak, and Jürgen König — Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany

We consider a quantum system coupled to a fermionic environment at a fixed temperature. Using the Redfield equation with time-dependent coefficients, we analyze the reduced evolution of the system. We find that the time-dependence of these coefficients can be described by an effective time-dependent contact temperature. In this way, we obtain a method which includes non-Markovian effects and can be applied to various types of Gorini-Kossakowski-Sudarshan-Lindblad equations. With this, we discuss its application to a simple setup consisting of quantum dots which may be realized experimentally. At short times, the effective temperature appears to be much higher than the true temperature of the environment but asymptotically it settles down towards the true environment value. This behavior follows from the formation of coherences between the system and the environment for short times, which is related to a transfer of energy from the coupling term of the Hamiltonian into the system.

DY 16.10 Tue 12:00 H 3005

Mean-field Decoupling of Single Impurity Anderson Model through Auxiliary Majorana Fermions — •Irakli Titvinidze[1], Julian Stobbe[1], Alexey N. Rubtsov[2], and Georg Rohringer[1] — [1]I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Moscow

We present a new method to study the time evolution of the single impurity Anderson model. We perform a mean-field decoupling of the impurity and the chain. This is achieved by introducing a pair of auxiliary Majorana fermions between the impurity and the chain. We obtain a self-consistent set of equations for the impurity and the chain. By solving them in equilibrium we obtain a phase transition between phases in which the mean field parameters are zero and we have a well-defined spin on the impurity, and the regime in which the mean field parameters take finite values and there is no well-defined spin. Once we know the equilibrium properties of the system, we quench one or more model parameters and study the time evolution of the impurity and the chain. Within our mean-field treatment, we obtain a coupled set of differential equations for the impurity and chain and find that the results converge to their equilibrium values for most quenches. For very strong interactions, the excitations are trapped and the oscillations never persist.

DY 16.11 Tue 12:15 H 3005

Emergence of unitary symmetry of microcanonically truncated operators in chaotic quantum systems — •jiaozi wang[1], jonas richter[2,3], mats lamann[1], robin steinigeweg[1], jochen

GEMMER[1], and ANATOLY DYMARSKY[4] — [1]U Osnabrück, Germany — [2]U Stanford, USA — [3]LU Hannover, Germany — [4]U Kentucky, USA

We study statistical properties of matrix elements entering the eigenstate thermalization hypothesis by studying the observables written in the energy eigenbasis and truncated to small micro- canonical windows. We put forward a picture, that below certain energy scale collective statistical properties of matrix elements exhibit emergent unitary symmetry. In particular, below this scale the spectrum of the microcanonically truncated operator exhibits universal behavior for which we introduce readily testable criteria. We support this picture by numerical simulations and demonstrate existence of emergent unitary symmetry scale for all considered operators in chaotic many-body quantum systems. We discuss operator and system-size dependence of this energy scale and put our findings into context of previous works exploring emergence of random-matrix behavior in narrow energy windows.

[1] J. Wang, M. Lamann, J. Richter, R. Steinigeweg, A. Dymarsky, J. Gemmer, Phys. Rev. Lett. 128 (2022) 180601
[2] J. Wang, J. Richter, M. H. Lamann, R. Steinigeweg, J. Gemmer, A. Dymarsky, arXiv: 2310.20264 (2023)

DY 16.12 Tue 12:30 H 3005

Periodically Driven Spin-1/2 XXZ Antiferromagnetic Chains — •DOMINIC WINDECKER[1], ASLAM PARVEJ[2], and SEBASTIAN EGGERT[1] — [1]University of Kaiserslautern-Landau, Landesforschungszentrum OPTIMAS — [2]Universität Hamburg

Time-periodically driven quantum systems are of great interest due the possibility of unconventional states of matter and Floquet engineering. The interplay of many-body interactions and time-periodic manipulations facilitate new phenomena in the steady state. We analyze the Floquet steady states of finite spin-1/2 XXZ antiferromagnetic chains with periodically driven anisotropy parameter at frequencies below the band width, so that resonances are in principle possible. We use three different numerical real-time approaches (TS1, TS2 and RK4) with an adiabatic time-evolution protocol by ramping up the driving amplitude of the external periodic drive to prepare a non-equilibrium Floquet steady state. Stability, accessibility, preparation and characteristics of parametric resonance states in finite systems are discussed.

DY 16.13 Tue 12:45 H 3005

Tuning the switching behavior of oligophenyls in metal-molecule-metal junctions by fluorine substituents — •SHENGMING ZHANG[1], ZHIQIANG LI[2], JOACHIM REICHERT[1], HAI BI[2], and JOHANNES BARTH[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Jihua Laboratory, Foshan, China

Single-molecule junctions represent a promising avenue in the realm of nanometer-scale electronic device development. Numerous investigations have concentrated on the I-V relationship, which often falls short in fully characterizing a single-molecule junction. In our study, we use Raman spectroscopy as a complementary tool to explore the vibrational states of individual, covalently bound molecules while sweeping the bias. Our focus is on a series of three terphenyl species. The first molecule incorporates four methyl side groups which aim to hinder the planarization of the neutral molecules. The molecules get transiently charged above a certain threshold voltage and coplanarize their phenyl rings. This conformational change goes along with an extension of the π-electron system, increases the polarizability and thus the Raman activity of the molecules significantly. In the second and third molecule, one resp. two methyl groups where fluorine substituted in order to tune the alignment of the HOMO to the Fermi level of the electrodes upon junction formation. This way, we can steer the threshold voltage where transient charging is planarizing the molecule. This approach underscores the tunability of characteristic transport properties in a molecular model system by intricate changes in its molecular structure.

DY 17: Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)

Time: Tuesday 9:30–13:00 Location: A 151

DY 17.1 Tue 9:30 A 151

Non-equilibration, synchronization, and time crystals in isotropic Heisenberg models — •JÜRGEN SCHNACK, PATRICK VORNDAMME, and PETER REIMANN — Bielefeld University

Isotropic, but otherwise largely arbitrary Heisenberg models in the presence of a homogeneous magnetic field are considered, including various integrable, non-integrable, as well as disordered examples, and not necessarily restricted to one dimension or short-range interactions. Taking for granted that the non-equilibrium initial condition and the spectrum of the field-free model satisfy some very weak requirements, expectation values of generic observables are analytically shown to exhibit permanent long-time oscillations, thus ruling out equilibration [1]. If the model (but not necessarily the initial condition) is translationally invariant, the long-time oscillations are moreover shown to exhibit synchronization in the long run, meaning that they are invariant under arbitrary translations of the observable [2]. Analogous long-time oscillations are also recovered for temporal correlation functions when the system is already at thermal equilibrium from the outset, thus realizing a so-called time crystal.

[1] P. Reimann, P. Vorndamme, J. Schnack, Phys. Rev. Research 5, 043040 (2023)
[2] P. Vorndamme, H.-J. Schmidt, Chr. Schröder, J. Schnack, New J. Phys. 23, 083038 (2021)

DY 17.2 Tue 9:45 A 151

Many-body localization in random exchange coupling Heisenberg chain — •YILUN GAO and RUDOLF A. RÖMER — Department of Physics, University of Warwick, Coventry, CV4 7AL

Disordered quantum systems have become an important research topic in modern condensed matter physics ever since the discovery of Anderson localization. The investigation of many-body localization in quantum interacting systems has received much recent attention following the increase of computational power and improvement in numerical methods. We focus on a Heisenberg spin chain with full SU(2) symmetry where the exchange couplings between neighboring spins are taken to be disordered. Sparse matrix diagonalization method is applied when calculating eigenvalues and eigenvectors of the Hamiltonian matrix. By understanding the structure of eigenvalues and eigenvectors in terms of spin symmetry, we investigate the participation ratio and entanglement entropy as a function of disorder strength. We average over many disorder realizations and compare the results for different system sizes. We find, for small system sizes, a clear distinction between the SU(2)-invariant random exchange model and the more often studied random field model.

DY 17.3 Tue 10:00 A 151

Long-range spectral statistics of the Rosenzweig-Porter model — •WOUTER BUIJSMAN — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The Rosenzweig-Porter model is a single-parameter random matrix ensemble that supports an ergodic, fractal, and localized phase. Introduced over sixty years ago, this model recently gained renewed interest as a toy model for the many-body localization transition. We construct a unitary (Floquet) equivalent of this model, for which we numerically study the long-range spectral statistics [1,2]. The construction is based on interpreting the Rosenzweig-Porter model as a Brownian quantum system [3]. Our main result is the observation that the transition between the ergodic and fractal phases can be probed through the spectral form factor. Complementing previous results on the level spacing distribution, this establishes that spectral statistics are sufficient to fully map out the phase diagram of the model. We quantitatively discuss the scaling of the Thouless time, and point out the possible universality of the spectral form factor at the transition between the fractal and the localized phases.

[1] W. Buijsman and Y. Bar Lev, *Circular Rosenzweig-Porter random matrix ensemble*, SciPost Phys. **12**, 082 (2022).
[2] W. Buijsman, *Long-range spectral statistics of the Rosenzweig-Porter model*, arXiv:2309.14043 (2023).
[3] W. Buijsman, *Efficient circular Dyson Brownian motion algorithm,* arXiv: 2309.07457 (2023).

DY 17.4 Tue 10:15 A 151

Interplay of many-body interactions and quasiperiodic disorder in the all-bands-flat diamond chain — •AAMNA AHMED[1], NILANJAN ROY[2], and AUDITYA SHARMA[3] — [1]University of Augsburg,

Germany — [2]Nanyang Technological University (NTU), Singapore — [3]Indian Institute of Science Education and Research (IISER) Bhopal, India

While the physics of flat band systems, quasiperiodic disorder and many-body interactions have been important fields of activity, the interplay of these features has only scantily been explored. This talk will discuss the effect of many-body interactions and quasiperiodic Aubry André (AA) disorder on the one-dimensional all-band-flat (ABF) diamond lattice**[1,2]**.

We show that coupling the ABF diamond lattice with nearest-neighbour interactions yields a non-ergodic phase independent of the strength of interaction. Interestingly, the resulting phases in the interacting diamond lattice depend on the symmetry and the strength of the applied quasiperiodic disorder. An exciting finding is the emergence of non-equilibrium quantum caging behaviour for specially engineered many-body initial states. Our work provides an insight into the phase diagram of an interacting flat band system subjected to quasiperiodic disorder via a non-equilibrium dynamical study.

1. Interplay of many-body interactions and quasiperiodic disorder in the all-band-flat diamond chain, **PRB 107, 245110 (2023)**

2.Flat-band-based multifractality in the all-band-flat diamond chain, **PRB 106, 205119 (2022)**

DY 17.5 Tue 10:30 A 151

Prethermalization in an Interacting Flat Band System — •Mirko Daumann and Thomas Dahm — Universität Bielefeld, Fakultät für Physik, Postfach 100131, D-33501 Bielefeld

Studying the influence of a weakly perturbed flat band on transport of interacting particles reveals anomalous diffusion and prethermalization. For very weak perturbations transport is getting slower than regular diffusion because of repulsive particle-particle interaction. The effect can be understood by a canonical transformation of dispersive and flat band eigenstates into a basis of light and heavy quasiparticles which are trapping each other. They are subjected to orbital conservation laws what enables a treatment of the phenomenon in terms of the Born-Oppenheimer approximation and allows an illustration in a familiar physical picture analogous to electrons and nuclei. This approach furthermore sheds light on the thermalization process in such a system in general.

Methodology: Transport properties are calculated by simulating the broadening of initially localized wave packets of spinless fermions in a quasi one-dimensional Hubbard model with three-orbital diamond structure. Initial states are constructed in the framework of dynamical quantum typicality. Time evolution is performed by either the Lanczos algorithm or full diagonalization if possible.

DY 17.6 Tue 10:45 A 151

Hilbert space fragmentation in anyonic chains — •Ludwig Zweng, Nico Kirchner, and Frank Pollmann — Technical University of Munich (TUM)

Hilbert spaces of chains of non-Abelian anyons are constrained by their fusion rules. These constraints may restrict the dynamics and lead to nontrivial thermalization behavior for such systems. As an examplary anyonic model with restricted thermalization, we suggest a one dimensional Fibonacci anyonic chain where the topological charges can perform braid moves around each other. We identify subspaces in the fusion space of this model which are left invariant by certain braid moves and by fine-tuning an additional magnetic field, we find various dynamically disconnected sectors. These sectors stem from the destructive interference of different braid processes and we expect that this model displays weak Hilbert space fragmentation. Moreover, we show that in global quenches certain initial states do not evolve to thermal states but display fidelity revivals up to late times.

DY 17.7 Tue 11:00 A 151

Quantum dynamical phase transition in Erdos-Renyi graph — •Tomohiro Hashizume[1], Felix Herbort[1], Joseph Tindall[2], and Dieter Jaksch[1] — [1]CUI, institute of quantum physics, University of Hamburg, Hamburg, Germany — [2]Centre for Computational Quantum Physics, Flatiron Institute, New York, USA

With the lack of the well-defined free energy, the dynamics of a closed quantum system reaching its equilibrium state is not constrained by the conventional statistical mechanical pricniples. In the light of expanding the temperature into the complex domain, the dynamical quantum phase transition manifests itself as non-analyticities in the logarithm of the survival probability of the initial state before the quench. Based on the duality between the equilibrium quantum phase of the transverse field Ising model and the same model on the probablistic random graph (Erdos-Rényi graph), we expand this duality to the non-equilibrium regime and study the dynamical phase transition in these models. We show that despite the consistency of the dynamical critical point for all probability of edge generalation, p, the anomality of the transition ceases to exist upon averaging the echo over all possible graphs for $p < 1$.

15 min. break

DY 17.8 Tue 11:30 A 151

Semiclassical eigenstate entanglement of bipartite Floquet systems — •Maximilian F.I. Kieler and Arnd Bäcker — TU Dresden, Institute of Theoretical Physics, Dresden, Germany

Strongly coupled quantum systems are expected to show the same amount of entanglement as random states. However, many body systems typically have an inherent multi-partite structure, and it is not clear, how this influences the entanglement. We show for the case of chaotic, bipartite quantum maps, that the eigenstate entanglement coincides up to leading order with the random matrix result. For this the eigenstate entanglement is transferred into a dynamical quantity and evaluated using semiclassical methods. The result is given in terms of periodic orbits of the subsystems. Interestingly, the coupling acts as synchronization between these orbits, only.

DY 17.9 Tue 11:45 A 151

Floquet-Anderson localization in the Thouless pump and how to avoid it — András Grabarits[1,2], Attila Takács[1,3], Ion Cosma Fulga[4,5], and •János K. Asbóth[1,6] — [1]Dept of Theor. Physics, Budapest University of Technology and Economics — [2]Dept of Physics and Materials Science, University of Luxembourg — [3]Universite de Lorraine, CNRS, Nancy, France — [4]Leibniz Institute for Solid State and Materials Research, IFW Dresden, — [5]Wurzburg-Dresden Cluster of Excellence ct.qmat, 01062 Dresden — [6]Wigner Research Centre for Physics, Budapest

We investigate numerically how onsite disorder affects conduction in the periodically driven Rice-Mele model, a prototypical realization of the Thouless pump, when run at finite period time T. We find that at any fixed period time and nonzero disorder, increasing the system size L to infinity always leads to a breakdown of the pump by Anderson localization of the Floquet states. In a properly defined thermodynamic limit, where L/T^θ is kept constant, Anderson localization can be avoided, and the charge pumped per cycle has a well-defined value (as long as the disorder is not too strong). The exponent θ is not universal, rather, depends on the disorder strength. Our findings are relevant for practical, experimental realizations of the Thouless pump, for studies investigating the nature of its current-carrying Floquet eigenstates, as well as the mechanism of the full breakdown of the pump, expected if the disorder exceeds a critical value.

DY 17.10 Tue 12:00 A 151

Deviations from random matrix entanglement statistics for kicked quantum chaotic spin-1/2 chains — •Tabea Herrmann, Roland Brandau, and Arnd Bäcker — TU Dresden, Institute of Theoretical Physics, Dresden, Germany

It is commonly expected that for quantum chaotic systems the statistical properties approach those of random matrices with increasing system size. We demonstrate for various kicked spin-1/2 chain models that the average eigenstate entanglement indeed approaches the random matrix result. However, the distribution of the eigenstate entanglement differs significantly. While for autonomous systems such deviations are expected, they are surprising for the more scrambling kicked systems. We attribute the origin of the deviations to the local 2×2 substructure. This is supported by similar deviations occurring in a local random matrix model with global diagonal coupling.

DY 17.11 Tue 12:15 A 151

The entanglement membrane in exactly solvable lattice models — •Michael A. Rampp, Suhail A. Rather, and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Entanglement membrane theory is an effective coarse-grained description of entanglement and operator growth in non-integrable quantum many body systems. The central quantity containing information about the dynamics is the entanglement line tension. However,

determining the entanglement line tension for microscopic models is difficult. We compute the entanglement line tension in a recently introduced class of exactly solvable unitary circuits, and show that it has a non-trivial form giving rise to a hierarchy of velocity scales, $v_E < v_B$. We find that these circuits saturate certain bounds on entanglement growth that are also saturated in holographic models. Furthermore, we relate the entanglement line tension to temporal entanglement and correlation functions. Our results shed light on entanglement membrane theory in microscopic Floquet lattice models and enable us to perform non-trivial checks on the validity of its predictions by comparison to exact calculations.

DY 17.12 Tue 12:30 A 151

Weak eigenstate thermalization hypothesis — Patrycja Łydzba[1], •Rafał Świetek[2,3], Marcin Mierzejewski[1], Marcos Rigol[4], and Lev Vidmar[2,3] — [1]Institute of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, 50-370 Wrocław, Poland — [2]Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia — [3]Department of Theoretical Physics, J. Stefan Institute, SI-1000 Ljubljana, Slovenia — [4]Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA

While the eigenstate thermalization hypothesis (ETH) is well established for quantum-chaotic interacting systems, its validity for other classes of systems remains a matter of intense debate. Focusing on quadratic fermionic Hamiltonians, we here argue that the weak ETH is satisfied for few-body observables in many-body eigenstates of quantum-chaotic quadratic (QCQ) Hamiltonians. In contrast, the weak ETH is violated for few-body observables in localized quadratic Hamiltonians. We argue that these properties can be traced back to the validity of single-particle eigenstate thermalization, and we highlight the subtle role of normalization of operators. Our results suggest that the difference between weak and no ETH in many-body eigenstates allows for a distinction between single-particle quantum chaos and localization. We test to which degree this phenomenology holds true for integrable systems such as the XYZ and XXZ models.

DY 17.13 Tue 12:45 A 151

Critical quantum dynamics of observables at eigenstate transitions — Simon Jiricek[1], •Miroslav Hopjan[2], Patrycja Łydzba[3], Fabian Heidrich-Meisner[1], and Lev Vidmar[2,4] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [2]Department of Theoretical Physics, J. Stefan Institute, SI-1000 Ljubljana, Slovenia — [3]Department of Theoretical Physics, Wroclaw University of Science and Technology, 50-370 Wroclaw, Poland — [4]Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia

It is an outstanding goal to unveil the fingerprints of universal quantum dynamics at eigenstate transitions. Focusing on quadratic fermionic Hamiltonians, we identify physical observables that exhibit critical behavior at the transition. Our result is based on two ingredients: (a) A relationship between the observable time evolution in a many-body state and the transition probabilities in single-particle states, and (b) a scale invariance of transition probabilities, which generalizes the recent result for survival probabilities [1]. We then show that these properties give rise to a critical behavior in the quantum quench dynamics of observables, which share the common eigenbasis with the Hamiltonian before the quench. We numerically demonstrate this phenomenon at the localization transition in the three-dimensional Anderson model, for which the critical bahavior can be detected in experimentally relevant observables such as site occupations and particle imbalance. [1] M. Hopjan and L.Vidmar, Phys. Rev. Lett. 131, 060404 (2023)

DY 18: Pattern Formation, Delay and Nonlinear Stochastic Systems

Time: Tuesday 9:30–13:00 Location: BH-N 128

Invited Talk DY 18.1 Tue 9:30 BH-N 128

Phase field method to model single cell locomotion and collective cell interactions — •Sergio Alonso — Group of Computational Biology and Complex Sytems, Department of Physics, Universitat Politècnica de Catalunya, Barcelona, Spain

The interior of the living cells is complex and different types of processes happens simultaneously. Such dynamics are regulated by biochemical reactions and the dynamics of different biochemical components which are commonly modeled by reaction-diffusion equations. Polarization is typically described by Reaction-Diffusion processes and determines the head and the tail of the motion of the cell. Such process has to be connected with cell deformation and cell locomotion. The definition of a dynamical phase field to determinate the interior of the cell is a common tool for biophysical modelers. Here, I will review this technique and note some application in the case of crawling amoebae.

DY 18.2 Tue 10:00 BH-N 128

Influence of physical interactions on spatiotemporal patterns — •Chengjie Luo, Lucas Menou, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Complex spatiotemporal patterns are often modeled by reaction-diffusion equations, which combine complex reactions between constituents with ideal diffusion. Such descriptions neglect physical interactions between constituents, which might affect resulting patterns. To overcome this, we investigate the influence of physical interactions on two representative chemical reactions: the Hill-Langmuir equation, generating static Turing patterns for ideal diffusion, and cyclic dominant reactions, like the seminal rock-paper-scissors (rps) game, yielding dynamic spiral waves. In the Hill-Langmuir system, we find that weak repulsion substantially lowers the required differential diffusivity and reaction nonlinearity for Turing pattern formation, while strong interactions induce phase separation. For cyclic-dominant reactions, we discover that weak interactions change the length- and time scales of spiral waves. In contrast, strong repulsive interactions typically generate oscillating lattices, and strong attraction leads to an interplay of phase separation and chemical oscillations. Despite the distinct nature of the two chemical reactions, physical interactions play a crucial role in pattern formation in both cases. We thus suggest that physical interactions are crucial for forming spatiotemporal patterns in nature, so they should be incorporated when modeling realistic systems.

DY 18.3 Tue 10:15 BH-N 128

Flower wave patterns in the CHD-BZ reaction in the presence of spatial heterogeneities — Sangram Gore[1], Binaya Paudyal[1], Oliver Steinbock[2], and •Azam Gholami[1] — [1]New York University, Abu Dhabi, UAE — [2]Florida State University, Tallahassee, Florida, USA

In this work, we investigate the effects of millimeter-sized obstacles on the chemical waves in the CHD-Belosouv-Zabotinsky reaction, in which the classical organic substrate malonic acid is replaced by 1,4-cyclohexanedione (CHD). Our experiments show that an arrangement of cylindrical obstacles can significantly influence the chemical waves in the CHD-BZ reaction. We observed circular waves with a period of about 1 min that started almost synchronously at the pillars and propagated outward. However, after two cycles of outward propagating circular waves, wavefront instability sets in and flower patterns form. Interestingly, the number of petals depends on the pillars diameters and is higher for larger diameters. This instability occurs in an open-lid environment where evaporation plays an important role. In a closed lid environment, the waves remain circular and do not break. These experiments underline the importance of evaporation, which, in addition to the chemical concentration gradient, contributes to the formation of Marangoni currents.

DY 18.4 Tue 10:30 BH-N 128

A universal description of stochastic oscillators — Alberto Pérez-Cervera[1], Boris Gutkin[2], Peter J. Thomas[3], and •Benjamin Lindner[4,5] — [1]Universidad Complutense de Madrid,Spain — [2]Ecole Normale Supérieure - Paris Science Letters University, France — [3]Case Western Reserve University, Cleveland, OH, USA — [4]Institut für Physik, Humboldt-Universität zu Berlin — [5]Bernstein Center for Computational Neuroscience Berlin

Systems in physics and biology exhibit oscillations which are shaped by randomness. Dynamically, such stochastic oscillations can be caused

by different mechanisms and are thus described by strongly different mathematical models, e.g. a linear dynamics with a stable focus and noise, limit-cycle systems perturbed by noise, or excitable systems in which random inputs lead to spikes. Here, we introduce a nonlinear transformation of stochastic oscillators to a complex-valued function that greatly simplifies and unifies the mathematical description of the oscillator's spontaneous activity, its response to an external time-dependent perturbation, and the correlation statistics of different, weakly coupled oscillators. The general framework (see Perez-Cervera et al. PNAS 2023) can be applied to the different example dynamics mentioned above but also to higher-dimensional systems such as two damped harmonic oscillators with thermal noise that are strongly coupled.

DY 18.5 Tue 10:45 BH-N 128

Detecting a periodic signal by a population of spiking neurons in the weakly nonlinear response regime — •Maria Schlungbaum[1,2] and Benjamin Lindner[1,2] — [1]Physics Department, Humboldt University Berlin — [2]Bernstein Center for Computational Neuroscience Berlin

Signal detection is a ubiquitous problem in several situations for living organisms. We are specifically interested in detecting a weak signal in the presence of a stronger stimulus and noise – known as cocktail party problem in auditory perception. We simplify this problem here and study the response to two periodic signals by a homogeneous population of stochastic leaky integrate-and-fire (LIF) neurons. Using a threshold-crossing of the population activity as a detection criterion, we show by the means of the receiver operating characteristics (ROC), that the detectability depends strongly on the stimulus amplitude but only weakly on the time window of observation. Interestingly, the detection of a weak periodic signal can be boosted by a strong periodic stimulus. This effect depends on the frequencies of the two signals and the dynamical regime in which the neurons operate. We also present an analytical approximation for the ROC curve based on the weakly nonlinear response theory for a stochastic LIF model.

DY 18.6 Tue 11:00 BH-N 128

Self-organizing patterns in crossing flows of pedestrians — •Pratik Mullick — Wroclaw University of Science and Technology, Wroclaw, Poland

Studying collective dynamics of human crowds are vital for enhancing pedestrian traffic flow, ensuring safety, and effective urban planning. In this research, we focus on the emergence of striped patterns when two streams of pedestrians cross, a manifestation of self-organized collective behavior. Using experimental data, we introduce numerical strategies, such as an edge-cutting algorithm and a Gabor function-based pattern-matching technique to study geometric properties of these patterns. Notably, an invariant property is revealed: stripes in crossing groups are consistently parallel, and perpendicular to the bisector of crossing angle. This work contributes to understanding and modeling crowd behavior, offering insights applicable to diverse scenarios like pedestrian traffic management and crowd safety during mass gatherings. In presenting this research, I aim to share innovative computational methods and findings that advance the comprehension of self-organizing patterns in human crowds.

15 min. break

DY 18.7 Tue 11:30 BH-N 128

Laminar chaos in systems with random delay — •David Müller-Bender[1] and Günter Radons[1,2] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]ICM - Institute for Mechanical and Industrial Engineering, 09117 Chemnitz, Germany

A type of chaos called laminar chaos was found in singularly perturbed dynamical systems with periodically time-varying delay [Phys. Rev. Lett. 120, 084102 (2018)]. It is characterized by nearly constant laminar phases, which are interrupted by irregular bursts, where the intensity levels of the laminar phases vary chaotically from phase to phase. While laminar chaos, which is observed in systems with a so-called dissipative delay, is a low-dimensional phenomenon, its counterpart called turbulent chaos is a high-dimensional type of chaos, which is typically found in systems with conservative (including constant) delays. In this talk, we demonstrate that laminar chaos can also be found in systems with randomly time-varying delay. Moreover, for short time correlated random delay variations it turned out that laminar chaos and its generalizations are observed in almost the whole delay parameter space spanned by the mean delay and the delay amplitude. This means that introducing such a random delay variation into the considered class of systems typically leads to a drastic reduction of the dimension of the chaotic attractor.

DY 18.8 Tue 11:45 BH-N 128

Temporal localized states in an injected Kerr Gires-Tournois Interferometer: The influence of phase modulation. — •Marc Hunkemöller[1], Thomas Seidel[1], Svetlana Gurevich[1,2], and Julien Javaloyes[3] — [1]Institute for Theoretical Physics, University of Münster, Germany — [2]Center for Nonlinear Science, University of Münster, Germany — [3]Departament de Física & IAC-3, Universitat de les Illes Balears, Spain

We study an injected Kerr Gires-Tournois interferometer (KGTI) in which a periodic modulation of the feedback phase is introduced that can be interpreted as a periodic potential. We investigate the first principle model based upon delay algebraic equations using direct numerical simulations and path continuation techniques. The micro-cavity's dispersion and Kerr effect combined with detuned injection give rise to temporal localized states (TLSs) which live on a continuous wave (CW) background and synchronize with the periodic potential. We show that the Arnold tongues limiting the synchronized regime are realized by a SNIPER bifurcation. Furthermore, we study the movement of the TLSs in the periodic potential, caused by third order dispersion. In the limit of weak injection and small cavity losses the system is compared to the Lugiato-Lefever equation. The linear part is solved by Hermite-Gauss modes therefore a mode decomposition is conducted.

DY 18.9 Tue 12:00 BH-N 128

Temporal localized states in an injected Kerr-Gires-Tournois interferometer in the regime of anomalous dispersion — •Tim Lohmann[1], Thomas G. Seidel[1], Julien Javaloyes[2], and Svetlana V. Gurevich[1,2,3] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany — [2]Departament de Física, Universitat de les Illes Balears and IAC-3, Cra. de Valldemossa, km 7.5, E-07122 Palma de Mallorca, Spain — [3]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstraße 2, 48149 Münster, Germany

We are interested in the dynamics of temporal localized states (TLSs) in an injected Kerr-Gires-Tournois interferometer (KGTI) in the regime of anomalous dispersion. In this regime and in the uniform field limit, the first principle model based upon delay algebraic equations can be approximated by the Lugiato-Lefever partial differential equation, giving rise to the formation of TLSs.Using the combination of numerical simulations and path continuation techniques, we demonstrate that for parameter values far away from the Lugiato-Lefever regime a new form of short high-intensity TLSs emerges.

DY 18.10 Tue 12:15 BH-N 128

Solitons beyond the uniform field limit in injected Kerr resonators — Thomas Seidel[1], Julien Javaloyes[2], and •Svetlana Gurevich[1,3] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany — [2]Departament de Física & IAC-3, Universitat de les Illes Balears, C/ Valldemossa km 7.5, 07122 Mallorca, Spain — [3]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, 48149 Münster, Germany

We elucidate the formation of temporal localized states (TLSs) in an injected Kerr-Gires-Tournois interferometer in the normal dispersion regime and operated far from the uniform field limit (UFL). Our first principle model is based upon time delayed algebraic equations whose uniform validity allows for a systematic exploration of all the parameter space. While in the weakly nonlinear regime the cavity response and the dynamics can be described by the Lugiato-Lefever equation (LLE), such a framework breaks down in the regimes of large detuning and injection. By using a combination of direct numerical simulations and path continuation techniques, we investigate these new regimes that departs from the UFL and find short, high-intensity TLSs which live on a single stable continuous wave (CW) background. In this regime, the previously stable upper CW solution becomes Turing unstable. Further, we analyze the transition between the LLE and the UFL and the change of the shape of the TLSs.

DY 18.11 Tue 12:30 BH-N 128

Stable semivortex solitons in a fermionic condensate — •Pablo Díaz — Departamento de Ciencias Físicas, Universidad de

La Frontera, Temuco, Chile

In the present work, we numerically show the existence of semivortex solitons in a two-dimensional fermionic spinor, which has never been previously reported in the literature. This soliton is free of two-dimensional potentials and includes a Rashba-type spin-orbit coupling. The theoretical framework consists of a mean-field theory applied to a Fermi superfluid. We obtain the gap solitons using an ansatz of semivortex type. This approach allows us to reduce the two-dimensional equations to a system of radial equations determined numerically for a parameter space given by the chemical potential and the cross-interaction between the spinors. To test the stability of the soliton solutions, we performed real-time computational simulations using finite differences with the Runge-Kutta 4 method. Our results show that the soliton stability zone only partially coincides with the Vakhitov-Kolokolov linear stability criterion. Interestingly, we have found stable solitons for times much larger than the simulations observed in similar works for bosonic systems. Moreover, this stability was tested by inducing oscillations of a soliton due to a step-like change of the Zeeman parameter. We compute the resulting fluctuations in the spin state of the soliton induced by the transfer of particles between the spinors.

DY 18.12 Tue 12:45 BH-N 128

Modeling 1/f noise using models with overlapping pulses — •Aleksejus Kononovicius and Bronislovas Kaulakys — Institute of Theoretical Physics and Astronomy, Vilnius University, Vilnius, Lithuania

White noise and Brownian motion are well understood types of noise and fluctuations in variety of materials, devices, and other physical and non-physical systems. Universal nature of 1/f noise remains an elusive problem. Earlier we have considered an elementary model with non-overlapping rectangular pulses in a conductive material [1, 2]. We have shown that pure 1/f noise can be obtained only with long pulses and power-law distributed gaps (or vice versa). Taking the point process limit results in perversion of 1/f noise, which suggests that allowing pulses to touch can also cause perversion. Here we show that this intuition is wrong, even a model with overlapping pulses exhibits pure 1/f noise.

[1] A. Kononovicius, B. Kaulakys, PRE 107: 034117 (2023).
[2] A. Kononovicius, B. Kaulakys, arXiv:2306.07009.

DY 19: Machine Learning in Dynamics and Statistical Physics II (joint session DY/SOE)

Time: Tuesday 9:30–13:00 Location: BH-N 243

DY 19.1 Tue 9:30 BH-N 243

Pareto-Based Selection of Data-Driven Ordinary Differential Equations — •Gianmarco Ducci, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Data-driven approaches enable the approximation of governing laws of physical processes with parsimonious equations. However, they face challenges due to inherent noise in data, which impacts the sparsity of the result. While a great effort over the last decade has been made in this field, data-driven approaches generally rely on the paradigm of imposing a fixed base of library functions. In order to promote sparsity, finding the optimal set of basis functions is a necessary condition but a challenging task to guess in advance.

In this work, we propose an alternative approach which consists of optimizing the very library of functions while imposing sparsity. The robustness of our results is not only evaluated by the quality of the fit of the discovered model, but also by the statistical distribution of the residuals with respect to the original noise in the data. The model selection is then chosen from a subset of optimal models obtained in a Pareto fashion. We illustrate how this method can be used as a tool to derive microkinetic equations from experimental data.

DY 19.2 Tue 9:45 BH-N 243

Accurate Memory Kernel Extraction from Discretized Time-Series Data — •Lucas Tepper — Department of Physics, Freie Universität Berlin

Memory effects emerge whenever the dynamics of complex many-body systems are projected onto low-dimensional observables. Accounting for memory effects using the framework of the generalized Langevin equation (GLE) has proven efficient, accurate and insightful, particularly when working with high-resolution time series data. However, in experimental systems, high-resolution data is often unavailable, raising questions about the effect of the data resolution on the estimated GLE parameters. Using molecular dynamics (MD) data of a small, alpha-helix-forming peptide, I demonstrate that the direct memory extraction remains accurate when the discretization time is below the memory time. For discretization times exceeding the memory time, I show that a Gaussian Process Optimization (GPO) scheme estimates accurate memory kernels by minimizing the deviation of discretized two-point correlation functions between MD and GLE simulations. The GPO scheme stays accurate for discretization times below the longest time scale in the data, typically the barrier crossing time.

DY 19.3 Tue 10:00 BH-N 243

Coarse-graining non-equilibrium systems with machine learning: from conceptual challenges to new approaches — •Patrick Egenlauf[1,2] and Miriam Klopotek[2] — [1]University of Stuttgart, Interchange Forum for Reflecting on Intelligent Systems, IRIS3D project, Stuttgart, Germany — [2]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany

Machine learning (ML) was previously shown to effectively coarse-grain configurations of many-body systems. We want to investigate ML applications to address the dynamic coarse-graining of non-equilibrium many-body systems. Our research aims to advance ML methods while avoiding conventional assumptions. The focus is on time-dependent datasets and their broader implications for understanding causality. We introduce innovative techniques by incorporating general theory, including the time-dependent generalized Langevin equation [1], for building and interpreting time-dependent learning techniques [2]. This provides a distinctive ML perspective that extends to various applications for dynamical systems beyond equilibrium states. This study offers new ways to improve our understanding and manipulation of complex non-equilibrium many-body dynamics using ML.

[1] Schilling, T. (2022). Coarse-grained modelling out of equilibrium. *Physics Reports*, 972, 1-45.
[2] Nakajima, K., and Fischer, I. (2021). *Reservoir Computing*. Springer Singapore.

DY 19.4 Tue 10:15 BH-N 243

Statistical criteria for the prediction of dynamical clustering in granular gases — •Sai Preetham Sata[1,2], Dmitry Puzyrev[2], and Ralf Stannarius[1,2] — [1]Institute of Physics, Otto-von-Guericke University, Magdeburg, Germany — [2]Department of Microgravity and Translational Regenerative Medicine and MARS, Otto von Guericke University, Magdeburg, Germany

Granular gases excited by external forces can undergo transitions from the homogeneous to a dynamical cluster state [1, 2], depending on filling fraction, excitation parameters and container geometry. We compare two statistical criteria for the clustering transition, viz. the Kolmogorov-Smirnov Test (KS-Test) on the particle number density profile and the so-called caging-effect based on the local packing fraction [2]. Both criteria are evaluated for various combinations of system parameters in the VIP-Gran experiment [3] and combined into one dataset. This allows us to compare existing clustering criteria and tune them to provide matching clustering thresholds. The aim is to develop improved threshold criteria. Machine learning models are trained with this dataset to predict whether particular parameters lead to homogeneous or dynamical cluster states.

This study is supported by DLR projects VICKI and EVA II(50WM2252 and 50WK2348)

References: [1] É. Falcon et al., Phys. Rev. Lett., 83:440-443, 1999 [2] E. Opsomer et al., Europhys. Lett., 99:40001, 2012 [3] S. Aumaître et al., Rev. Sci. Instr., 89, 2018.

DY 19.5 Tue 10:30 BH-N 243

Excitability and Memory in a Time-Delayed Optoelectronic Neuron — •Jonas Mayer Martins[1], Svetlana V. Gurevich[1],

and Julien Javaloyes[2] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9 and Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, 48149 Münster, Germany — [2]Departament de Física and IAC-3, Universitat de les Illes Balears, C/ Valldemossa km 7.5, 07122 Mallorca

We study the dynamics of an optoelectronic circuit composed of a nanoscale resonant-tunneling diode (RTD) in the excitable regime driving a nanolaser diode (LD) coupled via time-delayed feedback. Using a combination of numerical path-continuation methods and time simulations, we demonstrate that the RTD-LD system can serve as an artificial neuron, generating pulses in the form of temporal localized states (TLSs) that can be employed as memory for neuromorphic computing. In particular, our findings reveal that the prototypical delayed FitzHugh–Nagumo model previously employed to model the RTD-LD resembles our more realistic model qualitatively only in the limit of a slow RTD. We show that the RTD time scale plays a critical role in how the RTD-LD can be used as memory because it governs a shift in pulse interaction forces from repulsive to attractive, leading to a transition from stable to unstable multi-pulse TLSs. Our theoretical analysis uncovers novel features and challenges, including the multistability of TLSs and attractive interaction forces, stemming from the previously neglected intrinsic dynamics of the laser. These dynamics are crucial to consider for the memory properties of the RTD-LD.

DY 19.6 Tue 10:45 BH-N 243

Anisotropic diffusion analysis in confined geometries — •Kevin Höllring[1], Andreas Baer[1], Nataša Vučemilović-Alagić[2], David M. Smith[2], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Group of Computational Life Sciences, Ruđer Bošković Institute, 10000 Zagreb, Croatia

In various systems, liquid and particle transport are of major importance to the viability of chemical like catalysis or adsorption. Most of these systems involve interfaces and confined geometries, where the prerequesites for the application of classical analysis techniques like the Einstein/MSD or the Green-Kubo/ACF approach are not fulfilled. To facilitate the resolution of diffusion coefficients in such system, we propose a novel approach built around the analysis of time statistics of particles in subspaces of the system using the Smoluchowski equation. For simple point-like particles, we propose a explicit analytic formula to link mean lifetimes and diffusivity, with an extension to account for the impact of locally induced drift as a consequence of complex effective interaction potentials. For more complex particles like in ionic liquids, we provide an extended technique able to resolve the impact of internal degrees of freedom, through which we can not only analyze the evolution of transport but also characteristic changes in the conformational behavior of particles close to interfaces. Overall, this approach can be used to demonstrate a characteristic oscillatory behavior of particle diffusivity in confinement close to interfaces so far not reported in literature.

DY 19.7 Tue 11:00 BH-N 243

Data assimilation of cardiac dynamics by means of adjoint optimization — •Inga Kottlarz[1,2,3,4], Sebastian Herzog[2,4,5], Patrick Vogt[2,3], Stefan Luther[1,2,4], and Ulrich Parlitz[2,3,4] — [1]Institute for Pharmacology and Toxicology, UMG Göttingen, Germany — [2]MPI for Dynamics and Self-Organization, Göttingen, Germany — [3]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany — [4]German Center for Cardiovascular Research, Partner Site Niedersachsen, Göttingen, Germany — [5]III. Institute of Physics, University of Göttingen, Germany

Cardiac muscle tissue is an excitable medium that can exhibit a range of dynamics of different complexity, from planar waves to spiral waves to spatiotemporal chaos, the latter being associated with (fatal) cardiac arrhythmia.

Both the prediction of such high dimensional chaotic time series, as well as the reconstruction of their (not yet fully observable) complete dynamical state are ongoing challenges. In recent years, machine learning approaches have gained popularity for solving these problems, which can be advantageous if we do not have much knowledge about the dynamical system in question, but are limited by the large amounts of training data that is needed and often not available for biological systems. We present adoptODE, an adjoint optimization framework for estimating model parameters and unobserved variables. We showcase the adjoint method*s effectiveness in optimizing high-dimensional problems with thousands of unknowns, serving as a valuable tool for bridging the gap between empirical data and theoretical models.

15 min. break

DY 19.8 Tue 11:30 BH-N 243

Collective Variables for Neural Networks — •Konstantin Nikolaou[1], Samuel Tovey[1], Sven Krippendorf[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität, Germany

Neural Networks have witnessed extensive integration across diverse domains within physics. However, our focus shifts towards the inverse problem: How can neural networks benefit from physics? Learning with a neural network involves algorithmically assimilating information into a model. Nevertheless, the process of neural learning remains largely elusive, given the challenge of understanding how to extract information from its dynamics. Analogous to dynamical systems in statistical physics, describing neural network training involves an extensive number of degrees of freedom, which appears to benefit from a description through macroscopic quantities. To that end, we introduce Collective Variables for neural networks, tracing out microscopic degrees of freedom to describe and analyze the learning process at every stage. We investigate the initial state as well as the learning dynamics of the network in the context of the Collective Variables. We find a correlation between the initial network state and the generalization of the model computed after training. Moreover, we use the collective variables to identify and analyze stages arising in the dynamics of the learning process.

DY 19.9 Tue 11:45 BH-N 243

Fluctuating weight dynamics and loss landscape in deep linear networks — •Markus Gross — DLR, Institute for AI Safety and Security, Germany

Understanding how weights fluctuate during training of neural networks and how this impacts the loss landscape is key to optimizing training processes and performance. We investigate this dynamics in (deep) linear networks within the continuum limit of stochastic gradient descent. For a two-layer network, we highlight the role of the inter-layer coupling and analytically derive from first principles a recently discovered key relation between weight fluctuations and loss landscape. The uncovered behaviors are rooted in general statistical properties of the network architecture und training data.

Reference: https://arxiv.org/abs/2311.14120

DY 19.10 Tue 12:00 BH-N 243

Loss is More: Exploring the weight space of a perceptron via enhanced sampling techniques — •Margherita Mele[1], Roberto Menichetti[1], Alessandro Ingrosso[2], and Raffaello Potestio[1] — [1]Physics Department, University of Trento, via Sommarive, 14 I-38123 Trento, Italy — [2]The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy

Understanding how input data properties influence the learning process in artificial networks is crucial. The assumption of Gaussian i.i.d. inputs has long been foundational, yet questioning its constraints is now essential. Our approach utilises enhanced sampling methods from soft matter physics to exhaustively explore the loss profile and reconstruct the density of states of networks with discrete weights, addressing optimization in highly rugged landscapes even in simple architectures. These methods, effective in real datasets, enable exploration of data dimensionality and structure impact.

Employing benchmarks (e.g. MNIST, FashionMNIST) and in silico datasets, our study investigates the role of various input-data properties, including class imbalance, separation, item mislabelled, and input-output correlation. Our findings bridge theoretical and applied aspects, shedding light on the limitations and extensions of Gaussian i.i.d. assumptions. This work provides pivotal insights into the interplay between input data properties and network learning, advancing our understanding of how artificial networks adapt to different information contexts.

DY 19.11 Tue 12:15 BH-N 243

Emergent oscillating dimensionality transformations in deep learning — •Pascal de Jong, Felix J. Meigel, and Steffen Rulands — Arnold Sommerfeld Center for Theoretical Physics, Department of Physics, Ludwig- Maximilians-Universität, München, Germany

Artificial intelligence relies on deep neural networks (DNNs), which comprise a large set of nonlinear nodes connected by weights. The

functioning of DNNs and their ability to generalize to unseen data are examples of complex behavior, which due to their highly nonlinear nature is poorly understood. Here, we show that training DNNs universally leads to oscillating weight topologies that alter the embedding dimensions of hidden data representations in different layers. Specifically, using a path representation of DNNs, we derive equations for the time evolution of the weights. We show that training leads to a structure, in which weights are focused on a subset of nodes, and the degree of focusing oscillates across layers. We empirically confirm these findings by studying the training dynamics of large DNNs on different data sets. Finally, we show that these structures imply a repeated dimensional decrease and increase of the hidden data representations. Our results highlight that emergent dynamics during training can lead to universal network topologies with implications for their function.

DY 19.12 Tue 12:30 BH-N 243

Investigating the Evolution of Fisher Information for Neural Network Dynamics — •Marc Sauter, Samuel Tovey, Konstantin Nikolaou, and Christian Holm — Institute for computational physics, Stuttgart, Germany

Machine learning has proven to be a powerful tool with remarkable effectiveness for various physical applications. Even though Neural Networks offer great potential for solving complex tasks, their black-box nature limits the information obtainable about the underlying mechanisms they employ. Especially in physics, where the exact methodologies of solving tasks are just as important as finding solutions itself, advances in interpretable machine learning promise to aid the applicability of Neural Networks task-solving capabilities greatly. The Fisher Information Matrix (FIM) is a statistical measure known for its ability to identify second order phase transitions in physical systems. It can also be used for analyzing learning dynamics, where it expresses correlations between influences of parameters in Neural Networks. However, because of its size, computation of the FIM is currently intractable for Neural Networks used in common problem settings. As a way of obtaining parts of the information contained in the FIM, we introduce a novel mathematical relationship between the trace of the FIM and the Neural Tangent Kernel, a smaller observable of neural network training. We apply this approach for simple test models and discuss arising research topics.

DY 19.13 Tue 12:45 BH-N 243

Near-zero-cost post-training uncertainties for deep learning architectures — •Filippo Bigi, Sanggyu Chong, Michele Ceriotti, and Federico Grasselli — Laboratory of Computational Science and Modeling (COSMO), IMX, École Polytechnique Fédérale de Lausanne, Switzerland

Over the last decade, deep learning models have shown impressive performance and versatility on an extremely wide range of tasks. However, their probability estimates are unreliable, especially outside of the training distribution, with neural networks often returning overconfident results when queried on unfamiliar data. Although several uncertainty quantification schemes are available, their practical downsides hinder their widespread adoption. We propose a novel method for estimating the predictive uncertainties of deep learning architectures based on the interpretation of the last layer of neural networks as a linear Gaussian process. Contrary to previous methods, the proposed approach is simple, scalable, does not involve modification of the architecture or the training procedure, can be applied to trained models *a posteriori*, and generates uncertainty estimates with a single forward pass at negligible additional cost. We demonstrate the accuracy and practicality of our scheme on a wide range of machine learning datasets.

DY 20: Statistical Physics of Biological Systems I (joint session DY/BP)

Time: Tuesday 9:30–13:00 Location: BH-N 334

Invited Talk DY 20.1 Tue 9:30 BH-N 334

Dynamics of genome replication — •Simone Pigolotti — Okinawa Institute of Science and Technology

The DNA replication program of an organism determines the timing at which different genomic regions are replicated, with fundamental consequences for cell homeostasis and genome stability. I will present a method to infer the DNA replication program, by combining stochastic modeling and deep sequencing experiments. Our approach can be applied to a vast range of organisms from bacteria to eukaryotes. Applied to E. coli, our method reveals regular variations of replication speed, that correlate with previously measured variations of the mutation rate. In budding yeast, our method is able to infer the location of replication origins with remarkable accuracy.

DY 20.2 Tue 10:00 BH-N 334

Theory for Adaptive Systems: Collective Robustness of Genotype-Phenotype Evolution — •Tuan Pham and Kunihiko Kaneko — Niels Bohr Institute, University of Copenhagen

Biological and neural networks are adaptive - their connections slowly change in response to the state of the coupled elements making up the systems. The dynamics of such adaptive networks are intriguingly complex, rendering it extremely difficult to answer the fundamental question of how the resulting collective states of biological and neural systems are functionally robust against environmental stochasticity. We tackle this problem by developing a new framework based on the path-integral formalism of non-equilibrium statistical physics. We demonstrate the wide applicability of our framework to various very high-dimensional dynamical systems on multiple timescales, often encountered in biological evolution and neural network learning. As a specific example of our theory, we apply it to biological evolution, where phenotypes are shaped by gene-expression fast dynamics that are subjected to an external noise while genotypes are encoded by the configurations of a network of gene regulations. This network slowly evolves under natural selection with a mutation rate, depending on how adapted the shaped phenotypes are. Here we find phenotypes with a robust high-valued mean gene-expression level within an intermediate level of noise. The emergence of such robustness can be characterised analytically within our framework as the onset of instability of the attractor state with zero gene-expression levels.

DY 20.3 Tue 10:15 BH-N 334

Modelling antibiotic killing and tolerance dynamics in tuberculosis treatment — •Miriam Clincy[1], Vijay Srinivasan[2], Rosalind J Allen[2], and Martin R Evans[3] — [1]Hochschule Esslingen, Esslingen, Germany — [2]Friedrich-Schiller-Universität, Jena, Germany — [3]University of Edinburgh, Edinburgh, UK

The bacterium Mycobacterium tuberculosis (Mtb), which causes tuberculosis, is the leading global cause of deaths from infectious disease. The antibiotic treatment regime for tuberculosis is very long, because Mtb can switch into tolerant physiological states that are only slowly killed by antibiotic. Here we introduce a stochastic two-species birth-death model for antibiotic treatment of an Mtb infection accounting for this switching.

Solving analytically for the probability generating function describing the treatment phase in which neither state proliferates allows 1) to recover the mean subpopulation dynamics from which numerical estimates for the birth, death and switching rates specifically for Mtb can be derived, and 2) the calculation of the extinction probability as a function of time. From the latter, a numerical measure for the extinction time of the bacterial population is defined. Studying this extinction time reveals distinct regimes in which the required treatment time is limited by either the rate of killing of tolerant bacteria, or the rate of switching out of the tolerant state.

DY 20.4 Tue 10:30 BH-N 334

Information theory of chemotactic agents using both spatial and temporal comparison — Julian Rode[1], Maja Novak[2], and •Benjamin M. Friedrich[1] — [1]Physics of Life, TU Dresden, Germany — [2]University of Zagreb, Croatia

Biological system process information despite noise-corrupted input, often operating at physical limits. A prime example is chemotaxis, i.e., active navigation of biological cells in spatial fields of chemical cues. Intriguingly, cells of different size use two different chemotaxis strategies, comparing concentrations in either space or time. Only heuristic arguments exist to explain this evolutionary choice. We present an information theory of an ideal agent that combines both strategies to quantify 'chemotaxis in bits' [1]. This enables us to pre-

dict when each strategy provides more information as function of a new powerlaw that combines agent size, motility noise and sensing noise. We demonstrate our theory with a bio-inspired search robot. [1] https://www.biorxiv.org/content/10.1101/2023.10.14.562229v1

DY 20.5 Tue 10:45 BH-N 334

Relaxation and first passage properties of boundary driven run and tumble particle — •Pritha Dolai[1,2] and Arghya Das[3] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [3]TIFR Centre for Interdisciplinary Sciences, Tata Institute of Fundamental Research, Gopanpally, Hyderabad, 500046, India

We study the spatio-temporal properties of boundary-driven noninteracting Run and tumble particles (RTPs) in one-dimension. We found exact results for the steady state density and current. The spatial and internal degrees of freedom, combined together, possess a symmetry, using which we have analytically obtained the full eigen-spectrum. The eigenvalues are arranged in bands around 0 and -2ω where ω is the tumble rate of the RTP. In the large system size limit, the steady state and dynamical properties are closely approximated by an effective passive-like dynamics with an effective diffusivity. Interestingly, we found that the genuine signatures of activity in the dynamics appear only as subleading correction in system size. Further, there is a crossover from the system size independent relaxation rate to the diffusive relaxation as the system size is increased. Along the lines of equilibrium, we explored the possibility of defining an effective temperature in the single active particle case. It turns out that the effective temperature not only depends on the details of the system parameters, but on the quantities through which it is defined as well as the boundary conditions. We also studied the first passage properties of an RTP in the presence of absorbing boundaries.

DY 20.6 Tue 11:00 BH-N 334

Single particle analysis of sorbing tracers — •Timo Doerries[1], Aleksei Chechkin[1,2,3], and Ralf Metzler[1,4] — [1]Institute of Physics & Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]Faculty of Pure and Applied Mathematics, Hugo Steinhaus Center, Wrocław University of Science and Technology, Wyspianskiego 27, 50-370 Wrocław, Poland — [3]Akhizer Institute for Theoretical Physics National Science Center "Kharkiv Institute of Physics and Technology", 61108 Kharkiv, Ukraine — [4]Asia Pacific Center for Theoretical Physics, Pohang 37673, Republic of Korea

Based on a simple switching diffusion process we describe tau proteins changing between a mobile (diffusive) and an immobile state, leading to strong non-Gaussian displacements. For long but finite observation times the time averaged mean squared displacements have a significant spread, of which we obtain the exact distribution. This behaviour is similar to the well known continuous time random walk, which has instantaneous jumps in contrast to our model. We discuss the role of the non-zero mobile duration in our model compared to the instantaneous jumps in the continuous time random walk.

15 min. break

DY 20.7 Tue 11:30 BH-N 334

Furutsu-Novikov theorem for shot-noise driven systems — •Jakob Stubenrauch[1,2] and Benjamin Lindner[1,2] — [1]Physics Department of Humboldt University Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, Philippstraße 13, Haus 2, 10115 Berlin, Germany

We consider an arbitrary system (later exemplified by a spiking neuron) that is driven by an intensity-modulated Poisson process with intensity $\lambda(t) = \lambda_0 + \varepsilon s(t)$. We derive an exact relation between the input-output cross-correlation in the spontaneous state ($\varepsilon = 0$) and the response function for a weak time-dependent modulation of the input intensity ($\varepsilon > 0$). This can be regarded as a variant of the famous Furutsu-Novikov theorem (FNT) for the case of shot noise. Neurons in networks fluctuate spontaneously and respond if stimulated. Spontaneous fluctuations and response properties are linked, in correspondence to the fluctuation-dissipation theorem, as has recently been shown (Lindner, 2022). Such relations constrain the signal-to-noise ratio, they can be used to fit models, and to advance theories. However, for the biologically relevant case of shot-noise driven neurons, such relations have not been reported yet. As we demonstrate, we can use the new FNT to obtain a fluctuation-response-relation between the spontaneous fluctuations of a neuron's output and its systematic response to a time-dependent stimulus, extending the approach of (Lindner, 2022) from Gaussian noise to shot noise. The relations are numerically tested and their limitation to Poissonian input exemplified for the important example of a leaky integrate-and-fire neuron with alpha synapses.

DY 20.8 Tue 11:45 BH-N 334

Mesoscopic dynamics of spiking neuron population with quenched randomness — •Nils Erik Greven[1,2], Jonas Ranft[3], and Tilo Schwalger[1,2] — [1]TU Berlin — [2]BCCN Berlin — [3]IBENS, Ecole Normale Supérieure & CNRS

To understand the neural mechanisms underlying the response and variability dynamics of neuronal populations in the brain, simple mean-field models at the mesoscopic scale are required that faithfully describe the fluctuations of population activities and recurrent synaptic inputs in network of spiking neurons. We derive a nonlinear stochastic mean-field model for a network of spiking Poisson neurons with random connectivity. The quenched disorder of the connectivity is treated by an annealing approximation leading to a simpler fully connected network with additional noise in the neurons. This annealed network enables a reduction to a mesoscopic model as a two-dimensional closed system of coupled Langevin equations for the mean and variance of the neuronal membrane potentials. Compared to microscopic simulations, the mesoscopic model well describes the fluctuations and nonlinearities of finite-size neuronal populations and outperforms previous mesoscopic models that neglected the recurrent noise effect caused by quenched disorder. This effect can be analytically understood as a softening of the effective nonlinearity. The mesoscopic theory also shows that, in the presence of synaptic transmission delays, quenched disorder can stabilize the asynchronous state. Furthermore, our theory correctly predicts the effect of connection probability and stimulus strength on the variance of the population firing rate.

DY 20.9 Tue 12:00 BH-N 334

Low-dimensional stochastic dynamics of finite-size, spiking-neuron populations via eigenmode expansion — •Tilo Schwalger[1,2] and Bastian Pietras[3] — [1]Technical University Berlin, 10623 Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, 10115 Berlin, Germany — [3]Universitat Pompeu Fabra, Barcelona, Spain

Low-dimensional neural population models in the form of nonlinear Langevin equations provide an effective description of the collective stochastic dynamics of neural networks in the brain. However, existing population models are largely heuristic without a clear link to the underlying neuronal and synaptic mechanisms. Here, we derive a system of Langevin equations at the mesoscopic scale from a microscopic model of a finite-size, fully-connected network of integrate-and-fire neurons with escape noise. The theory is based on a stochastic integral equation for the mesoscopic dynamics of the neural network (Schwalger et al. PloS Comput Biol. 2017) and an eigenmode expansion of the corresponding refractory-density equation (Pietras at al., Phys. Rev. E 2020). Truncating the hierarchy of coupled spectral modes after the first M modes yields a $2M$-dimensional Langevin equation, permitting a systematic model reduction. Retaining only the dominant spectral mode, $M = 1$, already captures well oscillatory transients and finite-size fluctuations when compared to microscopic simulations. Our bottom-up theory thus connects biologically plausible spiking neural networks to the efficient firing-rate models often used in applcations.

DY 20.10 Tue 12:15 BH-N 334

The Effect of Temperature on Large Biochemical Networks — •Julian Voits[1] and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, University of Heidelberg, Heidelberg, Germany — [2]BioQuant-Center for Quantitative Biology, University of Heidelberg, Heidelberg, Germany

An increase of temperature of a few Kelvin might seem modest on the absolute temperature scale, but it can have a dramatic impact on complex biosystems. Instructive examples are fever, when a rise in body temperature of 2-3K has strong effects on our immune system, or climate change, when even smaller temperature changes lead to dramatic shifts in ecosystems. From the physics point of view, the main effect of increased temperature should be the exponential acceleration of biochemical reactions (Arrhenius equation). However, it is unclear how this law plays out in the large biochemical networks of complex systems. We have developed a universal theory that describes the effect of temperature on large biochemical networks. We approach this problem with a graph theoretical interpretation of the mean first passage times of a biochemical master equation. We show that in the limit

of large networks, one obtains quadratic forms of the Arrhenius plots, in excellent agreement with experimental data on developmental rates of Drosophila.

DY 20.11 Tue 12:30 BH-N 334

Tensile elasticity of multi-state flexible chains and loops — •Geunho Noh and Panayotis Benetatos — Department of Physics, Kyungpook National University, Daegu, Republic of Korea

Polymer loop structure commonly appears in biological phenomena, such as DNA looping and DNA denaturation. When a chain forms a loop, its elastic behavior differs from that of an open chain due to the loss of entropy. In the case of reversible loop formation, interesting behavior emerges related to the multi-state nature of the conformations. In this study, we model a multi-state reversible loop as a looping Gaussian chain which can bind to form a loop, or a zipping Gaussian loop which can zip to form a double-stranded chain. For each model, we calculate the force-extension relations in the fixed-force (Gibbs) and the fixed-extension (Helmholtz) statistical ensembles. Unlike the single Gaussian chain or loop, the multi-level systems demonstrate qualitatively distinct tensile elasticity and ensemble inequivalence. In addition, we investigate a Gaussian necklace consisting of reversible alternating blocks of the chain and loop, and obtain the temperature-force phase diagram. The phase diagram implies a force-induced phase transition from a completely looped (denatured) state to a mixed (chains and loops) state.

DY 20.12 Tue 12:45 BH-N 334

Manifestation of hidden degrees of freedom in dissipative self-assembly — •Seeralan Sarvaharman and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen 37077, Germany

Dissipative self-assembly is crucial for the development and healthy functioning of biological systems. By breaking time-reversal symmetry in either the binding or unbinding process of at least one of the components, living organisms are able to assemble structures with much more diverse compositions in a robust fashion. One such example that is of fundamental biological relevance are microtubules. Through a process called "dynamic instability" these microtubules, which are made up of several filaments, grow and shrink depending on the instantaneous compositions of the filaments. The observable that is often used to quantify such dynamic instability is the length of the assembled microtubule. However, the ability to infer the many-body effects underlying this instability from the projected length observable has remained elusive. Here we address this challenge by considering a stochastic Ising-type model of microtubule assembly with thermodynamically consistent driving. Using a mixture of analytical techniques and computational methods we uncover the manifestation of many-body physics encoded the time-ordering of the length of the assembly.

DY 21: Focus Session: Nanomechanical Systems for Classical and Quantum Sensing I (joint session TT/DY/HL/QI)

Nanomechanical and cavity-optomechanical systems have been recently established as a controllable and configurable platform that can be engineered to tackle outstanding sensing challenges both in the classical and in the quantum regime. With this focus session, experts from different but synergetically overlapping fields of nanomechanical sensing pursuing classical, non-linear and quantum approaches are brought together. The session shall provide an overview over the recent exciting developments of the techniques explored in micro- and nanomechanical systems and sensing concepts exploring quantum measurement schemes.
This joint session will be continued Wednesday afternoon (TT53) and Thursday morning (TT70). Organized by Eva Weig, Hubert Krenner, and Hans Hübl.

Time: Tuesday 11:45–13:00 Location: H 3007

DY 21.1 Tue 11:45 H 3007

Josephson Optomechanics — •Surangana Sengupta[1], Bjoern Kubala[1,2], Joachim Ankerhold[1], and Ciprian Padurariu[1] — [1]ICQ and IQST, Ulm University, Germany — [2]DLR-QT, German Aerospace Center, Ulm, Germany

In recent years, optomechanical cooling using microwave radiation has been realized in various superconducting circuits with a microwave cavity comprising a mechanical element. Circuits provide an opportunity to engineer nonlinear cavities, by using Josephson junctions, thereby generating quantum states of light for optomechanics experiments.
Here, we will theoretically describe an optomechanical setup where the cavity is realized by an LC circuit driven by a dc-biased Josephson junction. By engineering the nonlinearity, such a cavity becomes an effective N-level system, with $N = 2, 3, ...$, where the access to Fock states N and above is blocked. Consequently, the cavity emission spectrum shows Mollow-type side peaks, analogous to an optical cavity interacting with an atom. We show that at these Mollow side peaks, the system exhibits a new, nonlinear type of optomechanical cooling. We calculate the cooling rate using the spectral density of noise due to the radiation pressure [1] and highlight how its unusual features compared to conventional optomechanics, can be explained in a dressed state picture.
[1] F. Marquardt *et.al.*, Phys. Rev. Lett. **99** (2007) 093902

DY 21.2 Tue 12:00 H 3007

Logarithmic susceptibility of a quantum parametrically modulated oscillator — •Daniel Boness[1], Wolfgang Belzig[1], and Mark Dykman[2] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA

A weakly damped nonlinear oscillator modulated close to twice its eigenfrequency has two stable states, which have the same vibration amplitudes but opposite phases. The states are equally populated due to classical or quantum fluctuations.

An extra force at half the modulation frequency lifts the symmetry of the states. Even a weak force can result in a significant change of the populations, as it beats against the intensity of quantum and classical fluctuations. We develop an approach that allows us to find this population change.

We also study the effect of the extra force with frequency slightly detuned away from half the modulation frequency. For a detuning that is small compared to the switching rate the force leads to the imbalance of populations that is modulated at the frequency of the detuning. For larger detuning, the adiabatic picture breaks down and the wells are again equally populated. However, the rates of switching between the wells is exponentially increased. We calculate the change of the logarithm of the switching rate, termed logarithmic susceptibility, using the real-time instanton method. The results are relevant for controlling parametric oscillators and their application in quantum information systems.

DY 21.3 Tue 12:15 H 3007

Cavity optomechanics with carbon nanotube quantum dots — •Akong N. Loh, Furkan Özyigit, Fabian Stadler, Niklas Hüttner, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Carbon nanotubes (CNTs) are the smallest and lightest nanomechanical beam resonators. When suspended transversally between two electrodes (Ti/Au for example) and then gated, they can act as mechanical beam resonators with large quality factors and also as quantum dots. The motion of a CNT is coupled to other degrees of freedom, such as photons, spins, and electrons. The optomechanical coupling of a single wall carbon nanotube nanomechanical resonator to a microwave

cavity has been realized and quantified through optomechanically induced transparency measurements [1]. The quantum dot properties of the CNT were exploited (specifically the nonlinearity of the coulomb blockade) to significantly enhance the coupling strength [1,2]. Current work is directed towards achieving even stronger coupling and possibly groundstate cooling of the nanomechanical resonator through anti-Stokes processes. This requires significant improvement of the microwave cavity, CNT growth and transfer. All measurements are done at ∼10 mK in a dilution refrigerator.

[1] S. Blien *et al.*, Nat. Comm. **11** (2020) 1636
[2] N. Hüttner et al., Phys. Rev. Applied, in press (2023), arXiv:2304.02748

DY 21.4 Tue 12:30 H 3007

Signatures of Josephson force in a vibrating carbon nanotube junction — •Andreas K. Hüttel[1,2], Jukka-Pekka Kaikkonen[2], Keijo Korhonen[2], and Pertti Hakonen[2] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany — [2]Low Temperature Laboratory, Dept. of Applied Physics, Aalto University, Espoo, Finland

A carbon nanotube suspended between superconducting electrodes acts simultaneously as nanomechanical resonator and as a Josephson junction. Its energy-dependent density of states and with that displacement-dependent critical current further adds to the complexity of the system, as does both mechanical and electronic nonlinearity. Measurements on such a system display complex behaviour of the vibrational resonance with respect to junction biasing. Strikingly, the resonance frequency appears to decrease in a distinct parameter region where the biasing is similar in size to the junction switching current.

Using highly parallelized Julia code, we numerically solve the coupled differential equation system of the driven (via an ac gate voltage and ac current or voltage bias) system for realistic device parameters and characterize the evolving steady state. Specific attention is given to the impact of the Josephson junction behaviour on the mechanical resonance frequency and the vibration amplitude, and on the ac signal simultaneously acting on gate and bias.

DY 21.5 Tue 12:45 H 3007

Optimization of Flux-Tunable Microwave Resonators for Strong Single-Photon Optomechanics in Nano-Electromechanical Systems — •Korbinian Rubenbauer[1,2], Thomas Luschmann[1,2], Kedar Honasoge[1,2], Achim Marx[1,2], Kirill G. Fedorov[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, Munich, Germany

Quantum sensing leverages quantum properties to enhance the precision of sensing applications. One promising implementation for the detection of forces or accelerations are optomechanical systems which encode the displacement of a low-frequency mechanical element onto the properties of a high-frequency optical or electromagnetic resonator. We present a flux-tunable superconducting quantum circuit with an integrated superconducting quantum interference device (SQUID), where the mechanical element is embedded in the SQUID structure. This implements a magnetic field and flux tunable optomechanical interaction with the prospect of reaching the strong single-photon coupling regime. We discuss the design concept of the device and detail its optimization. We corroborate the conceptual improvements with experimental data demonstrating the performance improvements of the microwave resonator, the optomechanical coupling and the mechanical element.

DY 22: Focus Session: Recent Progresses in Criticality in the Presence of Boundaries and Defects I (joint session DY/TT)

In recent years there has been a renewed interest in critical systems in the presence of boundaries or, more generally, defects. This attention is driven by different perspectives. Numerical studies of quantum spin models have reported in some cases unexpected boundary critical behavior. This, in turns, has led to a reconsideration of the classical surface critical behavior problem, with the discovery of so-far overlooked boundary phases. In this context, numerous recent studies have considered the so-called symmetry-protected topological gapless systems, and in particular their boundary states. At the same time, advances in conformal field theory, specifically the conformal bootstrap program, have addressed the problem of boundaries and defects in conformally-invariant theories. This Focus Session brings together some of the main actors in the aforementioned advancements in boundary critical phenomena.

Organized by Francesco Parisen Toldin (Aachen) and Stefan Wessel (Aachen)

Time: Wednesday 9:30–12:30 Location: A 151

Invited Talk DY 22.1 Wed 9:30 A 151

Boundary behavior at classical and quantum phase transitions — •Max Metlitski — Physics Department, MIT, Cambridge, MA, USA

There has been a lot of recent interest in the boundary behaviour of materials. This interest is driven in part by the field of topological states of quantum matter, where exotic protected boundary states are ubiquitous. In this talk, I'll ask: what happens at a boundary of a system, when the bulk goes through a phase transition. While this question was studied in the context of classical statistical mechanics in the 70s and 80s, basic aspects of the boundary phase diagram for the simplest classical phase transitions have been missed until recently. I'll describe progress in this field, as well as some extensions to quantum phase transitions.

DY 22.2 Wed 10:00 A 151

Universal results for near-critical systems in presence of defects — •Gesualdo Delfino — SISSA, Trieste, Italy

We show how low-energy singularities in field theory lead to exact universal predictions for near-critical systems in presence of defects and present the results for the order parameter profiles in three different cases: the three-dimensional XY model with boundary conditions producing a vortex line [1], the three-dimensional Ising model with boundary conditions leading to the formation of an interface [2], and the time evolution from domain wall initial conditions in quantum one-dimensional ferromagnets [3]. In the three cases, the theoretical predictions are successfully compared with numerical results.

References:

[1] Gesualdo Delfino, Walter Selke and Alessio Squarcini, Vortex mass in the three-dimensional O(2) scalar theory, Phys. Rev. Lett. 122 (2019) 050602

[2] Gesualdo Delfino, Walter Selke and Alessio Squarcini, Particles, string and interface in the three-dimensional Ising model, Nucl. Phys. B 958 (2020) 115139

[3] Gesualdo Delfino and Marianna Sorba, Space of initial conditions and universality in nonequilibrium quantum dynamics, Nucl. Phys. B 983 (2022) 115910

DY 22.3 Wed 10:15 A 151

Emergent geometry at the critical point — •Giacomo Gori — Heidelberg University

Critical correlations in a bounded system with ordered boundary are argued to be function of a suitably chosen metric g. This isotropic metric rules the order parameter profile according to general scaling arguments. These statements are verified via extensive Monte Carlo simulations. A natural candidate for g is the solution of a differential geometry problem known as Yamabe problem i.e. find a local

rescaling of a metric making curvature constant. The correct Yamabe problem to be considered entails a fractional (anomalous in physics) generalization of the Ricci scalar curvature.

DY 22.4 Wed 10:30 A 151

Many-body correlations at wetting. Exact results — •Alessio Squarcini — Institute for Theoretical Physics, Innsbruck

The exact characterization of correlations in the presence of strongly fluctuating interfaces has always been considered a difficult problem in classical statistical mechanics. In this talk we present exact results for density correlations for an interface forming a droplet in two dimensions whose endpoints are pinned on a wall. Our framework, which hinges on recently developed field-theoretical techniques, applies to interfaces entropically repelled by a hard wall as well as to the regime of wetting transitions that we characterize also via the notion of interface structure factor in capillary wave theory. We will show that for entropically repelled interfaces the finite extent of the droplet yields finite-size corrections to correlation functions. These corrections are interpreted as adsorption of bubbles and self-interaction of the interface; their exact form is identified, interpreted in terms of Brownian excursions, and finally tested against high-precision Monte Carlo simulations in the absence of adjustable parameters. This analysis allows us to resolve a 40-years old discrepancy observed in early Monte Carlo studies. For the regime of wetting we present a recent conjectured expression for n-point correlation functions whose proof is a current work in progress.

A. Squarcini and A. Tinti, SciPost Phys. 15, 164 (2023). A. Squarcini and A. Tinti, Journal of High Energy Physics, 123 (2023). A. Squarcini and A. Tinti, J. Stat. Mech. (2023) 013206

DY 22.5 Wed 10:45 A 151

Emergent conformal boundaries from finite-entanglement scaling in matrix product states — •Rui-Zhen Huang — Department of Physics and Astronomy, University of Ghent, Belgium

The use of finite entanglement scaling with matrix product states (MPS) has become a crucial tool for studying 1+1d critical lattice theories, especially those with emergent conformal symmetry. We argue that finite entanglement introduces a relevant deformation in the critical theory. As a result, the bipartite entanglement Hamiltonian defined from the MPS can be understood as a boundary conformal field theory with a physical and an entanglement boundary. We are able to exploit the symmetry properties of the MPS to engineer the physical conformal boundary condition. The entanglement boundary, on the other hand, is related to the concrete lattice model and remains invariant under this relevant perturbation. Using critical lattice models described by the Ising, Potts, and free compact boson CFTs, we illustrate the influence of the symmetry and the relevant deformation on the conformal boundaries in the entanglement spectrum.

15 min. break

Invited Talk DY 22.6 Wed 11:15 A 151

Criticality senses topology — Oleg Vasilyev[2], •Anna Maciolek[1], and Siegfried Dietrich[2] — [1]Institute of Physical Chemistry Polish Academy of Sciences, Warsaw — [2]Max-Planck-Institute for Intelligent Systems, Stuttgart

It is well known that near the critical point, the behavior of a condensed matter system is characterized by the universality class. According to the concept of universality, the critical exponents governing the power law behavior of physical quantities, as well as the corresponding scaling functions, are the same within one universality class. In this lecture I will ask the question to what extent critical behavior "recognizes" the topology of the manifold supporting the critical system. This question is important because topological surfaces can either form spontaneously, such as vesicle membranes in biological systems, or they can be fabricated, such as Möbius rings, from microsized single crystals or from self-assembled chiral block copolymers. I will talk about our recent research that tried to answer this question for Ising-like systems, using Monte Carlo simulations of the Ising model on finite two-dimensional manifolds with different topologies.

DY 22.7 Wed 11:45 A 151

Critical Casimir forces for quenched surface disorder in the 2d Ising model — Luca Cervellera and •Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen

For the anisotropic square-lattice Ising model, the critical Casimir amplitude and force can be calculated exactly for many geometries and boundary conditions. From a recent exact solution for the cylinder with length L, circumference M, and with arbitrary quenched random boundary conditions at one boundary, we determine the full density of thermodynamic states $\omega(f^{(\mathrm{ex})}, m_{\mathrm{B}})$, with excess free energy per boundary spin $f^{(\mathrm{ex})}$ and boundary magnetization m_{B}, at criticality. From an analysis of this quantity we can derive the disorder averaged Casimir potential and Casimir force for different aspect ratios and disorder ensembles.

DY 22.8 Wed 12:00 A 151

Quantifying nonuniversal corner free energy contributions in weakly-anisotropic two-dimensional critical systems — •Florian Kischel and Stefan Wessel — RWTH Aachen University, Aachen, Germany

Confined two-dimensional critical systems with corners along the boundary of the spatial domain exhibit a logarithmic contribution to the free energy density. For conformal invariant bulk systems, this corner term has been derived by Cardy and Peschel in terms of the underlying central charge. However, for weakly anisotropic systems, the corner term deviates from this conformal field theory prediction, and the question arises, whether this anisotropy effect can be further quantified in a general way in terms of the asymptotic critical fluctuations. Here, we derive an exact formula for the corner free energy contribution of weakly-anisotropic two-dimensional critical systems in the Ising universality class on rectangular domains, expressed in terms of quantities that specify the anisotropic fluctuations. The resulting expression compares well to numerical exact calculations that we perform for the anisotropic triangular Ising model and quantifies the nonuniversality of the corner term for anisotropic critical two-dimensional systems. Our generic formula is exected to apply also to other weakly-anisotropic critical two-dimensional systems that allow for a conformal field theory description in the isotropic limit.

DY 22.9 Wed 12:15 A 151

Confinement of magnetic solitons and edge states in van-der Waals FeOCl — •Angela Möller[1], Martin Panthöfer[1], Stefanie Berinskat[1], Fabian Predelli[2], and Peter Lemmens[2] — [1]Dept. Chemistry, JGU Mainz, Mainz, Germany — [2]IPKM, TU Braunschweig, Braunschweig, Germany

In a comparative and systematic study of the isostructural van-der Waals materials ScOCl, ScOBr, FeOCl, the origin of unconventional magnetic properties of FeOCl has been investigated. Evidence for a size dependent order parameter and fluctuations are found in Mössbauer and Raman spectroscopy in conjunction with thermodynamic data and X-ray diffraction. We discuss our data in relation to soliton condensation into topological edge states.

Funding by the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) under the projects 443703006 (CRC 1487) and 442589410 is gratefully acknowledged. PL and FP acknowledge support by DFG GrK 1952/2, Metrology for Complex Nanosystems-NanoMet and DFG EXC-2123 QuantumFrontiers - Light and Matter 390837967.

DY 23: Stochastic Thermodynamics

Time: Wednesday 9:30–13:00 Location: BH-N 128

DY 23.1 Wed 9:30 BH-N 128

Entropy production and thermodynamic inference for stochastic swimmers — •Michalis Chatzittofi[1], Jaime Agudo-Canalejo[1], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — [2]University of Oxford, Oxford, Germany

The question of characterization of the degree of non-equilibrium activity in active matter systems is studied in the context of a stochastic microswimmer model driven by a chemical cycle. The resulting dynamical properties and entropy production rate unravel a complex interplay between the chemical and the hydrodynamic degrees of freedom beyond linear response, which is not captured by conventional phenomenological approaches. By studying the precision-dissipation trade-off, a new protocol is proposed in which microscopic chemical driving forces can be inferred experimentally. Our findings highlight subtleties associated with the stochastic thermodynamics of autonomous microswimmers.

DY 23.2 Wed 9:45 BH-N 128

An estimator of entropy production for partially accessible Markov networks based on the observation of blurred transitions — •Benjamin Ertel and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

A central task in stochastic thermodynamics is the estimation of entropy production for partially accessible Markov networks as these models correspond to the partial observation of real-world systems. We establish an effective transition-based description for partially accessible Markov networks with transitions that are not distinguishable and therefore blurred for an external observer. We demonstrate that, in contrast to the description of fully resolved transitions, this effective description is non-Markovian at any point in time. We derive an information-theoretic bound for this non-ideal observation scenario which reduces to an operationally accessible entropy estimator under specific conditions that are met by a broad class of systems. We illustrate the operational relevance of this system class and the quality of the corresponding entropy estimator based on the numerical analysis of various representative examples.

DY 23.3 Wed 10:00 BH-N 128

Fluctuating Entropy Production on the Coarse-Grained Level: Inference and Localization of Irreversibility — •Jann van der Meer, Julius Degünther, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Stochastic thermodynamics provides the framework to analyze thermodynamic laws and quantities along individual trajectories of small but fully observable systems. If the observable level fails to capture all relevant degrees of freedom, some form of effective, coarse-grained dynamics naturally emerges for which the principles of stochastic thermodynamics generally cease to be applicable straightforwardly. Our work unifies the notion of entropy production along an individual trajectory with that of a coarse-grained dynamics by establishing a framework based on snippets and Markovian events as fundamental building blocks. A key asset of a trajectory-based fluctuating entropy production is the ability to localize individual contributions to the total entropy production in time and space. As an illustration and potential application for inference we introduce a method for the detection of hidden driving. The framework applies equally to even and odd variables and, therefore, includes the peculiar case of entropy production in underdamped Langevin dynamics.

DY 23.4 Wed 10:15 BH-N 128

Thermodynamic cost for precision of general counting observables — •Patrick Pietzonka[1,2] and Francesco Coghi[3] — [1]School of Physics and Astronomy, University of Edinburgh, United Kingdom — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Nordita, KTH Royal Institute of Technology and Stockholm University, Sweden

We analytically derive universal bounds that describe the trade-off between thermodynamic cost and precision in a sequence of events related to some internal changes of an otherwise hidden physical system. The precision is quantified by the fluctuations in either the number of events counted over time or the times between successive events. Our results are valid for the same broad class of nonequilibrium driven systems considered by the thermodynamic uncertainty relation, but they extend to both time-symmetric and asymmetric observables. We show how optimal precision saturating the bounds can be achieved. For waiting time fluctuations of asymmetric observables, a phase transition in the optimal configuration arises, where higher precision can be achieved by combining several signals.

Preprint: arXiv:2305.15392

DY 23.5 Wed 10:30 BH-N 128

Thermodynamic cost of stochastic resetting — •Kristian S. Olsen[1], Deepak Gupta[2], Francesco Mori[3], and Supriya Krishnamurthy[4] — [1]Institut für Theoretische Physik II - Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Nordita, Royal Institute of Technology and Stockholm University, Sweden — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom — [4]Department of Physics, Stockholm University, Sweden

Stochastic resetting gives rise to non-equilibrium steady states, and is known to appear in a wide range of both natural and man-made systems. Recent experiments have implemented resetting by means of an external trap, whereby a particle relaxes to the minimum of the trap and as such is reset in a finite time. Here we present a framework able to fully characterise the thermodynamic work of such resetting protocols. Our results are valid for a wide range of system, with the only assumption being that of relaxation to equilibrium in the resetting trap. Optimal trap shapes that minimise the work are studied for the case of Brownian motion.

DY 23.6 Wed 10:45 BH-N 128

Decoding sample-to-sample fluctuations in the time-ordering of non-Markovian sample paths — •Felix Tippner and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Inherent to almost all measurements is the loss of information as only a small number of degrees of freedom can be simultaneously observed. These measurements track projections of higher dimensional stochastic processes. Besides introducing (or enhancing) non-Markovian effects, such projections often hide features like irreversible currents (i.e., driven vs. non-driven) or barriers in the energy landscape. By studying correlations and comparing (systematic) sample-to-sample fluctuations of path-wise observables, such as empirical densities and currents inferred from projected trajectories—which may correspond, e.g., to time series of single-molecule measurements—we are able to gain qualitative insight into the aforementioned hidden features that cannot be observed upon ensemble averaging.

DY 23.7 Wed 11:00 BH-N 128

Nonequilibrium fluctuations of chemical reaction networks at criticality — •Benedikt Remlein and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Chemical reaction networks can undergo nonequilibrium phase transitions upon variation of external control parameters like the chemical potential of one species. We investigate the critical fluctuations of the flux in the associated chemostats, which is proportional to the entropy production, for two paradigmatic models, the Schlögl model and the Brusselator. In both cases, numerical simulations show that the corresponding diffusion coefficient diverges at the critical point as a function of system size albeit with different exponents. In the vicinity of the transition, the diffusion coefficient in the Schlögl model follows a scaling form. We develop an analytical approach based on van Kampen's system size expansion that yields these exponents. For the Brusselator model, we numerically find that the diffusion coefficient as function of the control parameter develops a discontinuity while increasing the system size.

15 min. break

DY 23.8 Wed 11:30 BH-N 128

Thermodynamically efficient agents — •Paul C. Barth, Lukas

J. Fiderer, Isaac D. Smith, Marius Krumm, Fulvio Flamini, and Hans J. Briegel — Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria

Landauer's bound and its generalizations such as the information-processing second law provide energetic limits not only on information erasure but also on pattern manipulation and computations in general. In this work, we generalize these bounds further to account for agents which interact with an environment via a percept-action loop. Within our framework, we then design and analyze toy environments and thereby demonstrate that efficient agents, which maximize work production, do not always adhere to zero entropy production. Furthermore, we introduce a thermodynamic framework for learning by leveraging similarities between maximum work extraction and reward maximization in reinforcement learning. We apply this framework to an existing reinforcement learning scheme, namely projective simulation. We also discuss a possible quantization of our framework. This line of research promises new insights into the energetic aspects of adaptive behavior in natural and artificial system.

DY 23.9 Wed 11:45 BH-N 128

Thermodynamically consistent model of an active Ornstein-Uhlenbeck particle — •Jonas Fritz and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Identifying the full entropy production of active particles is a challenging task. We introduce a microscopic, thermodynamically consistent model that leads to active Ornstein-Uhlenbeck statistics in the continuum limit [1]. Our minimal model consists of a particle with a fluctuating number of active reaction sites which contribute to its active self-propulsion on a lattice. In addition, the model also takes ordinary thermal noise into account. This approach allows us to identify the full entropy production stemming from both thermal diffusion and active driving. Extant methods based on the comparison of forward and time-reversed trajectory underestimate the physical entropy production when applied to the Langevin equations obtained from our model. Constructing microscopic Markovian models can thus provide a benchmark for determining the entropy production in non-Markovian active systems.

[1] Jonas H. Fritz and Udo Seifert, J. Stat. Mech. (2023) 093204

DY 23.10 Wed 12:00 BH-N 128

Thermodynamics of active matter: Tracking dissipation across scales — •Robin Bebon, Joshua F. Robinson, and Thomas Speck — Institute for Theoretical Physics 4, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

The non-equilibrium "active" nature of living systems becomes manifest in the spatial and temporal organization of hierarchical structures, which provide essential functionality. Maintaining activity is necessarily coupled to continual energy consumption, which in turn posits dissipation as the central constraint of any such process. Here we derive exact expressions for the dissipation rate of catalytically propelled active particles, ranging across length scales from individual agents to large-scale collectives. Commencing from a microscopic model of a single catalytic particle that interacts with explicit solute molecules, we motivate a mesoscopic many-body description reminiscent of active Brownian particles. Through further coarse-graining, we obtain a macroscopic field theoretic description based on effective hydrodynamic equations and sketch how to treat scalar field theories. This systematic bottom-up construction enables precise bookkeeping of the degrees of freedom that partake in the stochastic energetics and shows that dissipation is, both locally and globally, accompanied by a continual solute flux between solute reservoirs. We employ our results to gain insights into the thermodynamic footprint of confinement and the role of dissipation in motility-induced phase separation. Moreover, we demonstrate how the phenomenological framework of linear irreversible thermodynamics unfolds from our microscopic approach.

DY 23.11 Wed 12:15 BH-N 128

Active matter under control — Luke K. Davis[1,2], Karel Proesmans[1,3], and •Etienne Fodor[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg — [2]Department of Mathematics, University College London, 25 Gordon Street, London, England — [3]Niels Bohr International Academy, Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100 Copenhagen, Denmark

Active constituents burn fuel to sustain individual motion, giving rise to collective effects that are not seen in systems at thermal equilibrium. There is a great potential in harnessing the striking phenomenology of active matter to build novel controllable and responsive materials that surpass passive ones. Yet, we currently lack a systematic roadmap to predict the protocols driving active systems between different states in a way that is thermodynamically optimal. Equilibrium thermodynamics is an inadequate foundation to this end, due to the dissipation rate arising from the constant fuel consumption in active matter. Here, we derive and implement a versatile framework for the thermodynamic control of active matter. Combining recent developments in stochastic thermodynamics and nonequilibrium response theory, our approach shows how to find the optimal control for either continuous- or discrete-state active systems operating arbitrarily far from equilibrium. Our results open the door to designing novel active materials which are not only built to stabilize specific nonequilibrium collective states, but are also optimized to switch between different states at minimum dissipation.

DY 23.12 Wed 12:30 BH-N 128

Optimizing the Energetics of the Finite-time Driving of Field Theories — •Atul Tanaji Mohite — Universität des Saarlands

Field theories have been extremely successful in characterizing the universal properties of various phase transitions, and in delineating a few canonical models which capture the essential Physics at play in a large class of systems. Interestingly, a generic framework for optimizing the energetic cost associated with the finite-time driving of such systems is still largely missing. Here, building on recent advances in stochastic thermodynamics and optimal transport theory, we show how to analytically derive the optimal driving protocols that minimize work, which we apply to cases with either conserved or non-conserved scalar order parameters in the weak noise regime. Moreover, we formulate a numerical multi-optimization problem to simultaneously optimize the mean and variance of work, leading to revealing a first-order phase transition in the corresponding Pareto front, which features the coexistence of multiple optimal protocols. Overall, our results elucidate how to drive field dynamics at a minimal energetic cost, with the potential to be deployed in a broad class of systems.

DY 23.13 Wed 12:45 BH-N 128

Geometrically frustrated systems which are as singles hotter than in company — •Wolfgang Bauer — Dept. of Internal Medicine I, UKW, Würzburg, Germany

Systems of same temperature, which are brought from initial isolation to weak thermal coupling, maintain their temperature, which is equivalent to that of the combined system. Any other scenario would be in conflict with our notion of thermal stability and the 2nd law of thermodynamics. Special geometrically frustrated systems (GFSs), which are constraint to reside at negative Boltzmann temperature, challenge the above notion. When brought in weak thermal contact, the assembly of GFSs is in equilibrium cooler than its constituents, and may even exhibit positive Boltzmann temperatures. The 2nd law of thermodynamics would imply heat flow related to the gradient of Boltzmann temperatures between a single GFS and the residual assembly under equilibrium conditions. This conflict is resolved by considering the canonical temperature of a GFS, derived from information theory, which differs from its Boltzmann temperature. We show, that the gradient of Boltzmann temperatures predicts the stochastic drift of the most probable state of a GFS within its environment, whereas the canonical temperature gradient defines the direction of heat flow, which restores the 2nd law of thermodynamics.

DY 24: Focus Session: New Trends in Nonequilibrium Physics – Conservation Laws and Nonreciprocal Interactions I

Nonequilibrium phase transitions and pattern formation are known from numerous examples of open systems, where external reservoirs and gradients prevent relaxation to thermodynamic equilibrium. In recent years, related research in biology and soft matter systems in physics and chemistry has increasingly focused on active matter, where energy is injected locally. This often involves mass conservation constraints and, in many cases, in addition non-reciprocal interactions of the involved entities, such as macromolecules or cells. Both have far reaching consequences on the universal dynamical behavior of a wide range of nonequilibrium systems and require classical concepts of nonlinear and statistical physics, such as phase transitions, to be reconsidered and developed further. For example, well-known approaches to nonequilibrium pattern formation require substantial extensions to address conserved systems. Thus, recent theoretical studies in this field have revealed many novel phenomena, such as arrested coarsening, odd elasticity, oscillatory phase separation, persistent wave dynamics, and active turbulence. Many of these aspects have by now been confirmed by experimental findings, for example, in intracellular pattern formation or collective dynamics in colloidal systems. This symposium will provide a well-balanced overview of experimental and theoretical progress in this new, exciting area.

Organized by Markus Bär (Berlin) and Carsten Beta (Potsdam)

Time: Wednesday 9:30–13:00 Location: BH-N 243

Invited Talk DY 24.1 Wed 9:30 BH-N 243

The nonreciprocal Cahn-Hilliard model - properties and significance — •Uwe Thiele[1,2], Tobias Frohoff-Hülsmann[1], and Daniel Greve[1] — [1]Institut für Theoretische Physik, Universität Münster, Germany — [2]Center for Nonlinear Science (CeNoS), Universität Münster, Germany

The phenomenologically introduced nonreciprocal Cahn-Hilliard (NRCH) model couples densities with mass-conserving dynamics via a nonreciprocal interaction [1]. After discussing types of nonreciprocity and their relation to a 'spurious' gradient dynamics form (allowing for a Maxwell construction) we show that the NRCH model features conserved-Turing and conserved-Hopf instabilities beside the usual Cahn-Hilliard instability. Then, we discus the model's role as a high-codimension amplitude equation (AE) placing it within a hierarchy of AE for the eight types of instabilities of uniform steady states in homogeneous isotropic systems resulting from the combination of three features: large- vs small-scale, stationary vs oscillatory, and with vs without conservation law(s) [2]. Further, a codimension-one AE for the conserved-Hopf instability is discussed and compared to [3].

[1] ZH You, A Baskaran, MC Marchetti, PNAS 117, 19767 (2020); S Saha, J Agudo-Canalejo, R Golestanian, PRX 10, 041009 (2020); T Frohoff-Hülsmann, J Wrembel, U Thiele, PRE 103, 042602 (2021). [2] T Frohoff-Hülsmann, U Thiele, PRL 131, 107201 (2023). [3] A Nepomnyashchy, S Shklyaev, J Phys A 49, 053001 (2016); A Förtsch, W Zimmermann, DY 4.4, DPG Spring Meeting 2023, Dresden; A Förtsch, Thesis Bayreuth 2023.

DY 24.2 Wed 10:00 BH-N 243

Field-theoretical modeling of a zombie apocalypse* — •Michael te Vrugt[1], Julian Jeggle[2], and Raphael Wittkowski[2] — [1]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom — [2]Institut für Theoretische Physik, Center for Soft Nanoscience, Universität Münster, 48149 Münster, Germany

The physics of systems with nonreciprocal interactions has attracted a significant amount of interest in recent years. A prototypical example are predator-prey systems. In this work [1], we connect the physics of nonreciprocal interactions to epidemiology by developing a dynamical density functional theory for a popular hypothetical infectious disease, namely a zombie outbreak. A numerical investigation of this model is used to compare different strategies for containing the spread of zombies.

[1] M. te Vrugt, J. Jeggle, and R. Wittkowski, arXiv:2307.00437 (2023)

*Funded by the Deutsche Forschungsgemeinschaft (DFG) under Project-IDs 525063330 (MtV) and 433682494 – SFB 1459 (RW).

DY 24.3 Wed 10:15 BH-N 243

Maxwell construction for a nonreciprocal Cahn-Hilliard model — •Daniel Greve[1], Tobias Frohoff-Hülsmann[1], and Uwe Thiele[1,2] — [1]Universität Münster — [2]Center for Nonlinear Science (CeNoS), Universität Münster

Two important models for active, anti-dissipative phenomena are the nonreciprocal two-field Cahn-Hilliard (NRCH) model [1, 2] and active model B+. The latter is a one-field model describing motility-induced phase-separation (MIPS), for which Solon et al. have analyzed phase coexistence through the derivation of a Maxwell construction in terms of a "generalized thermodynamics" [3]. Using a generalised unifying formalism, we provide phase diagrams for a NRCH model. In contrast to active model B+, where only a stationary large-scale instability occurs, the NRCH model exhibits a rich phenomenology, that includes large- and small-scale stationary as well as large-scale oscillatory instabilities [1, 2, 4]. This leads to the occurrence of a crystal-like phase whose coexistence with liquid-like phases we discuss. In passing, we also show how time-periodic behaviour may coexist with stationary one. Finally, we indicate that the relation of the obtained phase diagrams and the behaviour of corresponding finite-size systems resembles the one for passive systems.

[1] Z. H. You et al., Proc. Natl. Acad. Sci. U. S. A. 117, 19767 (2020).
[2] S. Saha et al., Phys. Rev. X 10, 041009 (2020).
[3] A. P. Solon et al., Phys. Rev. E 97, 020602 (2018).
[4] T. Frohoff-Hülsmann et al., Phys. Rev. E 103, 042602 (2021).

DY 24.4 Wed 10:30 BH-N 243

Non-reciprocal alignment can induce asymmetric clustering in active repulsive mixtures — •Kim L. Kreienkamp and Sabine H. L. Klapp — Technische Universität Berlin

It is now well established that non-reciprocal systems exhibit intriguing, novel dynamical phases, the characteristics of which are shaped by the type and degree of non-reciprocity [1-3]. Here, we study a paradigmatic model of non-reciprocal active matter, namely a binary mixture of motile particles with completely symmetric repulsive interactions and non-reciprocal alignment couplings [3]. Using a combination of hydrodynamic theory, linear stability analysis, and particle-based simulations, we find dynamical, asymmetrical clustering situations, in which weakly polarized clusters form out of only one of the two species. Importantly, these asymmetric clusters emerge even though the isotropic repulsive interactions do not distinguish one species. Instead, the clustering is driven solely by non-reciprocal orientational couplings. For systems with antagonistic (anti-)alignment couplings, the resulting single-species clusters move and chase more dilute accumulations of the other species. We present a full non-equilibrium phase diagram in the parameter space of inter-species coupling strengths and compare with particle-based simulations, highlighting the impact of non-reciprocity on various scales.

[1] Z. You et al., PNAS 117, 19767 (2020).
[2] M. Fruchart et al., Nature 592, 363 (2021).
[3] K. L. Kreienkamp and S. H. L. Klapp, New J. Phys. 24, 123009 (2022).

DY 24.5 Wed 10:45 BH-N 243

Mobility-induced condensation and (rotating) crystallization in a higher-order active Phase Field Crystal model — •Alina Barbara Steinberg[1], Max Philip Holl[2], and Uwe Thiele[1,3] — [1]Institut für Theoretische Physik, Universität Münster — [2]Department of Chemistry and Materials Science & Department of Bioproducts and Biosystems, Aalto University — [3]Center for Nonlinear Science, Universität Münster

Active soft matter consisting of self-propelled particles can show a variety of motility-induced phenomena, including phase separation and crystallization, i.e. the formation of clusters with respective liquid-like and crystal-like inner structure. We demonstrate this using an (active) Phase-Field-Crystal model [1-3] of higher order [4]. We consider active and passive cases, present morphological phase diagrams, and examples of localized states that represent the various types of clusters. Finally, we take a closer look at rotating crystallites and the dependence of their properties on control parameters.

[1] H. Emmerich et al., Adv. Phys., 61:665-743, 2012. [2] A. M. Menzel & H. Löwen, Phys. Rev. Lett., 110:055702, 2013. [3] L. Ophaus et al., Phys. Rev. E 98:022608, 2018. [4] Z.-L. Wang et al., Phys. Rev. Materials, 4:103802, 2020.

DY 24.6 Wed 11:00 BH-N 243

Deciphering the interface laws of Turing foams — Henrik Weyer[1], •Tobias Roth[1], and Erwin Frey[1,2] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany — [2]Max Planck School Matter to Life, Hofgartenstraße 8, D-80539 Munich, Germany

Protein pattern formation is central to the spatiotemporal self-organization of both prokaryotic and eukaryotic cells. It is also employed as a key spatial control system in the design of artificial cells. However, it remains unclear how the properties of the macroscopic, highly nonlinear reaction–diffusion patterns can be systematically linked to the underlying reaction network [1]. Here, we show—based on protein-mass conservation—that protein patterns are governed by an effective interfacial tension arising from cyclic steady-state currents of attachment and detachment at the interface. Furthermore, we recover generalized Plateau and von-Neumann laws for two-dimensional liquid foams in two-dimensional mesh patterns. This leads us to introduce "Turing foams," which show generic behavior governed by the interplay of interfacial-tension-driven dynamics and interrupted coarsening, and that we observe experimentally in the *in vitro* Min protein system. Our theory offers a new ansatz to find principles of macroscopic self-organization in mass-conserving systems far from equilibrium.

[1] Halatek, J., Brauns, F. & Frey, E. Philos. Trans. R. Soc. B Biol. Sci. 373, 20170107 (2018).

15 min. break

DY 24.7 Wed 11:30 BH-N 243

Traveling waves and arrested coarsening in a simple model for protein patterns on biomembranes — •Benjamin Winkler[1], Sergio Alonso[2], and Markus Bär[1] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]UPC, Barcelona, Spain

The formation of protein patterns on membranes is important for spatial organization, growth and division of biological cells. In many cases these dynamics is described by coupled, mass-conserving reaction-diffusion equations. Here, we study the dynamics emergent from the coupling of two well-known, mass-conserved systems. System A is given by a simplified reaction-diffusion model for the emergence of cell polarity by proteins undergoing active phase separation. The proteins are fast-diffusing in the bulk of the cell and become activated when they bind to the cell membrane. System B is a Cahn-Hilliard-like equation describing the mixing dynamics of two different lipids. When introducing a coupling between system A and B due to a concentration-dependent interaction affinity, we observe the emergence of traveling waves in system A and likewise, a systematic slowing of the coarsening in system B depending on the coupling strength between the two systems. The primary linear instabilities of the homogeneous steady for the coupled system are all stationary, hence the traveling wave emerge from a secondary instability of a stationary pattern. Our results exemplify the interaction between pattern forming systems with well-separated length scales and illustrate how complex behavior in biological systems can arise from the coupling of simpler subsystems.

DY 24.8 Wed 11:45 BH-N 243

Defect Solutions of the Non-reciprocal Cahn-Hilliard Model: Spirals and Targets — •Navdeep Rana[1] and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), D-37077 Goettingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We study the defect solutions of the Non-reciprocal Cahn-Hilliard model (NRCH). We find two kinds of defects, spirals with unit magnitude topological charge, and topologically neutral targets. These defects generate radially outward travelling waves and thus break the parity and time-reversal symmetry. For a given strength of non-reciprocity, spirals and targets with unique asymptotic wavenumber and amplitude are selected. We use large-scale simulations to show that at low non-reciprocity, a disordered state evolves into quasi-stationary spiral network. With increasing non-reciprocity, we observe networks composed primarily of targets. Beyond a critical threshold, a disorder-order transition from defect networks to travelling waves emerges. The transition is marked by a sharp rise in the global polar order.

DY 24.9 Wed 12:00 BH-N 243

Liquid mechanics - Exploring instabilities in active condensates — •Florian Rasshofer[1], Simon Bauer[1], Alexander Ziepke[1], Ivan Maryshev[1], and Erwin Frey[1,2] — [1]Arnold Sommerfeld Center for Theoretical Physics, LMU Munich, Germany — [2]Max Planck School Matter to Life, Munich, Germany

This study employs a theoretical framework to investigate the stability and morphology of active condensates. Active condensates, characterized by their consumption of chemical energy (fuel), exhibit unique features absent in passive systems. Their non-equilibrium nature allows for stationary pattern-forming states and more exotic phenomena such as self-propelled domains and dividing droplets.

We present a unifying theory that rationalizes dynamical instabilities observed in various systems, encompassing chemotactic motility-induced phase separation to enzymatically active droplets. Analytical results obtained from classical perturbation theory are shown to be in good agreement with finite element simulations, providing valuable insights into the intricate behavior of active condensates.

Beyond theoretical contributions, our work envisions practical applications. The emergent dynamical phases uncovered offer insights into the potential design of self-assembling micro machines capable of extracting work on a scale not admissible to classical mechanics.

DY 24.10 Wed 12:15 BH-N 243

Self-excited oscillations and motion of sessile drops covered by autocatalytic surfactants — •Florian Voss and Uwe Thiele — Institute for Theoretical Physics, University of Münster, Germany

We consider shallow sessile drops of a nonvolatile liquid covered by a mixture of surfactants that can transform into each other via a simple autocatalytic conversion reaction. Based on the form of a passive gradient dynamics model for fields with conserved and nonconserved dynamics we develop a fully reciprocal three-field model with two conservation laws that captures coupled droplet hydrodynamics [1] and a chemical reaction [2]. We then drive the mechanically, thermodynamically and chemically reciprocal system permanently out of equilibrium by in- and outfluxes of surfactants controlled by external chemostats. Then, we study the resulting active system using linear stability analysis, numerical continuation and time simulations. As the chemostat driving strength is varied, we find, inter alia, the emergence of surfactant (Turing) patterns, breathing and swaying drop oscillations, and oscillatory self-propulsion.

[1] U. Thiele, A. J. Archer, M. Plapp, Phys. Fluids, 2012, 24, 102107
[2] D. Zwicker, Curr. Opin. Colloid Interface Sci., 2022, 61, 101606

DY 24.11 Wed 12:30 BH-N 243

Escaping kinetic traps using non-reciprocal interactions — Saeed Osat[1], •Jakob Metson[1], Mehran Kardar[2], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Göttingen, Germany — [2]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, United States — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

A prominent problem for systems trying to find a global energy minimum is getting trapped in deep local minima. In this work we show that by using non-reciprocal interactions we can drive systems out of

these kinetic traps to end up at a global minimum. We use multifarious self-assembly as a model system, where systems are designed to store and assemble multiple different structures. Firstly we demonstrate that by introducing non-reciprocal interactions we enable systems to escape from chimeric states (kinetic traps), which with only reciprocal interactions are practically impossible to escape from. Then we look in more detail at the escape dynamics in our model system. The principle escape mechanism is interface growth. We find that the interface dynamics in our non-reciprocal system falls into the KPZ universality class. Furthermore, we study escape via spiraling point defects. These can either annihilate pairwise, leaving the system trapped, or reach the boundary of the structure which leads to successful escape. Although we focus on multifarious self-assembly as a model system, in principle these ideas can be applied to a wide range of complex systems, being particularly impactful for systems with rough energy landscapes.

DY 24.12 Wed 12:45 BH-N 243

Correlation effects in the non-reciprocal Ising system — •Kristian Blom[1], Uwe Thiele[2], and Aljaz Godec[1] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen — [2]Universität Münster, Münster

Non-variational continuum models like the non-reciprocal Cahn-Hilliard model are typically constructed using phenomenological reasoning, and their full consistency with microscopic models may thus not be taken for granted. In this talk, we focus on the bottom-up construction of a non-reciprocal phase field system, starting from a pair of opposing non-reciprocally coupled Ising models evolving according to Kawasaki or Glauber dynamics. To analyze the thermodynamic properties of the system, we develop a kinetic variant of the Bethe-Guggenheim approximation that explicitly accounts for pair-correlations, and thus goes beyond the mean field reasoning. Unlike the mean field approximation, our approach provides results for both, the magnetization and local defects within and between the lattices. The coupling between the magnetization and defects gives rise to a rich kinetic phase diagram. Our results reveal the conditions under which the various phases are stable, and how they depend on both, the reciprocal and non-reciprocal coupling between spins.

DY 25: Active Matter III (joint session DY/BP/CPP)

Time: Wednesday 9:30–13:00 Location: BH-N 334

Invited Talk DY 25.1 Wed 9:30 BH-N 334

Emergent chemotaxis in synthetic active matter — •Abhinav Sharma[1,2], Hidde Vuijk[1], Pierluigi Muzzeddu[3], Holger Merlitz[2], and Jens-Uwe Sommer[2] — [1]Universität Augsburg, 86159 Augsburg — [2]Leibniz Institute für Polymerforschung, Dresden — [3]SISSA, Trieste, Italy

Active particles with their characteristic feature of self-propulsion are regarded as the simplest models for motility in living systems. The accumulation of active particles in low activity regions has led to the general belief that chemotaxis requires additional features and at least a minimal ability to process information and to control motion. We show that self-propelled particles display chemotaxis and move into regions of higher activity if the particles perform work on passive objects, or cargo, to which they are bound. The origin of this cooperative chemotaxis is the exploration of the activity gradient by the active particle when bound to a load, resulting in an average excess force on the load in the direction of higher activity. In fact chemotaxis should emerge in all those structures which allow cooperative exploration of the activity landscape. We demonstrate this in simple assemblies of active molecules, which show robust chemotaxis both under static and dynamic activity landscapes.

DY 25.2 Wed 10:00 BH-N 334

Active particles interacting via phase-separating chemicals — •Dennis Schorn, Aritra K. Mukhopadhyay, and Benno Liebchen — Institut für Physik Kondensierter Materie, Technische Universität Darmstadt, Germany

Synthetic active particles self-propel by catalyzing a certain chemical reaction and moving up or down the resulting concentration gradient. In this talk, we present our study of the collective dynamics of chemotactic active particles which interact via self-produced chemicals that have an intrinsic tendency to phase separate. When the chemical interactions are attractive (chemoattraction), the particles aggregate to form a large cluster. In contrast, chemorepulsive particles exhibit two distinct patterns: a stationary foam-like structure and an oscillating stripe pattern. We explain the origins of these structures through a comprehensive linear stability analysis of our system. Our findings underscore that the intricate interplay between chemical phase separation and particle chemotaxis induces new instabilities, leading to the formation of unique patterns.

DY 25.3 Wed 10:15 BH-N 334

Towards the cybernetics of active matter — •Alexander Ziepke[1], Ivan Maryshev[1], Igor S. Aranson[2], and Erwin Frey[1,3] — [1]Arnold Sommerfeld Center and CeNS, LMU, Munich, Germany — [2]Dept. Biomed. Eng., Penn State University, University Park, PA, USA — [3]Max Planck School Matter to Life, Munich, Germany

Cybernetics describes the self-organized behavior of collectives of individual units in response to their environment, often taking inspiration from biological processes. Different organisms have developed various communication strategies to control such collective responses. For instance, social amoeba use chemical signaling to form localized aggregates in response to starvation, insects such as ants secrete pheromones for navigation, and bats and birds employ acoustic signals to form cohesive swarms. Our research focuses on how chemical and acoustic communication enables the formation of collective states with cooperative functionality, a targeted specification of the units, and the control of a coordinated response. In particular, we show that acoustic signaling of oscillatory agents leads to the formation of synchronized localized clusters and collectively propagating snake- and larva-like structures with distinct acoustic signatures. By emitting acoustic waves, these emergent structures are able to sense environmental changes, such as approaching reflective objects, and respond with a coordinated change in phenotype. This study provides insights into design principles for unsupervised microrobots, able to form adaptive, multi-functional structures with population-level cognitive capabilities (Ziepke, Maryshev, Aranson, Frey., Nat Commun 13, 6727 (2022)).

DY 25.4 Wed 10:30 BH-N 334

Active Spaghetti: Collective Organization in Cyanobacteria — •Jan Cammann[1], Mixon K. Faluweki[2,3], Lucas Goehring[2], and Marco G. Mazza[1] — [1]Loughborough University, UK — [2]Nottingham Trent University, UK — [3]Malawi Institute of Technology

Filamentous cyanobacteria can show fascinating examples of nonequilibrium self-organization, which, however, are not well understood from a physical perspective. We investigate the motility and collective organization of colonies of these simple multicellular lifeforms. As their area density increases, linear chains of cells gliding on a substrate show a transition from an isotropic distribution to bundles of filaments arranged in a reticulate pattern. Based on our experimental observations of individual behavior and pairwise interactions, we introduce a nonreciprocal model accounting for the filaments large aspect ratio, fluctuations in curvature, motility, and nematic interactions. This minimal model of active filaments recapitulates the observations, and rationalizes the appearance of a characteristic length scale in the system, based on the Péclet number of the cyanobacteria filaments.

Reference: M. Faluweki, J. Cammann, et al. Phys. Rev. Lett. 131, 158303 (2023)

DY 25.5 Wed 10:45 BH-N 334

Collective dynamics and pair-distribution function of active Brownian ellipsoids* — Stephan Bröker[1], •Michael te Vrugt[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Universität Münster, 48149 Münster, Germany — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

While the collective dynamics of spherical active Brownian particles is relatively well understood by now, the much more complex dynamics of nonspherical active particles still raises interesting open questions. Previous work has shown that the dynamics of rod-like or ellipsoidal active particles can differ significantly from that of spherical ones. In this

work [1], we obtain the full state diagram of active Brownian ellipsoids depending on the Péclet number and packing density via computer simulations. The system is found to exhibit a rich state behavior that includes cluster formation, local polar order, polar flocks, and disordered states. Moreover, we obtain numerical results and an analytical representation for the pair-distribution function of active ellipsoids. This function provides useful quantitative insights into the collective behavior of active particles with lower symmetry and has potential applications in the development of predictive theoretical models.

[1] S. Bröker, M. te Vrugt, and R. Wittkowski, arXiv:2307.15535 (2023)

*Funded by the Deutsche Forschungsgemeinschaft (DFG) under Project-IDs 525063330 (MtV) and 283183152 (WI 4170/3) (RW).

DY 25.6 Wed 11:00 BH-N 334

Flow and orientational properties of active nematic liquid crystals under an electric field — •Yutaka Kinoshita and Nariya Uchida — Department of Physics, Tohoku University, Sendai, Japan

Active nematic liquid crystals are materials where each constituent has nematic symmetry and produces dipolar flow along its axis. Examples include microtubule-kinesin suspensions and actomyosin networks. Because of the input of energy into the system, the state is driven out of thermodynamic equilibrium and shows a chaotic flow called active turbulence. The flow patterns are controlled by external field, confinement, and friction. An external field induces reorientation of the active elements and suppresses chaotic flow. Here we numerically simulate the effects of an electric field on the dynamics of two-dimensional active nematics [1].

We found transitions among three states that are characterized by the degree of flow anisotropy: the active turbulence, laning state, and uniformly aligned state. The average flow speed and its anisotropy are maximized in the laning state. We also found localization of vortices and topological defects associated with periodic shifts between active turbulence and laning state, which is similar to experimentally observed oscillations in a friction-controlled system. Our results might lead to a further understanding of the dynamical states of active nematics under an external field.

[1] Y. Kinoshita and N. Uchida, Phys. Rev. E **108**, 014605 (2023)

15 min. break

DY 25.7 Wed 11:30 BH-N 334

From Active Chiral Particles to the Active Model B + — •Erik Kalz[1], Abhinav Sharma[2,3], and Ralf Metzler[1,4] — [1]University of Potsdam, Germany — [2]University of Augsburg, Germany — [3]Leibniz-Institute for Polymer Research, Dresden, Germany — [4]Asia Pacific Centre for Theoretical Physics, Pohang, Republic of Korea

A first-principles approach for active chiral hard disks is presented, that explicitly accounts for steric interactions on the two-body level. With a handle on the full derivation, we explicitly point out the necessary assumptions to derive the field-theoretical description for Active Chiral Particles. By considering different regimes of the Péclet number, the well-known models in active matter can be obtained through our consideration. Explicitly, we derive the phenomenological Model B. By going to higher orders in the closure scheme, we show that this first-principles approach results in the recently introduced Active Model B +, a natural extension of Model B for active processes. Contrary to systems without chirality and to previous derivations, we find that chirality can change the sign of the characteristic activity parameters. This has profound consequences for the already shown effects in the Active Model B +. Finally, we draw a connection between Active Chiral Particles and Odd Diffusion, a phenomenon that has attracted considerable attention recently, and for which Active Chiral Particles are handled as an exemplary system.

Ref: E. Kalz, A. Sharma, and R. Metzler: *arXiv preprint arXiv:2310.16691*, 2023

DY 25.8 Wed 11:45 BH-N 334

Phase Behaviour of a Minimal Chiral Active Ising Lattice Model — •Boyi Wang[1,3], Frank Jülicher[1,4,5], and Patrick Pietzonka[2,1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom — [3]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [4]Center for Systems Biology Dresden (CSBD), Dresden, Germany — [5]Cluster of Excellence, Physics of Life, TU Dresden, Dresden, Germany

We introduce chiral activity into a lattice model with Ising interactions, achieved by locally rotating a random selected 2×2 neighbourhood of lattice site each time step only in clockwise direction. Monte Carlo simulations at low temperature reveal a path to condensate formation, marked by the evolution of the droplet's edge into a particular tilted orientation relative to the square lattice. This tilt angle depends on the local rotation direction, thus reflecting the chirality of the model on a macroscopic scale.

Furthermore, we investigate the stability of the chiral tilted angle in the droplet's lattice field. We identify a persistent edge current flowing along the droplet's interface. By an equivalent 1D model, we also quantify this current-angle dependence, allowing us to identify the angles that emerge in the stationary state.

Our findings provide a novel perspective on chiral non-equilibrium systems in a discrete and analytical framework, expanding our understanding of how chiral driving forces influence the formation and interface behaviour of active droplets.

DY 25.9 Wed 12:00 BH-N 334

Long-range fluctuation-induced forces in chiral active fluids — Hashem Fatemi[1], Hamidreza Khalilian[1], Jalal Sarabadani[1], and •Reza Shaebani[2] — [1]Institute for Research in Fundamental Sciences (IPM), Iran — [2]Department of Theoretical Physics, Saarland University, Germany

We study long-range fluctuation-induced (FI) interactions in chiral active matter systems. We show that the combination of self-rotation and self-propulsion can lead to large FI forces, depending on the elongation of active particles. Such strong forces can contribute to self-organization of chiral active matter into dynamic structures and patterns. We numerically measure the FI forces between intruders immersed in chiral active fluids and find that the influence of chirality depends on the particle elongation in the active bath. For round active objects, the FI force monotonically decreases with increasing chirality since the active bath structure gradually changes from rotating flocks and vortices to localized spinners. Contrarily, for elongated active objects there is an optimal chiral angle at which the magnitude and range of the FI interaction are maximized. We explain how the balance of collisions around the intruders varies with chirality and separation between the intruders.

DY 25.10 Wed 12:15 BH-N 334

Self-Solidifying Active Droplets Showing Memory-Induced Chirality — •Aritra K. Mukhopadhyay[1], Kai Feng[2], José Carlos Ureña Marcos[1], Ran Niu[2], Qiang Zhao[2], Jinping Qu[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany. — [2]Huazhong University of Science and Technology, 430074 Wuhan, China.

Synthetic microswimmers have yet to achieve the autonomy and versatility of their biological counterparts, particularly in terms of energy supply and motion diversity. Here, we introduce an all-aqueous droplet swimmer that shows remarkable autonomy and rich dynamics without any external driving mechanism [1]. Comprising a surface tension-lowering polyelectrolyte mixture, the droplets undergo self-solidification on acidic water surfaces, gradually emitting polyelectrolytes into the surroundings. A spontaneous asymmetry of the emitted polyelectrolyte concentration along the droplet surface induces Marangoni flows, which causes the droplet to self-propel. The slowly diffusing polyelectrolytes form long-lived chemical trails creating memory effects that drive a dynamic transition from linear to chiral motion. This showcases the droplet's ability to navigate its environment in a persistent, directional manner requiring no externally imposed symmetry breaking. Practical applications are highlighted through the droplets' highly efficient uranium removal from wastewater. Our results provide a route to fueling self-propelled agents that can autonomously perform chiral motion and collect toxins.

[1] K. Feng et al., Advanced Science 10, 2300866 (2023).

DY 25.11 Wed 12:30 BH-N 334

Optimising transport of active magnetic particles with finite internal magnetic anisotropy — Andrey Kuznetsov[1], Ekaterina Novak[2], Vladimir Zverev[2], Tatyana Belyaeva[2], and •Sofia Kantorovich[1] — [1]University of Vienna, Vienna, Austria — [2]Ekaterinburg, Russia

In recent years, we have observed a rapid development in synthesis techniques that opens up new avenues for tailoring magnetic nanopar-

ticles, including their size, shape, and internal anisotropy. The concept of creating magnetically controllable colloids with finely tuneable rheological properties on the nano- or micro-scale has sparked significant experimental and theoretical efforts but remains not fully realised. In this contribution, we employ molecular dynamics computer simulations to investigate the interplay between internal particle magnetic relaxation dynamics and particle self-propulsion. Our findings demonstrate that optimal transport can be achieved by selecting the strength of an applied magnetic field based on the particle's material and size. This, in turn, opens up an avenue for active magnetic particle sorting.

DY 25.12 Wed 12:45 BH-N 334

The Role of Anisotropy in Pulsating Active Matter — •Luca Casagrande, Alessandro Manacorda, and Etienne Fodor — University of Luxembourg, Department of Physics and Material Science

Contraction waves have been observed in different biological systems where contractile tissues are present. Some examples can be found in embryonic development, cardiac arrhythmogenesis and uterine contraction. Recently, a particle-based model reproducing the spontaneous emergence of contraction waves has been proposed. In this model, a dense system of active particles is considered, where each particle features isotropic repulsion with neighbors, and has an internal drive that periodically changes its size.*However, it is well know that cells in tissues are not isotropic. Therefore, we consider an additional degree of freedom which embodies the ability of particles to change their eccentricity. It enables us to investigate the role of particle anisotropy in pulsating collective dynamics. The resulting dynamics are studied through numerical simulations. Also an analytical hydrodynamics approach is used through coarse-graining methods. We present the full phase diagram that illustrates the stationary regime as a function of the control parameters of the model. Our model elucidates the interplay between nematic order and phase synchronization in pulsating active matter, and it paves the way towards studying how to control the emergence of contractile waves in biological tissues.

DY 26: Focus Session: Inference Methods and Biological Data (German-French Focus Session) (joint session BP/DY)

Time: Wednesday 15:00–17:45 Location: H 2032

Invited Talk DY 26.1 Wed 15:00 H 2032

Inhibitor-induced transitions in pattern formation and their role to morphogenesis robustness — •Silvia Grigolon — Laboratoire Jean Perrin (UMR 8237), CNRS & Sorbonne Université, Paris, France

Development relies on the finely coordinated expression of morphogens, proteins driving cell differentiation and organ formation. Cell fate specification is achieved thanks to the establishment of morphogen patterns, which act as signals for cells in a concentration dependent manner. By the aid of reaction-diffusion systems, intense studies over the past decades were dedicated to the identification of the underlying microscopic processes leading to robust pattern formation and the classification of the emergent different mechanisms induced by these. In this work, we show that the presence of negative feedbacks in reaction-diffusion systems can lead to a transition in the modes of pattern formation during morphogenesis and induce memory and robustness. We apply this to the study of zebrafish early morphogenesis and show that the aforementioned mechanisms can indeed be found in this system.

DY 26.2 Wed 15:30 H 2032

Bayesian Model Inference for Biological Tracking Data — •Jan Albrecht[1], Lara S. Bort[1], Carsten Beta[1], Manfred Opper[2,3], and Robert Grossmann[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]TU Berlin, Fakultät IV-MAR 4-2, Marchstraße 23, 10587 Berlin, Germany — [3]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom

In order to understand and predict the motion patterns of microorganisms, robust methods to infer motility models from time discrete experimental data are required. Due to the internal complexity of the organisms, their movements appear to have random components which motility models need to account for. Bayesian statistical methods provide a way to efficiently extract information from the trajectory data and provide model parameter estimates together with a measure of uncertainty. We showcase that Bayesian methods are especially well suited when the models contain additional layers of stochasticity, for example population heterogeneity or temporal dependence of parameters. Furthermore, we demonstrate how challenges that arise when multidimensional dynamics is only partially observed, e.g. second order dynamics, colored noise or non-observed internal degrees of freedom, can be addressed.

DY 26.3 Wed 15:45 H 2032

Inference and modelling of the stochastic dynamics of cell shape during cellular state transition — •Wolfram Pönisch[1], Iskra Yanakieva[1], Belle Sow[1], Aki Stubb[2], Alex Winkel[1], Guillaume Salbreux[3], and Ewa Paluch[1] — [1]University of Cambridge, UK — [2]MPI for Molecular Biomedicine, Münster, Germany — [3]University of Geneva, Switzerland

The development of an organism involves a series of state transitions in which cells progressively specialize. Many state transitions coincide with changes in cell shape, with emerging evidence suggesting a strong crosstalk between shape and states. An example is epithelial-to-mesenchymal transition (EMT) which plays a crucial role in development and pathogenesis. Yet, there is very limited knowledge about cell morphodynamics during EMT. Here, we present a morphometric pipeline to analyse individual cell shapes in 3D as cells undergo EMT. By modelling the dynamics as a Langevin process, we infer the potential driving EMT and capture temporal dynamics of cell shape fluctuations during the transition. Our findings reveal a peak in cell shape fluctuations coinciding with the time of spreading during EMT. We hypothesize that downstream biomechanical mechanisms are controlling cell shape fluctuations during EMT and combine computational modelling of cell morphodynamics with molecular perturbation experiments. Overall, by combining morphometric approaches with stochastic inference and mathematical modelling, we create a comprehensive understanding of the biophysical basis of shape changes associated with state transitions.

DY 26.4 Wed 16:00 H 2032

From two to three cells: Are three-body interactions important in collective cell migration? — •Agathe Jouneau[1], Tom Brandstätter[2], Emily Brieger[1], Chase Broedersz[2], and Joachim Rädler[1] — [1]Faculty of Physics and Center for NanoScience, LMU Munich, Germany — [2]Department of Physics and Astronomy, VU Amsterdam, Netherlands

During collective cell migration, for example in embryo development or cancer invasion, cells coordinate their movement by actively interacting with each other. How cell-cell interactions shape the dynamics and emergent properties of the cell assembly is not fully understood. In recent work, we showed that the dynamics of two cells interacting on a dumbbell pattern can be captured by a particle model, including cell-cell interaction terms directly inferred from experimental data. However, we do not know if the collective dynamics of more than two cells can be described by pairwise interactions between cells, or if higher-order interactions come into play. To answer this question, we use time-lapse microscopy to record the dynamics of three cells interacting together in a tailored confinement. We collect a large number of cell trajectories and use them to infer the cell-cell interactions by adapting the framework of the two-cell study. Our work reveals that the pairwise interactions between cells appear to be preserved in the presence of a third cell. However, the superposition of the inferred pairwise interactions is not sufficient to fully capture the observed three-cell dynamics. This could indicate the presence of three-body interactions, with possible implications for large-scale collective behavior.

DY 26.5 Wed 16:15 H 2032

Model selection in stochastic dynamical systems — •Andonis Gerardos and Pierre Ronceray — Aix Marseille Univ, CNRS, CINAM, Turing Center for Living Systems, Marseille, France

Analyzing the dynamics of complex biological systems requires stochastic dynamical models; a common choice is stochastic differential equations (SDE). Given a time series, we developed a method that selects, among a class of SDE models, the one that best captures the dynamics and infers its parameters. This method corresponds to an adaptation of the Akaike information criterion (AIC) to SDE. We validated it using synthetic data generated with stochastic Lorenz and competitive Lotka-Volterra equation. Looking ahead, we envision applications of our data-driven method to unravel the hidden mechanisms of dynamical systems.

15 min. break

Invited Talk DY 26.6 Wed 16:45 H 2032

Bayesian inference of chromatin looping dynamics from live-cell measurements — •Christoph Zechner[1], Michele Gabriele[2], Hugo B Brandão[2], Simon Grosse-Holz[2], Asmita Jha[2], Gina M Daily[3], Claudia Cattoglio[3], Tsung-Han Hsieh[3], Leonid Mirny[2], and Anders S Hansen[2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]University of California, Berkeley, Berkeley, USA

Recent live-cell microscopy techniques allow the simultaneous tracking of distal genomic elements, providing unprecedented ways to study chromatin dynamics and gene regulation. However, drawing robust conclusions from such data is statistically challenging due to substantial technical noise, intrinsic fluctuations and limited time-resolution. I will present recent progress we have made in addressing some of these challenges; specifically, we developed a new statistical method to quantify CTCF/cohesin-mediated chromatin looping dynamics from two-point live-cell imaging experiments. The method combines a simple polymer model with a Bayesian filtering approach to infer loop lifetimes and frequencies. Its application to experimental data revealed that chromatin loops are surprisingly rare (~5% looped fraction) and short-lived (~20mins loop lifetime). I will discuss potential implications of these findings and outline future challenges.

DY 26.7 Wed 17:15 H 2032

Rigorous inference of stochastic reaction networks based on moment constraints via semidefinite optimisation — •Zekai Li, Barahona Mauricio, and Philipp Thomas — Imperial College London, London, United Kingdom

Stochastic reaction networks are used in many fields to model the behaviour of complex systems with uncertainty. Inference of the rate parameters has been an essential and challenging task for accurately understanding the network. While numerous inference methods have been proposed and implemented, the uncertainty measures associated with these methods often lack theoretical guarantees. Here, we propose a novel inference approach to obtain rigorous bounds on the parameters via convex optimisation over sets constrained by moment equations and moment matrices. Under the condition that the moment intervals, obtained through bootstrap from the original data, contain the true stationary moments, our bounds on the parameters are guaranteed to contain the true parameters. Our method is also capable in the case that there exists latent species or observation error, and in the former case, we can bound the stationary moments of the latent species.

DY 26.8 Wed 17:30 H 2032

Information rates of neural activity on varying time scales — •Tobias Kühn and Ulisse Ferrari — Institut de la Vision, Sorbonne Université, CNRS, INSERM

Evaluating electrophysiological recordings, time is normally discretized in bins. If one aims at determining the information rate, i.e. the mutual information per time, the time-bin size has to be chosen with care because the result will appreciably depend on it. The framework we suggest gives freedom in this choice because our single-neuron model is not restricted to a binary representation of neural activity - as is the case for Ising-like models of neural networks.

Our method allows to faithfully estimate the entropy of the neural activity and eventually the mutual information between neural activity and stimulus for a given time scale. Like in the Ising model, we restrict ourselves to pairwise interactions, so that we just need the mean activities and the covariances (across neurons or across time) to compute entropies. This estimate requires a number of measures growing only quadratically in the number of neurons, as opposed to the exponential growth associated to the estimate of the full probability distribution, which prohibits using the latter for real data. More concretely, to compute entropies, we use a small-correlation expansion, expressed in a novel diagrammatic framework (Kühn & van Wijland 2023), avoiding the explicit inference or even a concrete choice of a single-neuron model. Our approach enables studying the dependence of information rate on the time scale on which the information is registered, which is crucial to understand how dynamic stimuli are processed.

DY 27: Focus Session: Nanomechanical Systems for Classical and Quantum Sensing II (joint session HL/DY/TT/QI)

Nanomechanical and cavity-optomechanical systems have been recently established as a controllable and configurable platform that can be engineered to tackle outstanding sensing challenges both in the classical and in the quantum regime. With this focus session, experts from different but synergetically overlapping fields of nanomechanical sensing pursuing classical, non-linear and quantum approaches are brought together. The session shall provide an overview over the recent exciting developments of the techniques explored in micro- and nanomechanical systems and sensing concepts exploring quantum measurement schemes.

Organized by Eva Weig, Hubert Krenner, and Hans Hübl.

Time: Wednesday 15:00–17:45 Location: EW 202

DY 27.1 Wed 15:00 EW 202

Quantum backaction evasion in cavity magnomechanics — •Victor Augusto Sant Anna V Bittencourt[1], Clinton A. Potts[2], John P. Davis[3], and Anja Metelmann[1,4,5] — [1]ISIS (UMR 7006), Universite de Strasbourg, 67000 Strasbourg, France — [2]Kavli Institute of NanoScience, Delft University of Technology, PO Box 5046, 2600 GA Delft, Netherlands — [3]Department of Physics, University of Alberta, Edmonton, Alberta T6G 2E9, Canada — [4]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology, 76131, Karlsruhe, Germany — [5]Institute for Quantum Materials and Technology, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany

Magnetic excitations (magnons) hosted in a solid can couple to mechanical vibrations of the material (phonons) via a radiation-pressure like interaction due to magneto-elastic effects. When the magnet is loaded on a microwave cavity, phonons can be driven and measured via the microwave while having the tunability of the magnetic excitations. Nevertheless, the noise added to mechanics can hinders both potential applications of the system at the quantum level and measurements of the phonon mode. Here, we propose a scheme to evade quantum backaction on a phonon mode of a cavity magnomechanical system by using a two-tone microwave drive. We study the robustness of the different possible backaction evading schemes, and show that measurements of the phonon mode can be performed with added noise below the standard quantum limit.

DY 27.2 Wed 15:15 EW 202

Optical detection of guided GHz acoustic phonons in a semiconductor hybrid microcavity — •Mingyun Yuan[1], Antonio Crespo-Poveda[1], Alexander S. Kuznetsov[1], Klaus

Biermann[1], Alexander Poshakinskiy[2], and Paulo V. Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5, 10117 Berlin, Germany — [2]ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Spain

The interaction between acoustic phonons and optical quasiparticles has profound implication in both understanding of light-matter interaction and acousto-optical applications. We report on the optical detection of phonon echos resulting from the interaction between acoustic phonons and exciton polaritons in a hybrid (Al,Ga)As microcavity grown by molecular beam epitaxy. The microcavity spacer embedding multiple quantum wells is surrounded by Bragg mirrors designed to enable polariton formation. Simultaneously, the spacer-quantum wells and the Bragg reflectors act as the core and cladding regions, respectively, of an acoustic waveguide sustaining GHz acoustic phonons propagating along [110], excited by side bulk-acoustic-wave transducers. The acoustic modulation gives rise to an optical comb in the polariton photoluminescence, in which both the guided phonon modes and the substrate phonon modes are identified via Fourier transform. Our results demonstrate the robust generation of guided acoustic phonons above 6 GHz as well as their effective coupling to the polaritons, and showcase the sensitive optical detection of acoustic modes.

DY 27.3 Wed 15:30 EW 202

Topological phononic waveguides with ultralow loss — •Ilia Chernobrovkin[1], Xiang Xi[1], Jan Kosâta[2], Oded Zilberberg[3], Anders Sørensen[1], and Albert Schliesser[1] — [1]Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100 Copenhagen, Denmark — [2]Institute for Theoretical Physics, ETH Zürich, 8093 Zürich, Switzerland — [3]Department of Physics, University of Konstanz, 78464 Konstanz, Germany

Topological insulators have long intrigued researchers in terms of fundamental physical properties as well as potential applications. The advantages of topological insulators have been extended to the realm of bosonic defects or waveguiding systems and overturned some of conventional views of photonic or phononic wave manipulation. However, the existing topological phononic waveguides still have large transportation loss, which limits its applications.

In our work, we combine the so-called soft-clamping technique - which can dramatically suppress mechanical losses - with non-trivial topology, designed to enable valley-locked propagation along a topological edge. Our systems are based on sub-100 nm thin, highly stressed membrane made of silicon nitride membranes. Our preliminary experimental results show a measured Q-factor above 1 million for whispering-galley megahertz-frequency elastic modes along a closed triangular path of length of ˜10 mm, which corresponds to a classical coherent length of tens of meters. Our system can be considered promising for use in phononic circuits for coherent microwave signal processing or interconnection.

DY 27.4 Wed 15:45 EW 202

Dry processing of high Q 3C-silicon carbide nanostring resonators — •Felix David, Philipp Bredol, and Eva Weig — Technical University of Munich - Chair of Nano and Quantum Sensors, Garching, Germany

We fabricate string resonators from strongly stressed 3C-silicon carbide (SiC) grown on a silicon substrate. The conventional fabrication process involves electron-beam lithography with PMMA to define a metallic hard mask for the subsequent dry-etching step via a liftoff process. This requires some wet-chemical process steps, which can destroy our samples. Here we describe an alternative process, which avoids all wet-chemical process steps to enable superior quality. It involves the use of a negative electron-beam resist as an etch mask, as well as the completely reactive-ion etching-based release of the nanostrings. The dry-processed nanostrings can be fabricated with a high yield and exhibit high mechanical quality factors at room temperature. Due to the high reliability combined with the high process speed, it also allows us to investigate material-intensive questions, such as the influence of etching depth and undercut on the mechanical quality factor.

DY 27.5 Wed 16:00 EW 202

Spatial Mode Mapping of 2D Mechanical Resonators — •Lukas Schleicher, Leonard Geilen, Alexander Holleitner, and Eva Weig — TU München, Garching, Deutschland

We present studies on the spatial mapping of mechanical modes of 2D resonators based on monolayer transition-metal dichalcogenides. A spatially resolved mode mapping allows us to investigate non-isotropic pre-strain and other transfer-related artefacts, such as cracks and surface contaminations, which may result from the fabrication process. We compare the mechanical properties of drums with various sizes and fabrication methods of the 2D resonators.

15 min. break

DY 27.6 Wed 16:30 EW 202

Electrochemical etching strategy for shaping monolithic 3D structures from 4H SiC wafers — •André Hochreiter, Fabian Gross, Morris Niklas Möller, Michael Krieger, and Heiko Weber — Lehrstuhl für Angewandte Physik Universität Erlangen-Nürnberg, Germany

Silicon Carbide's (SiC) as wide bandgap semiconductor has outstanding material properties, which enable applications like already available commercial power-electric devices, and applications in quantum sensing. For mechanical applications of SiC, extremely high quality factors are predicted, but on-chip 3D shaping of SiC is difficult due to its chemical robustness. We report on an electrochemical etching (ECE) strategy, which solely relies on a doping contrast introduced by targeted ion-implantation of p-dopants on n-type material. With such a dopant-selective etching, n-doped regions remain inert and p-type regions are removed. We present devices as diverse as monolithic cantilevers, membranes and disk-shaped optical resonators etched out a single crystal wafer. The electrochemically etching process leaves the etched surface with low roughness, which can even be improved by annealing.

DY 27.7 Wed 16:45 EW 202

Probing the Mechanical Loss of Individual Surfaces of a Nanomechanical String Resonator — •Philipp Bredol, Felix David, and Eva Weig — Technical University of Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany

Stressed nanostring resonators are a promising platform for sensing applications and quantum technologies because of their small footprint and high mechanical quality factors. In this contribution we show that the dissipation caused by sidewall surfaces and the dissipation caused by bottom and top surfaces can be individually determined from the mechanical response spectrum. This information helps to evaluate and adjust fabrication parameters such as etchant chemistry, etch mask materials and possible annealing steps. Being able to characterize the mechanical loss mechanisms that limit a given device is important for integration with other structures and to further push the performance of nanostring resonators.

DY 27.8 Wed 17:00 EW 202

Parametric normal mode splitting for coupling strength estimation — •Ahmed A. Barakat, Avishek Chowdhury, Anh Tuan Le, and Eva M. Weig — Technical University of Munich, Munich, Germany

The experimental estimation of the linear coupling strength between two nanomechanical modes is a challenging task. For dielectrically actuated nano-string resonators, the coupling strength between in-plane and out-of-plane modes is usually estimated by tuning the modal eigenfrequencies using a bias voltage up to the occurrence of the avoided crossing. In this contribution, we introduce a novel approach using parametric excitation to estimate the linear coupling strength at any bias voltage.

In addition to a broadband noise excitation, the proposed approach involves parametrically driving in the direction of at least one of the eigenmodes with a frequency that resonates with the difference between both eigenfrequencies causing a parametric normal mode splitting. Using the dependence of the splitting width on the coupling strength, a mathematical model is introduced and perturbed around the parametric excitation frequency using the multiple scales method. The locus of the splitting is derived analytically and agrees well with the experimental results, leading to an accurate estimation of the coupling strength.

DY 27.9 Wed 17:15 EW 202

Tunable near-infrared exciton-polariton optomechanical GHz rulers of light — •Alexander Kuznetsov, Klaus Biermann, and Paulo V. Santos — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Frequency combs, which consist of many equidistant optical lines, are photonic analogues of spatial rulers. Such rulers of light can be used for high-resolution spectroscopy, ranging, optical and atomic clocks, and for large-scale quantum systems. On-chip miniaturized and low-power comb-sources are, therefore, of great importance. Here, we demonstrate generation of tunable combs using spatially confined light-matter quasiparticles – exciton-polaritons – coherently modulated by GHz phonons inside a hybrid photon-phonon (Al,Ga)As patterned microcavity. Using non-resonant optical excitation, we create polariton Bose-Einstein-like condensates (BEC) with long temporal coherence reaching $\tau_{BEC} \approx 2$ ns. The BEC is modulated by piezoelectrically generated strain of bulk acoustic wave (BAW) phonons with frequency $f_{BAW} = 7$ GHz and RF-tunable amplitude. Since $\tau_{BEC} \gg 1/f_{BAW}$, the modulation is coherent and leads to the emergence of well-resolved phonon sidebands, separated by f_{BAW}, in the polariton emission spectrum. For large BAW amplitudes, the comb contains up to 50 well-resolved lines with nearly-flat profile. The demonstrated RF-induced comb functionality may be useful for the realization of on-chip arrays of tunable GHz optical combs as well as coherent optical-to-microwave bi-directional conversion.

DY 27.10 Wed 17:30 EW 202

Imaging acoustic fields on metasurfaces — •Alessandro Pitanti[1,2,3], Mingyun Yuan[1], Simone Zanotto[3], and Paulo Ventura Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., 5-7 Hausvogteiplatz, Berlin 10117, Germany — [2]Dipartimento di Fisica E. Fermi, Università di Pisa, Largo B. Pontecorvo 3, Pisa 56127, Italy — [3]NEST, CNR Istituto Nanoscienze and Scuola Normale Superiore, piazza San Silvestro 12, Pisa 56127, Italy

The last decades have witnessed a rich activity towards the integration of acoustic technologies within electro-optical circuits in high-frequency hybrid devices. The main role in this trend has been played by surface acoustic waves (SAW), easily integrable in several material platforms via piezoelectricity. Given their high frequency and quality factors, simple SAW delay-line resonators have found application as sensors, filters, and oscillators for telecommunication applications. More complex manipulation of acoustic waves would boost SAW-based technologies, becoming a key for the transition to 6G; complete wave manipulation and control in the GHz range would offer the most promise for integration with modern communication technologies.

In this context, we illustrate the use of light-interferometry and atomic force microscopy based scanning probe techniques for a fine investigation of GHz acoustic fields in mechanical metasurfaces. Focusing on the role of symmetries in wave scattering, we show complex wave manipulation, leading to asymmetric negative refraction and anisotropic transmission of mechanical waves.

DY 28: Networks: From Topology to Dynamics I (joint session SOE/DY)

Time: Wednesday 15:00–18:30 Location: TC 006

DY 28.1 Wed 15:00 TC 006

Implicit models, latent compression, intrinsic biases, and cheap lunches in community detection in networks — •Tiago Peixoto — Central European University, Vienna, Austria

The task of community detection, which aims to partition a network into clusters of nodes to summarize its large-scale structure, has spawned the development of many competing algorithms with varying objectives. Some community detection methods are inferential, explicitly deriving the clustering objective through a probabilistic generative model, while other methods are descriptive, dividing a network according to an objective motivated by a particular application, making it challenging to compare these methods on the same scale. In this talk I present a solution to this problem that associates any community detection objective, inferential or descriptive, with its corresponding implicit network generative model. This allows us to compute the description length of a network and its partition under arbitrary objectives, providing a principled measure to compare the performance of different algorithms without the need for ground truth labels. Our approach also gives access to instances of the community detection problem that are optimal to any given algorithm, and in this way reveals intrinsic biases in popular descriptive methods, explaining their tendency to overfit. Using our framework, we compare a number of community detection methods on artificial networks, and on a corpus of over 500 structurally diverse empirical networks.

[1] Tiago P. Peixoto, Alec Kirkley, Phys. Rev. E 108, 024309 (2023)

DY 28.2 Wed 15:15 TC 006

ESABO Co-Abundance Analysis: cases where the binarization threshold matters — •Devi Chandran and Jens Christian Claussen — School of Computer Science University of Birmingham, UK

Population dynamics including their complex interactions lead, in societies and microbial populations, to rich co-abundance patterns, and often only the (co)abundance pattern data is measured – whereby the precise interactions remain unknown. Here, ESABO [1] has been introduced to grasp interactions that remain unseen especially for low-abundant species. In [1], using ESABO we have recovered positive and negative interactions between agents (or species) within the population based on co-abundance data. However, in the medium abundance region, instead of a binarization threshold of 1, might it be worth to consider larger binarization thresholds? We investigate, based on two datasets, whether higher thresholds can lead to a higher information gain (in the sense of ESABO), and demonstrate cases of higher information gain for higher thresholds, but also confirm that the original threshold of 1 can be optimal for other datasets.

[1] J.C.Claussen at al., PlosCB (2017) 13(6): e1005361.

DY 28.3 Wed 15:30 TC 006

Interplay of synchronization and cortical input in models of brain networks — •Eckehard Schöll[1,2,3] and Jakub Sawicki[2] — [1]Technische Universität Berlin — [2]Potsdam Institute for Climate Impact Research (PIK) — [3]Bernstein Center for Computational Neuroscience (BCCN) Berlin

It is well known that synchronization patterns and coherence have a major role in the functioning of brain networks, both in pathological and in healthy states. In particular, in the perception of sound, one can observe an increase in coherence between the global dynamics in the network and the auditory input. In this work, we show that synchronization scenarios are determined by a fine interplay between network topology, the location of the input, and frequencies of these cortical input signals [1]. To this end, we analyze the influence of an external stimulation in a network of FitzHugh-Nagumo oscillators with empirically measured structural connectivity, and discuss different areas of cortical stimulation, including the auditory cortex. [1] J. Sawicki and E. Schöll: Europhys. Lett. (2024), invited Perspective.

DY 28.4 Wed 15:45 TC 006

Neuronal avalanches in weakly coupled FitzHugh-Nagumo oscillators — Max Contreras[1], Everton Medeiros[2], Igor Franović[3], and •Philipp Hövel[4] — [1]Technische Universität Berlin, Germany — [2]Carl von Ossietzky University Oldenburg, Germany — [3]University of Belgrade, Serbia — [4]Saarland University, Germany

The activity in the brain cortex remarkably shows a simultaneous presence of robust collective oscillations and neuronal avalanches, where intermittent bursts of pseudo-synchronous spiking are interspersed with long periods of quiescence. The mechanisms allowing for such coexistence are still a matter of an intensive debate. Here, we demonstrate that avalanche activity patterns can emerge in a rather simple model of an array of diffusively coupled neural oscillators with multiple timescale local dynamics in the vicinity of a canard transition. The avalanches coexist with the fully synchronous state where the units perform relaxation oscillations. We show that the mechanism behind the avalanches is based on an inhibitory effect of interactions, which may quench the spiking of units due to an interplay with the maximal canard. The avalanche activity bears certain heralds of criticality, including scale-invariant distributions of event sizes. Furthermore, the system shows increased sensitivity to perturbations, manifested as critical slowing down and reduced resilience.

Reference: Max Contreras, Everton S. Medeiros, Anna Zakharova, Philipp Hövel, and Igor Franović: *Scale-free avalanches in arrays of FitzHugh-Nagumo oscillators*, Chaos **33**, 093106 (2023).

DY 28.5 Wed 16:00 TC 006

On the inadequacy of nominal assortativity for assessing homophily in networks — •Fariba Karimi[1] and Marcos Oliveira[2] — [1]Graz University of Technology — [2]Exeter University

Nominal assortativity (or discrete assortativity) is widely used to characterize group mixing patterns and homophily in networks, enabling researchers to analyze how groups interact with one another. Here we demonstrate that the measure presents severe shortcomings when applied to networks with unequal group sizes and asymmetric mixing. We characterize these shortcomings analytically and use synthetic and empirical networks to show that nominal assortativity fails to account for group imbalance and asymmetric group interactions, thereby producing an inaccurate characterization of mixing patterns. We propose the adjusted nominal assortativity and show that this adjustment recovers the expected assortativity in networks with various level of mixing. Furthermore, we propose an analytical method to assess asymmetric mixing by estimating the tendency of inter- and intra-group connectivities. Finally, we discuss how this approach enables uncovering hidden mixing patterns in real-world networks.

DY 28.6 Wed 16:15 TC 006

Unveiling homophily beyond the pool of opportunities — •Sina Sajjadi[1,2], Samuel Martin-Gutierrez[1], and Fariba Karimi[1,3] — [1]Complexity Science Hub Vienna, Vienna, Austria — [2]Central European University, Vienna, Austria — [3]Graz University of Technology, Graz, Austria

We introduce a robust methodology for quantifying and inferring choice homophily, reflecting individuals' preferences for connecting with similar others beyond structural factors that determine the pool of opportunities. Our approach employs statistical network ensembles to estimate and standardize homophily measurements. We control for group size imbalances and activity disparities by counting the number of possible network configurations with a given number of inter-group links using combinatorics. Our framework is suitable for undirected and directed networks, and applicable in scenarios involving multiple groups. Tested on synthetic networks, our approach outperforms traditional metrics, accurately capturing generative homophily despite additional tie-formation mechanisms. Preferential attachment has no effect on our measure, and triadic closure's impact is minor, especially in homophilic scenarios. We apply our model to scientific collaboration and friendship networks, demonstrating its effectiveness in unveiling underlying gender homophily. Our method aligns with traditional metrics in networks with balanced populations, but we obtain different results when the group sizes are imbalanced. This finding highlights the importance of considering structural factors when measuring choice homophily in social networks.

15 min. break

DY 28.7 Wed 16:45 TC 006

Nonequilibrium Nonlinear Dynamics I: Nonlinear Shift and Tipping — Julian Fleck[1], Moritz Thümler[1], Malte Schröder[1], Seungjae Lee[1], and •Marc Timme[1,2] — [1]Center for Advancing Electronics Dresden (cfaed) and Institute for Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Lakeside Labs, 9020 Klagenfurt am Wörthersee, Austria

The collective nonlinear dynamics and reliable function of complex networked systems fundamentally underlie our daily lives, whether in biological cells, in power grids or in ecosystems. Most complex systems from the natural and engineering sciences are externally driven, and may exhibit intrinsically nonlinear state shifts or undergo tipping that disrupt the systems* intended or desired functionality. While state-of-the-art theoretical concepts and method development have focused on linear responses suitable for weak driving signals, it is far less understood how to characterize, predict and design complex systems responding to strong perturbations, that e.g., may ultimately lead to tipping. Here we report average response offsets that scale nonlinearly at asymptotically small amplitudes. At some critical driving amplitude, responses cease to stay close to a given operating point and may diverge. Standard response theory fails to predict these amplitudes even at arbitrarily high orders. We propose an integral self-consistency condition that captures the full nonlinear response dynamics. We illustrate our approach for a minimal one-dimensional model and capture the nonlinear shift of voltages in the response dynamics of AC power grid networks.

DY 28.8 Wed 17:00 TC 006

Nonequilibrium Nonlinear Dynamics II: Strong Perturbations — •Julian Fleck, Moritz Thümler, Malte Schröder, Seungjae Lee, and Marc Timme — Institute for Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

Analytical studies of driven nonlinear dynamical systems often focus on linear response theory or extensions thereof in the asymptotic limit of small driving amplitudes. However, standard perturbation series are incapable of faithfully describing driving-induced system disruptions such as driving-induced tipping. In recent work (see part I: Nonlinear Shift and Tipping), we have proposed a self-consistency condition to estimate at which driving amplitudes non-equilibrium nonlinear system dynamics may tip. Here we propose to predict the tipping point by a large-perturbation expansion evaluated inside the self-consistency condition. We compare small-amplitude with the novel large-amplitude ansatz. The approach we propose may help to quantitatively predict intrinsically nonlinear response dynamics as well as bifurcations emerging at large driving amplitudes in non-autonomous dynamical systems.

DY 28.9 Wed 17:15 TC 006

Transport networks with dynamical metric: when noise is advantageous — •Frederic Folz[1], Kurt Mehlhorn[2], and Giovanna Morigi[1] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany — [2]Algorithms and Complexity Group, Max-Planck-Institut für Informatik, Saarland Informatics Campus, 66123 Saarbrücken, Germany

The interplay of nonlinear dynamics and noise is at the basis of coherent phenomena, such as stochastic resonance, synchronization, and noise-induced phase transitions. While the effect of noise in these phenomena has been partially analyzed, the impact of the specific form of the nonlinear dynamics on noise-induced phase transitions is unknown. In this work, we analyze transport on a noisy network where the nonlinearity enters through a dynamical metric, which depends nonlinearly on the local current. We determine network selforganization for different functional forms of the metric in a geometry of constraints simulating the network of metro stations of the city of Tokyo. We consider Gaussian noise and show that the resulting dynamics exhibits noise-induced resonances for a wide range of the model parameters, which manifest as selforganization into the most robust network with a resonant response to a finite value of the noise amplitude. We analyze in detail the specific features and perform a comparative assessment. Our study sheds light on the interplay between nonlinear dynamics and stochastic forces, highlighting the relevance of their mutual interplay in determining noise-induced coherence.

DY 28.10 Wed 17:30 TC 006

Crossword puzzle percolation — •Alexander K. Hartmann — University of Oldenburg, Germany

Games are a popular subject, also for physicists. Many games have a lattice or network representation. A crossword puzzle consists of *black* (blocked) and *white* sites, the latter can be *empty* or *occupied* with letters. A word is *known* in the puzzle if a complete horizontal or vertical segment of white sites, usually between two black sites, is occupied (periodic boundary conditions are used, words may also take a full column or row).

Here the crossword puzzle is considered as percolation problem: Two known words are *connected* if they are perpendicular to each other and share one occupied site. A configuration is considered as *percolating* if there exists a path of connected words around the system, in either direction.

Numerical simulations for two-dimensional crosswords up to size 1000×1000 are performed. For uncorrelated occupation with probability p for the white sites, percolation transitions at critical thresholds p_c, depending on the fraction of black sites, are found. The results are analyzed by finite-size scaling and indicate that the problem is in the universality class of standard two-dimensional percolation. This changes, when the real game case is considered where full words are known with a probability $p_w(x)$ which depends on the fraction x of already known letters in the word, introducing correlations. The universality class depends on the shape of $p_w(x)$.

DY 28.11 Wed 17:45 TC 006

Network percolation provides early warnings of abrupt changes in coupled oscillatory systems: An explanatory analysis — Noémie Ehstand[1], •Reik V. Donner[2,3], Cristóbal López[1], and Emilio Hernández-García[1] — [1]IFISC, Palma de Mallorca, Spain — [2]Magdeburg-Stendal University of Applied Sciences,

Magdeburg, Germany — [3]Potsdam Institute for Climate Impact Research, Potsdam, Germany

Functional networks are powerful tools to study statistical interdependency structures in spatially extended or multivariable systems. In particular, percolation properties of correlation networks have been employed to identify early warning signals of critical transitions. Here, we further study the potential of percolation measures for the anticipation of different types of sudden shifts in the state of coupled irregularly oscillating systems. For a ring of diffusively coupled noisy FitzHugh-Nagumo oscillators that are nearly completely synchronized, the percolation-based precursors successfully provide very early warnings of the rapid switches between the two states of the system. We clarify the mechanisms behind the percolation transition by separating global trends given by the mean-field behavior from the synchronization of individual stochastic fluctuations. We then apply the same methodology to real-world data of sea surface temperature anomalies during different phases of the El Niño-Southern Oscillation. This leads to a better understanding of the factors that make percolation precursors effective as early warning indicators of incipient El Niño and La Niña events. [N. Ehstand et al., Phys. Rev. E, 108, 054207, 2023]

DY 28.12 Wed 18:00 TC 006

Bond percolation and tree decompositions of real-world networks — •Konstantin Klemm — IFISC (CSIC-UIB), Palma de Mallorca, Spain

Percolation is a class of models with numerous applications in spreading processes including epidemics and social interactions. For most real-world and model-generated networks, percolation studies rely on Monte-Carlo sampling or approximate calculations such as (heterogeneous) mean-field. The present contribution introduces a method for exact numerical estimates of expected cluster sizes in bond percolation. The method is efficient on networks with a narrow tree-decomposition, a property shared by empirical networks of interest [Klemm, Journal of Physics: Complexity 1, 035003 (2020)]. Generalization of the approach to other processes in statistical physics are discussed [Klemm, arXiv:2111.04766].

DY 28.13 Wed 18:15 TC 006

Between mechanisms and behaviors in higher-order systems — •Thomas Robiglio[1], Davide Coppes[2], Cosimo Agostinelli[2], Matteo Neri[3], Maxime Lucas[4], Federico Battiston[1], and Giovanni Petri[4,5] — [1]Department of Network and Data Science, Central European University, Vienna, Austria — [2]Department of Physics, University of Turin, Via Pietro Giuria 1, 10125 Turin, Italy — [3]Institut de Neurosciences de la Timone, Aix Marseille Université, UMR 7289 CNRS, 13005, Marseille, France — [4]CENTAI, Corso Inghilterra 3, 10138 Turin, Italy — [5]NPLab, Network Science Institute, Northeastern University London, London, UK

Mechanism and behavior are the two fundamental facets of the study of the dynamical properties of complex systems. Mechanism describes how a system is structured and what the microscopic rules governing its dynamic are while behavior accounts for its emergent properties.

Using tools from information theory, we systematically explore the relationship between higher-order (i.e. beyond pairwise) mechanisms and higher-order behaviors. Considering two dynamical models with group interactions -a simplicial Ising model and the simplicial model of social contagion- we find a region of the parameter space in which higher-order synergistic behaviors and group mechanisms co-occur.

We also apply higher-order information theoretical metrics to characterize the behavior of the stock market across time and show that we can identify periods of economic crisis that are overseen by the corresponding low-order metrics.

DY 29: Focus Session: Recent Progresses in Criticality in the Presence of Boundaries and Defects II (joint session DY/TT)

In recent years there has been a renewed interest in critical systems in the presence of boundaries or, more generally, defects. This attention is driven by different perspectives. Numerical studies of quantum spin models have reported in some cases unexpected boundary critical behavior. This, in turns, has led to a reconsideration of the classical surface critical behavior problem, with the discovery of so-far overlooked boundary phases. In this context, numerous recent studies have considered the so-called symmetry-protected topological gapless systems, and in particular their boundary states. At the same time, advances in conformal field theory, specifically the conformal bootstrap program, have addressed the problem of boundaries and defects in conformally-invariant theories. This Focus Session brings together some of the main actors in the aforementioned advancements in boundary critical phenomena.

Organized by Francesco Parisen Toldin (Aachen) and Stefan Wessel (Aachen)

Time: Wednesday 15:00–16:15 Location: A 151

Invited Talk DY 29.1 Wed 15:00 A 151

Conformal boundary conditions of symmetric quantum critical states — •Long Zhang — University of Chinese Academy of Sciences, Beijing 100190, China

Some quantum critical states cannot be smoothly deformed into each other without either crossing some multicritical points or explicitly breaking certain symmetries even if they belong to the same universality class. This brings up the notion of "symmetry-enriched" quantum criticality. While recent works in the literature focused on critical states with robust degenerate edge modes, we propose that the conformal boundary condition (b.c.) is a more generic characteristic of such quantum critical states. In the first part of this talk, we show that in two families of quantum spin chains, which generalize the Ising and the three-state Potts models, the quantum critical point between a symmetry-protected topological phase and a symmetry-breaking order realizes a conformal b.c. distinct from the simple Ising and Potts chains at both the physical and the entangling boundaries. Furthermore, we argue that the conformal b.c. can be derived from the bulk effective field theory, which realizes a novel bulk-boundary correspondence in symmetry-enriched quantum critical states. In the second part, we will show the effect of finite-entanglement scaling of matrix-product states on their conformal b.c. at both the physical and the entangling boundaries.

DY 29.2 Wed 15:30 A 151

Universal fragility of spin-glass ground-states under single bond changes — Mutian Shen[1], Gerardo Ortiz[2], Yang-Yu Liu[3], •Martin Weigel[4], and Zohar Nussinov[1] — [1]Department of Physics, Washington University, St. Louis, MO 63160, USA — [2]Department of Physics, Indiana University, Bloomington, IN 47405, USA — [3]Harvard Medical School, Boston, MA, 02115, USA — [4]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

We examine the effect of changing a single local bond on ground states of the Edwards-Anderson Ising spin-glass in two and three dimensions and with a Gaussian distribution of couplings. We find such ground states to be exceedingly fragile: altering the strength of only a single bond beyond a critical threshold value leads to a new ground state that differs from the original one by a cluster ("critical zero energy droplet") of flipped spins whose boundary and volume diverge with system size — an effect that is reminiscent of the more familiar phenomenon of disorder chaos. At the same time, these elementary clusters provide the lowest-energy macroscopic excitations in short-range spin-glasses above the lower critical dimension. The presence of such excitations with fractal boundaries provides a strong characterization of the spin-glass phase in these systems. Within numerical accuracy, the size of these clusters is governed by a nearly universal power-law distribution

with exponents depending on the spatial dimension of the system. The critical coupling strengths follow a stretched Gaussian distribution that is largely set by the local coordination number of the lattice.

DY 29.3 Wed 15:45 A 151

Random Matrices and the Free Energy of Ising-Like Models with Disorder — •Nils Gluth, Thomas Guhr, and Fred Hucht — Fakultät für Physik, University of Duisburg-Essen, Duisburg, Germany

We consider an Ising model with quenched surface disorder, the disorder average of the free energy is the main object of interest. Explicit expressions for the free energy distribution are difficult to obtain if the quenched surface spins take values of ± 1. Thus, we choose a different approach and model the surface disorder by Gaussian random matrices. The distribution of the free energy is calculated. We chose skew-circulant random matrices and compute the characteristic function of the free energy distribution. We show numerically the distribution becomes log-normal for sufficiently large dimensions of the disorder matrices, and in the limit of infinitely large matrices the distributions are Gaussian. Furthermore, we establish a connection to the central limit theorem.

DY 29.4 Wed 16:00 A 151

The Griffiths phase and beyond: a large deviations study — •Lambert Münster[1], Alexander K. Hartmann[2], and Martin Weigel[1] — [1]Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany

The Griffiths phase is a temperature range in systems with quenched disorder that reaches from the critical temperature of the pure system to the corresponding critical temperature in the presence of disorder. In this phase, the possibility of large fluctuations in the disorder degrees of freedom leads to broad distributions in response functions. For example, inside the Griffiths phase of the two-dimensional bond-diluted Ising model the distribution of the magnetic susceptibility is expected to have an exponential tail [1]. A large-deviation Monte Carlo algorithm is used to sample this distribution [2,3], and the exponential tail is extracted over a wide range of the support down to probabilities of the order of 10^{-300}. A connection between the local fraction of ferromagnetic bonds and the size of the magnetic susceptibility is demonstrated numerically. Furthermore the distribution of the magnetic susceptibility is also investigated at the ferromagnetic phase transition, inside the ferromagnetic phase and at zero temperature, revealing interesting differences and similarities between the cases.

[1] A. J. Bray, Phys. Rev. Lett. **59**, 586 (1987).
[2] A. K. Hartmann, Phys. Rev. E **65**, 056102 (2002).
[3] K. Hukushima, Y. Iba, J. Phys. Conf. Ser. **95**, 012005 (2008).

DY 30: Focus Session: New Trends in Nonequilibrium Physics – Conservation Laws and Nonreciprocal Interactions II

Nonequilibrium phase transitions and pattern formation are known from numerous examples of open systems, where external reservoirs and gradients prevent relaxation to thermodynamic equilibrium. In recent years, related research in biology and soft matter systems in physics and chemistry has increasingly focused on active matter, where energy is injected locally. This often involves mass conservation constraints and, in many cases, in addition non-reciprocal interactions of the involved entities, such as macromolecules or cells. Both have far reaching consequences on the universal dynamical behavior of a wide range of nonequilibrium systems and require classical concepts of nonlinear and statistical physics, such as phase transitions, to be reconsidered and developed further. For example, well-known approaches to nonequilibrium pattern formation require substantial extensions to address conserved systems. Thus, recent theoretical studies in this field have revealed many novel phenomena, such as arrested coarsening, odd elasticity, oscillatory phase separation, persistent wave dynamics, and active turbulence. Many of these aspects have by now been confirmed by experimental findings, for example, in intracellular pattern formation or collective dynamics in colloidal systems. This symposium will provide a well-balanced overview of experimental and theoretical progress in this new, exciting area.

Organized by Markus Bär (Berlin) and Carsten Beta (Potsdam)

Time: Wednesday 15:00–16:30 Location: BH-N 243

Invited Talk DY 30.1 Wed 15:00 BH-N 243

Continuum Approach for Studying Morphological Deformations of Multiple-Phase Renewable Energy Devices — •Arik Yochelis — Swiss Institute for Dryland Enviremental and Energy Research, Ben-Gurion University of the Negev, Sede Boqer Campus, Midreshet Ben-Gurion 8499000, Israel — Department of Physics, Ben-Gurion University of the Negev, Be'er Sheva 8410501, Israel

Optimizing the morphological properties of soft-matter renewable energy devices is not only challenging technologically but also reveals novel physical and mathematical puzzles. For example, recent experimental studies of bulk heterojunction (BHJ) organic photovoltaics (OPV) show that phase separation can surprisingly inhibit morphological changes in three-phase (donor/mixed/acceptor) constellations. Motivated by BHJ observations, the development of a continuum model (dissipative parabolic-elliptic PDEs) that undertakes the coupling between the spatiotemporal evolution of the material and generated charge dynamics along with charge transfer at the device electrodes, will be presented. Model analysis in the spirit of reaction-diffusion-type mechanisms uncovers the bending (zigzag mode) and the pinching (cross-roll mode) of the donor/acceptor stripes, where the latter leads to the formation of disconnected domains and hence to loss of charge flux near the electrodes. In the end, a similar approach is applied to renewable Ni (Edison-type) batteries in which charge/discharge electrochemical reactions and capacity are associated with fingering instability between the multiplicity of Ni phases.

DY 30.2 Wed 15:30 BH-N 243

Collective behavior of cohesive, aligning particles — •Jeanine Shea and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin, Germany.

Collective behavior is all around us, from flocks of birds to schools of fish. These systems are immensely complex, which makes it pertinent to study their behavior through minimal models. We introduce a minimal model for cohesive and aligning self-propelled particles. In contrast to former models of this type, we establish group cohesion through non-reciprocal torques [1] as opposed to attractive forces. These torques cause constituents to effectively turn towards one another. We additionally incorporate an alignment torque. By changing the strength and range of these torque interactions, we uncover a vast array of dynamics ranging from long filaments to pear-shaped clusters. We present state diagrams to identify these different dynamic states.

[1] Knežević, M., Welker, T. and Stark, H. Collective motion of active particles exhibiting non-reciprocal orientational interactions. Sci Rep 12, 19437 (2022).

DY 30.3 Wed 15:45 BH-N 243

Aligning self-propelled particles beyond mean-field: the active Boltzmann equation — Jakob Mihatsch[1], •Horst-Holger

Boltz[1], Rüdiger Kürsten[2], and Thomas Ihle[1] — [1]Universität Greifswald, Greifswald, Deutschland — [2]Universitat de Barcelona, Barcelona, Spanien

Models of active matter are commonly discussed within mean-field approaches. Going beyond mean-field by assuming one-sided molecular chaos, we show that it is possible to explicitly account for the finite duration and range of actual interactions in particular active matter leading to the active Boltzmann equation. One principle outcome is a derivation of the entropy production.

We demonstrate the quantitatively accurate realization of this methodology, both analytically and numerically, for ensembles of Vicsek-style self-propelled particles with finite-ranged alignment interactions. For anti-aligning interactions in the absence of noise, this system displays deterministically chaotic dynamics under the existence of an additional conservation law that affects the large-scale statistics.

We use an asymptotically exact solution to predict a novel flocking transition in heterogeneous systems wherein all couplings are anti-aligning, which we corroborate by agent-based direct simulations, and show how the formalism can successfully be expanded to non-reciprocal interactions.

References: Ihle, Kürsten, Lindner (2023) arXiv:2303.03354, 2303.03357; Kürsten, Mihatsch, Ihle (2023) arXiv: 2304.05476

DY 30.4 Wed 16:00 BH-N 243

Formation of trails and bands of signaling active particles — •Zahra Mokhtari[1], Robert Grossmann[2], Robert Patterson[3], and Felix Höfling[1,4] — [1]Institut für Mathematik, Freie Universität Berlin — [2]Institut für Physik und Astronomie, Universität Potsdam — [3]WIAS Berlin — [4]Zuse Institute Berlin

To shed light on pattern formation of active particles with nonreciprocal interactions, we study self-propelled agents that interact via self-generated fields: individual particles deposit traces of pheromones which encode their current walking direction, in turn influencing the direction of motion of passing agents. In contrast to direct binary alignment interactions, the communication via self-generated fields constitutes a type of time-delayed, non-reciprocal feedback. The system exhibits different stable patterns: the collective dynamics is of the Vicsek type in the limit of short-lived traces, thus forming transversely moving bands. For prolonged pheromone lifetime, particles are found to gather along macroscopic narrow trails along the direction of motion. To elucidate the transitions between these states, we derive hydrodynamic equations within a mean-field approximation, unraveling a nuanced phase diagram dependent on pheromone lifetime. Combining numerics and a linear stability analysis reveals that transversal bands are destabilized in favor of the emergence of *longitudinal* trails. Thereby, this work provides a first steps towards an understanding of the role of nonreciprocal, delayed feedback interactions for the symmetry and structure of a novel type of emergent patterns forming under nonequilibrium conditions.

DY 30.5 Wed 16:15 BH-N 243

Two-species Janus colloids with non-reciprocal interactions — •Gennaro Tucci, Suropriya Saha, and Ramin Golestanian — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

We are examining two interacting populations of Janus colloids, each distinguished by their catalytic caps and mobility. The dynamics of these colloids are characterized by their position and orientation, influencing and being influenced by the density distribution of a single chemical substrate. Specifically, the particles can produce or consume the chemical and interact with its concentration gradient through chemotaxis. This chemically-mediated coupling gives rise to an effective non-reciprocal interaction between the two colloid species, resulting in novel configurations of instability. We derive the equation of motion for both density and the polar order parameter through a systematic coarse-graining of the microscopic dynamics. Subsequently, a linear stability analysis of the reference state, featuring constant densities and disordered polarity, allows us to elucidate the mechanisms by which it may become unstable. Initially, we demonstrate how the system exhibits one-species-like behavior in a certain parameter subspace. Finally, we explore phases that can be obtained through the non-reciprocal nature of the two-species interaction.

DY 31: Poster: Statistical Physics

Time: Wednesday 15:00–18:00 Location: Poster C

DY 31.1 Wed 15:00 Poster C

Localisation in one-dimensional random tight-binding models — •Luca Schäfer and Barbara Drossel — Technische Universität Darmstadt, Darmstadt, Germany

We compare the localisation characteristics of three different one-dimensional disordered quantum systems described by the tight-binding model, using exact and partial diagonalisation of the Hamiltonian to obtain the eigenvalue spectrum and the associated participation ratios (P), and the transfer-matrix method to determine the localisation length (ξ). The degree of localisation is evaluated based on the scaling of P and ξ with the system size. The first model is the well-known Anderson model (AM) featuring on-site disorder, for which all states are localised. The second model has no on-site disorder, but random couplings (RCM). In this scenario, solely the state with $E = 0$ is extended, and ξ increases proportional to the negative logarithm of E. We show that the eigenstate in the band centre can be mapped on a random walk, thus explaining its properties. The third model can be represented as a harmonic chain with random coupling (HCM), where the on-site potential is correlated with the coupling strengths such that the model has a conserved quantity. This choice is motivated by applications in ecological and diffusion networks. We find, in agreement with existing analytical calculations, that the number of extended states for $E \approx 0$ grows proportional to the square root of the system size, and we related this power law to the power laws that characterise the statistics of P and E and ξ and the relation between them.

DY 31.2 Wed 15:00 Poster C

Inferring hidden dynamics from empirical densities and currents of projected observables — •Francesco Malcangi and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Single-molecule experiments typically probe one-dimensional projections of complex high-dimensional dynamics, lumping many distinct microscopic configurations into the same observable state. The projection induces memory in the evolution of the observable but otherwise buries features of the underlying potential landscape. We show how the sample-to-sample fluctuations of functionals of projected paths may be utilized to infer hidden features of the landscape such as hidden intermediates and buried free energy barriers.

DY 31.3 Wed 15:00 Poster C

Acoustic properties of phononic crystal defect Lieb Lattices and the time evolution of its compactly localised states — •Katarzyna E. Sopińska, Peter Thomas, and Rudolf A. Römer — University of Warwick, Coventry, CV 7AL, United Kingdom

Lieb lattices are known to support so-called compactly localized states (CLS) in degenerate electronic flat-bands. As a wave phenomenon, CLS should also exist for acoustic waves. We model eigenstates of the acoustic wave equation in macroscopic Lieb lattice-like arrangements of steel rods arranged in air. Alternatively, we also consider the possibility of ultrasound CLSs in metal plates with air holes in Lieb lattice-like geometry. Both situations have obvious experimental realizations. We investigate the conditions for the existence of the CLS. We study frequency dependence as well as pressure amplitudes.

DY 31.4 Wed 15:00 Poster C

Analysis of the Mpemba effect in magnetic systems — •Janett Prehl and Martin Weigel — Technische Universität Chemnitz, Chemnitz, Deutschland

The Mpemba effect, first discovered by Mpemba and Osborne for water [1], is observed when a hot sample cools faster than an initially colder one, when both are refrigerated in the same thermal reservoir. During the last years this effect has also been found to take place in the general context of magnetic phase transitions of different orders. Here, we investigate and discuss the occurrence of this non-equilibrium process

for different ferromagnetic models exhibiting a phase transitions at a critical temperature T_c. We aim to analyze how different initial temperatures, structural properties or updating dynamics influence the time behavior of quantities such as energy E or the average domain length l in order to get a deeper insight in the occurring mechanism of the Mpemba effect for the systems under consideration.

[1] Mpemba, E.B. and Osborn, D.G., *Phys. Educ.* **4**, 172 (1969)

DY 31.5 Wed 15:00 Poster C

Controlling Uncertainty of Empirical First-Passage Times in the Small-Sample Regime — •Rick Bebon and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Central to the kinetics of target-search processes, first-passage phenomena find successful applications across virtually all scientific domains. Here, we address the challenge of controlling uncertainty of empirical first-passage times $\overline{\tau}_n \equiv \sum_{i=1}^{n} \tau_i/n$, i.e., the sample-mean inferred from under-sampled experimental or simulation data. Understanding the ramifications of the small-sample regime, such as non-Gaussian fluctuations, is crucial for obtaining trustworthy estimates but yet remains a daunting task not amenable to standard error-analysis techniques. Consequently, we outline a non-asymptotic theory that enables robust error control in empirical first-passage times of reversible Markov processes regardless of sample-size under minimal assumptions. Key results include concentration inequalities that bound deviations of the sample-mean from the true mean first-passage time from above and sharp two-sided bounds on the expected maximum and minimum deviation from the mean in any given sample.

DY 31.6 Wed 15:00 Poster C

Stress fluctuations and adiabatic speed of sound in liquids: A simple way to estimate it from simulations — Taras Bryk[1,2], Giancarlo Ruocco[3,4], and •Ari Paavo Seitsonen[5] — [1]Institute for Condensed Matter Physics of National Academy of Sciences of Ukraine, Lviv — [2]Institute of Applied Mathematics and Fundamental Sciences, Lviv National Polytechnic University, Lviv — [3]Centre for Life Nano Science @Sapienza, Istituto Italiano di Tecnologia, Rome — [4]Dipartimento di Fisica, Università di Roma La Sapienza — [5]Département de Chimie, École Normale Supérieure, Paris

One of the fundamental quantities in dynamics of the liquid state, the adiabatic speed of sound c_s, is difficult to predict from computer simulations, especially in simulations where the electronic structure is explicitly solved during the simulation, like the density functional theory-based molecular dynamics (DFTbMD). Here we derive an expression for the instantaneous correlator of fluctuations of longitudinal component of stress tensor, which contains c_s along with others quantities easy accessible via computer simulations. We show that the proposed methodology works well in the case of Lennard-Jones and soft-sphere simple fluids, Kr-Ar liquid mixture in connection with simulations with effective pair interactions as well as for liquid Sb, fluid Hg and molten NaCl from DFTbMD simulations.

DY 31.7 Wed 15:00 Poster C

Discovery of the Rapid Increase of Distances in the Early Universe Via Temperature — •Philipp Schöneberg[1], Hans-Otto Carmesin[1,2,3], Jannes Ruder[1], and Phil Immanuel Gustke[1] — [1]Gymnasium Athenaeum, Harsefelder Straße 40, 21680 Stade — [2]Hohenwedeler Weg — [3]Universität Bremen, Fachbereich 1, Postfach 330440, 28334 Bremen

Using general relativity, we derive the following astonishing property of the early universe: The Planck temperature is reached even though the corresponding size of the Hubble radius is still many orders of magnitude larger than the Planck length. Accordingly, the Hubble radius as a function of time must have increased rapidly in the early universe, in a manner not described by general relativity. That era of rapid increase of distances is usually called 'cosmic inflation'. We derive consequences about the era of 'cosmic inflation'.

Literature: Carmesin, H.-O. (2023): Geometrical and Exact Unification of Spacetime, Gravity and Quanta, Berlin: Verlag Dr. Köster.

DY 31.8 Wed 15:00 Poster C

The Macroscopic Dynamics of the Big Bang is Derived from the Microscopic Dynamics — •Hans-Otto Carmesin — Gymnasium Athenaeum, Harsefelder Straße 40, 21680 Stade — Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — Universität Bremen, Fachbereich 1, Postfach 330440, 28334 Bremen

The Schwarzschild metric describes the microscopic dynamics at an object in general relativity. With it, the Friedman Lemaitre equation of the macroscopic dynamics of the Big Bang is derived. Thereby, the flatness problem is solved.

Moreover, the microscopic dynimcs implies the Schrödinger equation and the postulates of quantum physics.

Consequences of these dynamical results are outlined. Especially, the unification of micro- & macrocosm and of general relativity & quantum physics is derived exactly, and this unification will be discussed.

Literature:

Carmesin, H.-O. (2023): Geometrical and Exact Unification of Spacetime, Gravity and Quanta, Berlin: Verlag Dr. Köster.

Carmesin, H.-O. (2022): Explanation of Quantum Physics by Gravity and Relativity. PhyDid B, pp. 425-438.

DY 31.9 Wed 15:00 Poster C

Thermodynamic inference in partially accessible, periodically driven Markov networks using transition-based waiting time distributions — •Alexander Maier, Julius Degünther, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Infering information on the dynamics including thermodynamic quantities of an only partially accessible physical system is one of the challenges of stochastic thermodynamics. In this work, we consider distributions of waiting times between consecutive detectable transitions in partially accessible, periodically driven Markov networks. These distributions allow us to infer dynamical properties like the period of the driving and time-dependent transition rates as well as thermodynamic quantities like estimators of the entropy production rate. Moreover, we conjecture a lower bound of the entropy production rate that is operationally accessible for arbitrary periodic driving.

DY 31.10 Wed 15:00 Poster C

Inference of entropy production beyond the mean — •Julius Degünther, Jann van der Meer, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

The laws of thermodynamics apply to biophysical systems on the nanoscale as described by the framework of stochastic thermodynamics. The theory provides universal, exact relations for quantities like heat or work, which have been verified for experiments where these quantities as well as the system are accessible. Complementary studies in the field consider partially hidden, coarse-grained descriptions, in which the mean entropy production typically is bounded in terms of observable quantities. In contrast, we discuss a fluctuating entropy production that applies to individual trajectories in a coarse-grained description under time-dependent driving. Thus, the concept is applicable to the broad and experimentally significant class of model systems subject to time-dependent driving in which not all relevant states can be resolved.

DY 31.11 Wed 15:00 Poster C

Entropy estimators based on waiting-time distributions for overdamped Langevin dynamics — •Ellen Meyberg and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Deutschland

Stochastic systems are usually only accessible on the meso-scale rather than on the micro-scale leading to the need of an effective, coarse-grained description that is often only partially accessible. Usually, coarse-graining is done by lumping many states together into one compound state. Recently, it has been shown that a complementary coarse-graining based on transitions between Markov states can provide bounds on the entropy production [1]. The logarithmic ratio of waiting-time distributions between two successive transitions in forward and backward direction is a measure of time-irreversibility and thus yields a lower bound on the entropy production. This bound is exact in the case of a uni-cyclic network and can be applied without knowing the steady-state distribution. How can the result obtained for Markov jump processes be applied to an overdamped Langevin dynamics? We explain how transitions can be defined for a continuous dynamics using the milestoning approach [2] and show that the entropy estimator for a uni-cyclic network based on this definition yields the full one.

[1] J. van der Meer, B. Ertel, and U. Seifert, Phys. Rev. X 12, 031025 (2022).

[2] D. Hartich and A. Godec, Phys. Rev. X 11, 041047 (2021).

DY 31.12 Wed 15:00 Poster C

Ein Statistischer Algorithmus für Makroskopische Koeffizienten aus Mikroskopischen Parametern — •Bin Su — Institut fuer Theoretische Physik, TU-Berlin, Germany

Dieser Artikel präsentiert einen Algorithmus aus der dynamischen Statistik, um makroskopische Koeffizienten eines Systems zu erhalten, das sich nicht nur in der Nähe vom Gleichgewicht (wenn das wirkende Außenfeld konstant ist) sondern auch fern vom Gleichgewicht (in Form der nichtlinearen Abhängigkeit von dem Außenfeld) befindet. Die konkrete Anwendung des Algorithmus im Artikel ist die nichtlinear optische Suszeptibilität der Zähflüssigkeit, deren mikroskopische Bestandteile aus anisotropieförmigen Teilchen moduliert wird. Die in den Ergebnissen erscheinenden makroskopischen Koeffizienten bestehen aus einer Reihe der Nichtlineare von dem Außenfeld. Die höheren Ordnungen der Koeffizienten entsprechen mehrfach der einfallenden Frequenz als zweite harmonische Generation usw. und Summenfrequenzgeneration. Der vorliegende statistische Algorithmus würde hier dazu beitragen, bei der Konstruktion eines Teilchensystems, ein homogenes Modell für Plasmas, zu entwickeln und die makroskopischen Messwerte zu erklären.

DY 31.13 Wed 15:00 Poster C

Far-from-equilibrium relaxation in long-range interacting stochastic few-body systems — •Felipe Pereira-Alves and Aljaž Godec — Mathematical bioPhysics group, Max Planck Institute for Multidisciplinary Sciences, Göttingen 37077, Germany

The dynamics of non-equilibrium systems in the presence of long-range interactions still pose great challenges for theory. A paradigm for such systems is Dyson's Brownian motion, for which exact calculations of certain physical observables and correlations are feasible. In our work, we interrogate the relaxation dynamics of the Dyson model prepared by a far-from-equilibrium temperature quench. It was predicted and recently experimentally confirmed that the relaxation, in the form of heating and cooling for an optically trapping colloidal particle, is fundamentally asymmetric. Here, we investigate the corresponding dynamical regimes and underlying (a)symmetries of heating versus cooling of a Dyson chain of trapped Brownian particles interacting with a long-range logarithmic potential.

DY 31.14 Wed 15:00 Poster C

Lane formation in gravitationally driven colloid mixtures consisting of up to three different particle sizes — •Kay Hofmann[1], Marc Isele[2], Artur Erbe[3], Paul Leiderer[2], and Peter Nielaba[2] — [1]Universität, Mainz, Deutschland — [2]Universität, Konstanz, Deutschland — [3]Helmholtz-Zentrum, Dresden, Deutschland

We utilized Brownian dynamics simulations to investigate segregation phenomena of gravitationally driven colloids in two-dimensional confined channels. In the present work, we introduce a third particle species to further our understanding of colloidal systems. The interaction between the colloids is modeled by the Weeks-Chandler-Andersen potential, and the confinement of the colloids is realized by hard walls. A difference in the driving force is established through variation in colloid sizes while maintaining a constant mass density. We observe for binary and ternary systems that a driving force difference induces a transition to lanes. In ternary systems, we investigate the tendency for lane formation in dependence of the medium-sized colloid diameter. Here, we find an optimal ratio between colloid diameters for lane formation in ternary systems. Moreover, we examine the interaction between colloids of varying sizes at the channel walls. Recently, we found that driven large colloids displace smaller ones towards the walls, leading to the formation of small particle lanes during the early stages of simulation. Additionally, we discover that these thin lanes are unstable and gradually dissolve over extended time frames.

DY 31.15 Wed 15:00 Poster C

Heat exchange fluctuation relation for the transition from a micro-canonical to a canonical ensemble in a classical harmonic oscillator — Leonel F. Ardila[1], Nicolás Torres-Domínguez[2], José D. Muñoz[1], and •Carlos Viviescas[2] — [1]Simulation of Physical Systems Group and Center of Excellence in Scientific Computing: CoE-SciCo, Department of Physics, Universidad Nacional de Colombia, Bogotá, Colombia. — [2]Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia.

In this work we present the analytical derivation and the numerical verification of an original heat fluctuation relation for a harmonic oscillator evolving at constant temperature from a micro-canonical to a canonical ensemble. We found that the probabilities $P(Q)$ and $P(-Q)$ of gaining or loosing a heat Q, respectively, are related as

$$\frac{P(Q)}{P(-Q)} = e^{-2Q/k_B T} \quad , \tag{1}$$

with T the temperature. This result is numerically validated through molecular dynamics simulations with an overdamping Langevin equation algorithm [1]. Our results give insight on the probabilistic behavior of a system undergoing thermalization and contributes to extend fluctuation relations to micro-canonical initial states [2].

[1] P. Talkner, M. Morillo2, J. Yi and P. Hänggi, New J. Phys. **15**,095001(2013).

[2] N. Goga, A.J. Rzepiela, A.H. de Vries, S.J. Marrink, and H.J.C. Berendsen, J. Chem. Theory Comput., **8** 3637-3649 (2012)

DY 31.16 Wed 15:00 Poster C

On the emergence of memory in equilibrium versus non-equilibrium systems — •Xizhu Zhao[1,2], David Hartich[1], and Aljaž Godec[1] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]Max Planck School Matter to Life, Heidelberg, Germany

Experiments often probe observables that correspond to low-dimensional projections of high dimensional dynamics. In such situations distinct microscopic configurations become lumped into the same observable state. It is well known that correlations between the observable and the hidden degrees of freedom give rise to memory effects. However, how and under which conditions these correlations emerge remains poorly understood. Here we shed light on two fundamentally different scenarios of the emergence of memory in minimal stationary systems, where observed and hidden degrees of freedom evolve either cooperatively or are coupled by a hidden non-equilibrium current. In the reversible setting strongest memory manifests when the time-scales of hidden and observed dynamics overlap, whereas, strikingly, in the driven setting maximal memory emerges under a clear time-scale separation. Our results hint at the possibility of fundamental differences in the way memory emerges in equilibrium versus driven systems that may be utilized as a "diagnostic" of the underlying hidden transport mechanism. [1]

[1] X. Zhao, D. Hartich, & A. Godec, arXiv:2311.12788 (2023)

DY 31.17 Wed 15:00 Poster C

In pursue of the tetratic phase in hard rectangles — •Denis Dertli and Thomas Speck — Institut für Theoretische Physik IV der Universität Stuttgart, Stuttgart, Deutschland

We consider two-dimensional systems of hard rectangles motivated by the collective behavior of self-assembled DNA-based nanostructures. We investigate this system in the NPT ensemble through extensive hard-particle Monte Carlo simulations. The phase behavior is controlled by the packing fraction and the aspect ratio of the particles. Both the equation of state and free-energy profiles of order parameters point to a continuous Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) two-step melting/freezing scenario interpolating between the smectic and isotropic phase. While rod-like particles with large aspect ratio assemble in an intervening nematic phase, a "tetratic" phase is found for moderately elongated rectangles. Our approach demonstrates the distinct properties of these phases and provides a quantitative determination of phase boundaries. Our findings can be verified in recent experiments of biological systems composed of DNA-based nanostructures.

DY 31.18 Wed 15:00 Poster C

Transgenerational trajectory statistics of dividing and interacting cells — •Leif Peters[1,2] and Philip Bittihn[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen 37077, Germany — [2]Institute for the Dynamics of Complex Systems, Göttingen University, Göttingen 37077, Germany

In growing dense active matter, growth and mechanical interactions give rise to non-trivial single-particle trajectories and complex collective motion. However, finite particle lifetimes in such systems pose a fundamental challenge to their characterization using traditional statistical-physics approaches. We use simulations of a minimal agent-based model to describe and quantify the movement of single cells in a growing active bath. To analyze the long-term statistics, we define observables like a transgenerational mean squared displacement. We evaluate these observables for different ensembles based on ances-

tral relationships between cells and distinct ways to deal with trajectory multiplicity. In systems in homeostasis with random removal and therefore turnover of cells, our results show similarities between the movement of single cells and noise driven dynamics.

DY 31.19 Wed 15:00 Poster C

Effect of burst packages on coding by primary sensory afferents in weakly electric fish — •Maria Schlungbaum[1,2], Alexandra Barayeu[3,4], Jan Grewe[3,4], Jan Benda[3,4], and Benjamin Lindner[1,2] — [1]Physics Department, Humboldt University Berlin — [2]Bernstein Center for Computational Neuroscience Berlin — [3]Institute for Neurobiology, Eberhard Karls Universität Tübingen — [4]Bernstein Center for Computational Neuroscience Tübingen

How burst spikes influence the coding of time-dependent signals is not well understood. We study the impact of burst packages on the output statistics of sensory neurons, namely the first- and second-order response functions, the spike train power spectrum, and the coherence function. Burst packages modulate these response functions in a frequency-dependent manner; they can have either an increasing or diminishing effect (low frequencies) or no effect at all (large frequencies) on all these statistics. In particular, we demonstrate that bursting can boost the nonlinear response in certain frequency regions. Assuming a random number of burst spikes endowed with a temporal jitter, we calculate theoretical formulas for the spectral statistics. In this framework, we do not take stimulus-driven effects on bursting into account. We compare our analytical results to spike train data from P-unit electroreceptors of the electric fish *Apteronotus leptorhynchus* and inspect how well our theoretical results can describe the differences between coding with and without burst spikes in these cells.

DY 31.20 Wed 15:00 Poster C

Large-deviation simulation of the Brownian Bee model — •Hartmut Schoon and Alexander K. Hartmann — Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

The Brownian Bee model is a version of Branching Brownian motion, evolving into a nonequilibrium steady state. The model consists of N particles performing independent Brownian motion. Every particle has the ability to randomly branch and create a new particle at the same position. At those branching events the farthest particle from its origin will be deleted, resulting in a conservation of the particle count. Berestycki *et al.* [1] showed that at long times the particles form a spherical steady state with radius l_0 which depends on the spatial dimension d. Meerson and Sasorov [2] investigated the probability $\mathcal{P}(l,N,T)$ of the maximum distance l of a particle from the origin within a very large time interval $0 < t < T$. They concluded, that this probability follows a large-deviation form $-\ln \mathcal{P}(l,N,T) \simeq NTR_d(l)$. Asymptotics for the rate function $R_d(l)$ were provided for $l \ll l_0$ and $l \gg l_0$ and a full analytical solution is given for $d = 1$. We implemented Brownian Bees numerically and computed $\mathcal{P}(l,N,T)$ by a large-deviation simulation [3] for various dimensionalities d which allowed us to obtain the distribution down to exponential small probability densities like $\mathcal{P} \sim 10^{-100}$.

[1] J. Berestycki, et al., Ann. Prob. **50**, 2133-2177 (2022)
[2] B. Meerson and P. Sasorov, Phys. Rev. Lett., **103**, 032140 (2021)
[3] A.K. Hartmann, Phys. Rev. E , **89**, 052103 (2014)

DY 31.21 Wed 15:00 Poster C

Josephson diode as a heat engine — •Konstantinos Kontogeorgiou[1], Inanc Adagideli[2,3,4], and Fabian Hassler[1] — [1]Institute for Quantum Information, RWTH Aachen University, Germany — [2]Faculty of Engineering and Natural Sciences, Sabanci University, Orhanli-Tuzla, Istanbul, Turkey — [3]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands — [4]TUBITAK Research Institute for Fundamental Sciences, 41470 Gebze, Turkey

Non-reciprocal superconducting elements, called Josephson diodes, have received increased attention in the past years. Here we explore the possibility of utilizing the reciprocity breaking to realize a thermal engine. To this end, we study the system coupled to two reservoirs at different temperatures. We investigate the influence of the different parameters in order to maximize the efficiency.

DY 31.22 Wed 15:00 Poster C

Cluster percolation in the 3D $\pm J$ random-bond Ising model — •Lambert Münster and Martin Weigel — Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

Single-replica clusters are successful in describing phase ordering in systems without frustration [1]. For models with frustration such as spin glasses where the order parameter, the overlap, is defined with respect to two replicas, it is convenient to define clusters which include multiple replicas [2]. In this work we numerically study multiple replica clusters in the 3D $\pm J$ random-bond Ising model with the fraction of ferromagnetic bonds set to $p = 0.9$ and $p = 0.5$, respectively, to investigate how different types of clusters can be used to describe phase ordering when there exists a ferromagnetic phase and when the ordering is of spin-glass type.

[1] A. Coniglio and A. Fierro, Correlated percolation, in Complex Media and Percolation Theory, edited by M. Sahimi and A. G. Hunt (Springer, New York, 2021), p. 61.
[2] J. Machta, C. M. Newman, and D. L. Stein, J. Stat. Phys. **130**, 113 (2008)

DY 31.23 Wed 15:00 Poster C

Correlation, crossover and broken scaling in the Abelian Manna Model — •Letian Chen[1], Hoai Nguyen Huynh[1,2], and Gunnar Pruessner[1] — [1]Department of Mathematics, Imperial College London, United Kingdom — [2]Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore

The role of correlations in self-organised critical (SOC) phenomena is investigated by studying the Abelian Manna Model (AMM) in two dimensions. Local correlations of the debris left behind after avalanches are destroyed by re-arranging particles on the lattice between avalanches, without changing the one-point particle density. It is found that the spatial correlations are not relevant to small avalanches, while changing the scaling of the large (system-wide) ones, yielding a crossover in the model's scaling behaviour. This crossover breaks the simple scaling observed in normal SOC.

DY 31.24 Wed 15:00 Poster C

Amorphous topological insulator: towards quantum Hall criticality — •Johannes Dieplinger[1], Soumya Bera[2], and Naba P Nayak[2] — [1]Institute of Theoretical Physics, University of Regensburg, D-93040 Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

We numerically investigate the critical properties of a topological transition in a two-dimensional lattice with randomly distributed points. The trivial to topological Anderson insulator transition belongs to the unitary class A of the ten-fold symmetry classification of non-interacting fermions. The model intrinsically breaks the time-reversal symmetry without the need for an external mag- netic field, often referred to as the Chern insulator. This transition is induced by varying the density of lattice points or adjusting the mass parameter. Using the two-terminal conductance and multi- fractality of the wavefunction, we found that the amorphous topological insulator exhibits the same universality as the integer quantum Hall transition. The localization length exponent is between $\nu = 2.55$ - 2.61 regardless of the approach to the critical point, thus pointing towards the universal nature of the transition across the topological phase boundary in the non-crystalline model. The irrelevant exponent, y for both observables, is y = 0.3(1), slightly smaller than values obtained using transfer matrix analysis in the Chalker-Coddigton network. Additionally, the analysis of the entire distribution function of the inverse participation ratio reveals a potentially non-parabolic multi- fractal spectrum at the critical point of the quantum anomalous Hall transition.

DY 32: Poster: Active Matter, Soft Matter, Fluids

Time: Wednesday 15:00–18:00 Location: Poster C

DY 32.1 Wed 15:00 Poster C

Modelling electrokinetic two-phase flows applicable to porous media — •Alexander Reinauer and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

The simulation of electrolytic multiphase flow is a highly complex task that requires to simulate a large number of explicit particles or to solve a highly coupled set of non-linear partial differential equations, namely the Navier-Stokes and the Nernst-Planck equations in a continuous picture. At the cost of the molecular details, the continuum scale description enables the investigation of larger-scale systems that are relevant for oil-recovery and biological systems. An application is the electrophoresis of liquid droplets, which displays various complex phenomena including phase separation and transport in biological systems. Several choices of solvers exist for the continuum scale description, our implementation is based on the color-gradient extension to the lattice Boltzmann method to simulate immiscible multiphase flow as well as a custom Nernst-Planck solver to describe the transport of dissolved charged chemical species. By developing a coupling between these two methods, we allow for the inclusion of preferential solubilities of the chemical species. For the implementation, the pystencils/lbmpy framework is used, providing a highly optimized code-generation tool for CPU and GPU that allows for rapid prototyping of stencil-code in Python. In order to assess our model, we conduct a simulation study of freely suspended liquid droplets under the application of an external electric field.

DY 32.2 Wed 15:00 Poster C

Nucleation and Growth of Sessile Chemically Active Droplets — •Noah Ziethen and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Driven chemical reactions can control the macroscopic properties of droplets, like their size. Moreover, such reactions control their formation from a homogeneous phase, e.g., for structuring biological cells. Inside cells, various organelles coexist and potentially interact with the complex cytoplasm. Understanding how the interaction of droplet material with boundaries modifies the droplet formation of size-controlled droplets is thus crucial.

Our numerical simulations reveal that reactions generally suppress nucleation in the presence of a boundary, as expected from homogeneous nucleation. Intriguingly, we uncover a coupled effect of wall interaction and chemical reactions, leading to shapes that deviate from spherical caps. We establish that these distortions result from anisotropic fluxes responding to the boundary conditions dictated by the Young Dupré equation. These findings demonstrate how the properties of stationary active droplets can deviate from their passive counterparts. In a biological context, such shape deformations may serve as a mechanism for cells to transition from a droplet state to a wetted film along the boundary.

DY 32.3 Wed 15:00 Poster C

Droplets on soft and flexible sheets — •Salik Sultan, Josua Grawitter, and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Droplets sitting on flexible sheets deform the sheets and assume the shape of a lens. One promising application of this phenomenon is the potential for designing tunable fluidic lenses. In our ongoing research we build on our established droplet model, developed using the boundary element method (BEM), to investigate dynamic wetting on thin flexible sheets. Central to our study is the nuanced interplay between the mechanical attributes of the sheet and droplet behavior, with a particular emphasis on contact angle during wetting. Drawing inspiration from biological membranes, we have integrated the Skalak model for elastic deformations and the Helfrich Hamiltonian for bending mechanics into our approach. This enables us to dissect how tension forces and sheet rigidity impact droplet shape and wetting dynamics, and ultimately allows us to steer droplets along the sheet. While our model has implications in material science, its versatility allows for insights into interfacial biology, illuminating the fascinating interactions between soft substrates and liquid interfaces.

DY 32.4 Wed 15:00 Poster C

Nonreciprocal Model B and the role of nonreciprocal interfacial forces — •Bibhut Sahoo[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen — [2]Department of Mathematics, King's College London, London

Recently it has been shown that the Cahn-Hilliard model for phase separation with nonreciprocal interaction can give rise to travelling states. While the Cahn-Hilliard description comes from a magnetic analogy, we explore here the corresponding nonreciprocal model B dynamics as the continuum theory for a particle mixture. We explore the topology of the phase diagram for binary mixtures, determining where spinodal instabilities occur and where these lead to travelling states because the relevant eigenvalues are complex. Simulations show that in addition to pure travelling states, coexistence of stable, equilibrium-like domains with strongly fluctuating patterns in the rest of the system can also occur, a feature that has not been observed in the Cahn-Hilliard setting. We argue further, based on a nonreciprocal version of Dean's equation, that coarse graining into a model B description should generically lead to nonreciprocal forces also at interfaces, rather than only in the bulk as assumed in nonreciprocal field theories to date. We explore the effects of such nonreciprocal interfacial forces and find that they can convert conventional spinodal instabilities into ones producing travelling patterns. This indicates that interfacial nonreciprocity can have important implications for the spinodal dynamics of phase separating mixtures, and potentially also for their long-time dynamics.

DY 32.5 Wed 15:00 Poster C

PT Symmetry and Non-Hermitian Band Topology — •Kang Yang[1], Zhi Li[2], Lukas König[3], Lukas Rødland[3], Marcus Ståhlhammar[4], and Emil Bergholtz[3] — [1]Freie Universität Berlin, Berlin, Germany — [2]Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada — [3]Stockholm University, Stockholm, Sweden — [4]Nordita, Stockholm, Sweden

Non-Hermitian matrices are ubiquitous in the description of nature ranging from classical dissipative systems, including optical, electrical, and mechanical metamaterials, to scattering of waves and open quantum many-body systems. Multiple non-Hermitian bands exhibit intriguing exceptional points, spectral braids and crossings. In this work we develop a topological description based on non-Hermitian band gaps and separation gaps. We provide a unified classification of both gapped and nodal systems in the presence of physically relevant parity-time (PT) and pseudo-Hermitian symmetries using homotopy theory. This uncovers new stable topology stemming from both eigenspectra and wavefunctions, and remarkably also implies distinct fragile topological phases. In particular, we reveal different Abelian and non-Abelian phases in PT-symmetric systems, described by frame and braid topology. The corresponding invariants are robust to symmetry-preserving perturbations that do not induce (exceptional) degeneracy, and they also predict the deformation rules of nodal phases. We further demonstrate that spontaneous PT symmetry breaking is captured by Chern-Euler and Chern-Stiefel-Whitney descriptions, a fingerprint of unprecedented non-Hermitian topology overlooked in previous study.

DY 32.6 Wed 15:00 Poster C

AMEP: Active Matter Evaluation Package — •Kai Luca Spanheimer, Lukas Hecht, Kay-Robert Dormann, Aritra Mukhopadhyay, Mahdieh Ebrahimi, Suvendu Mandal, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, D-64289 Darmstadt, Germany

The Active Matter Evaluation Package (AMEP) is a Python library for analysing simulation data of particle-based and continuum simulations. It provides a powerful and simple interface for handling large data sets based on the HDF5 data format. Main features are various methods for calculating observables, visualising results, and analysing simulation data of molecular dynamics simulations, Brownian-dynamics simulations, and continuum simulations. The methods are developed for analysis of active matter systems but are applicable to passive systems as well. AMEP is written in pure Python and leverages powerful libraries such as NumPy, SciPy, Matplotlib, and scikit-image. Computationally expensive methods are parallelised and optimised to run efficiently on workstations, laptops, and high-performance computing

architectures. AMEP provides the first unified framework for analysing results of both particle-based and continuum simulations. This allows users to easily analyse their data of simulations that combine particle-based and continuum techniques, e.g. as used to study the motion of bacteria in chemical fields or modelling particle motion in a flow field.

DY 32.7 Wed 15:00 Poster C

Consequence of anisotropy on flocking: the truly discretized Vicsek model — •Mintu Karmakar[1], Swarnajit Chatterjee[2], Raja Paul[1], and Heiko Rieger[2,3] — [1]School of Mathematical & Computational Sciences, Indian Association for the Cultivation of Science, Kolkata – 700032, India. — [2]Center for Biophysics & Department for Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany. — [3]INM - Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken, Germany.

We numerically study a "true" discretization of the Vicsek model (TDVM) on an off-lattice two-dimensional domain to probe the transition of collective motion as the system switches its symmetry from discrete to continuous. The TDVM consists of particles able to execute motion on a plane in q discrete angular directions like the active clock model (ACM) and follows dynamical rules of particle alignment and movement inspired by the prototypical Vicsek model (VM). We find a novel cluster phase for small q and noise and observe the formation of microphase and cross-sea in the phase coexistence region as q is increased and the system approaches the VM. We find that although the giant number fluctuations for large q corroborate with the nature of phase separation in the coexistence region, the large length-scale behavior of the direction of the global order and correlations does not correspond with it. We also investigate the stability of the ordered liquid phase and find it metastable to the nucleation of droplets of different polarization.

DY 32.8 Wed 15:00 Poster C

Tuning kinetics of chemically fueled droplets — •Lennard Holschuh and Joachim Dzubiella — Physikalisches Institut, Albert-Ludwigs Universität Freiburg, Germany

Membraneless organelles like centrosomes play an essential part in intracellular structuring. A similar behaviour can be mimicked by active droplets resulting from phase separation introduced by a chemical reaction that depends on the available fuel. Recent experiments with synthetic molecules in a chemically fueled reaction cycle explore the non-equilibrium behaviour of these active droplets. In our work, a two-state chemical reaction is modeled with a two-dimensional reactive Brownian dynamics simulation and compared to a macroscopic description with the Fokker-Planck equation. In the simulation, particles with state 0 are soluble and particles in state 1 - which are activated via the consumption of fuel - become attractive and are able to accumulate to droplets. In the case of a saturated system, expected power laws for the radius of the droplets as well as for the number of droplets are recovered. A coordination-dependent distinction of 'internal' and 'external' particles of the droplet gives further control over the deactivation process. The simulation shows that deactivation of only external particles slows down the decay and stabilizes the droplets, whereas the deactivation of only internal particles can lead to a temporary encapsulation of deactivated particles where the chemically active particles serve as shell. Similarities and differences to related experiments are discussed.

DY 32.9 Wed 15:00 Poster C

Collective Hall current in chiral active fluids: Coupling of phase and mass transport through traveling bands — Frank Siebers[1], •Robin Bebon[2], Ashreya Jayaram[2], and Thomas Speck[2] — [1]Institute for Theoretical Physics 4, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7-9, 55128 Mainz, Germany

Active fluids, composed of motile entities, have garnered enormous interest owing to the programmability of their collective spatiotemporal behavior that can be controlled by tuning physical properties at the individual level. We report a novel phase exhibited by locally aligning chiral particles – (meta-)stable, dispersionless traveling bands that couple phase and mass transport. Intriguingly, the particle current is neither parallel nor perpendicular to the direction of phase propagation, with magnitudes depending on the self-propulsion and angular speeds of particles. We thus report the first instance of a self-organized Hall (or Magnus) effect in chiral active fluids with a tunable Hall angle. Through particle-based simulations, we reveal the mechanism underlying this phenomenon and corroborate our results using a minimal hydrodynamic theory. Within this framework we show that bands arise as non-dispersive soliton solutions that fully explain the properties observed in simulations.

DY 32.10 Wed 15:00 Poster C

Phase Separation in Cycloactive Matter — •Theo Spornhauer[1], Johannes Zierenberg[1,2], and Benoît Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany

Living systems that generate activity from environmental resources are dependent on environmental conditions. In nature, these conditions are typically not static, but have a strong temporal profile, as seen for example in the day-night cycle that affects photosynthesis. Here, we numerically investigate the effect of cyclic activity variations in a minimal model of active Brownian particles, focusing in particular on how they affect the phenomenon of motility-induced phase separation (MIPS). Performing simulations at various driving amplitudes and frequencies, our results show that MIPS is robust to the introduction of cyclic activity. For cycles crossing the transition point, measures of phase separation exhibit a characteristic hysteresis, which we find to be most pronounced when the timescales associated with activity and cyclic driving are comparable. We also discuss how the geometric properties of MIPS clusters are affected by the presence of the cyclic drive.

DY 32.11 Wed 15:00 Poster C

Collective actuation in active elastic solids — •Katherina E. Hemmo, Kim L. Kreienkamp, and Sabine H. L. Klapp — Technische Universität Berlin

Collective motion is ubiquitous in various biological systems consisting of interacting active agents. Many of the coupling mechanisms rely on alignment couplings based on an exchange of heading vector information. However, collective motion can also emerge without explicit alignment interactions, solely through positional information exchange [1]. Building upon previous research on elastically coupled active solids [1-2], we here focus on active particles coupled via springlike interactions, leading to self-alignment in direction of displacement. For large enough activity, collective actuation, characterized by nearly synchronized oscillations of all particles around their equilibrium positions, can be observed [1-2]. Here, we address the question of how stable the collective actuation is when mixed groups include non-conforming members. Specifically, we introduce dissenters into the system, which do not engage in the self-alignment interactions but behave as Brownian particles in the otherwise active elastic sheet. Using particle-based simulations and normal mode analysis we find that an increasing number of dissenters weakens the collective actuation. We examine various geometric configurations of dissenters across different noise strengths to assess the most stable configurations and understand how the presence of dissenters impacts the elastic active solid as a whole.

[1] E. Ferrante, et al., New J. Phys. 15.9, 095011 (2013).
[2] P. Baconnier, et al., Nature 18.10, 1234 (2022).

DY 32.12 Wed 15:00 Poster C

Active fractalytes — •Sebastian Fehlinger and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Non-reciprocal interactions occur widely in nature. For the specific case of a binary mixture of passive particles, where one species non-reciprocally attracts the other one, the breaking of the action reaction principle can lead to formation of active colloidal molecules which are capable of self-propulsion. For small systems, such active molecules have already been realized in experiments [1,2]. The focus of the present work is to understand the collective behavior of many active molecules. Using particle based simulations, in a wide range of the parameter space, we find that active molecules self-organize into ballistically moving structures that feature holes, gaps and a fractal dimension. We call them active fractalytes [3]. Besides structural properties, which clearly distinguish them from aggregates emerging from diffusion-limited aggregation, we analyze the dynamics and the scaling properties of active fractalytes and complement our work with a continuum theory.

[1] F. Schmidt et al. J. Chem. Phys. 150, 094905 (2019).
[2] J. Grauer et al. Nat. Commun. 12, 6005 (2021)
[3] S. Fehlinger, B. Liebchen. Phys. Rev. Res. 5, L032038 (2023).

DY 32.13 Wed 15:00 Poster C

Flocking of two unfriendly species — •Matthieu Mangeat[1], Swarnajit Chatterjee[1], Chul-Ung Woo[2], Jae Dong Noh[2], and Heiko Rieger[1] — [1]Saarland University, Saarbrücken, Germany — [2]University of Seoul, Seoul, Korea

Complex systems are typically heterogeneous as individuals vary in their properties, their response to the external environment and to each other. In particular, many biological systems that show flocking involve self-propelled particles with heterogeneous interactions, which motivates the study of populations with multiple species. In this work, we consider the two-species variant of the Vicsek model (TSVM) and the active Ising model (TSAIM), consisting of two kinds of self-propelled particles that tend to align with particles from the same species and to antialign with the other. These two-species models show a flocking transition that is reminiscent of the original one-species model, as a liquid-gas phase transition, and display phase-separation in the coexistence region where dense liquid bands of each species propagate in a gaseous background. The interesting feature of these models is the appearance of two dynamical states in the coexistence region: the PF (parallel flocking) state in which all bands of the two species propagate in the same direction, and the APF (antiparallel flocking) state in which the bands of two different species move in opposite directions. PF and APF states perform stochastic transitions from one to the other only in TSVM, and the APF liquid phase of the TSVM is replaced by a high density PF state in the TSAIM. We also study the impact of particle switching from one species to another.

DY 32.14 Wed 15:00 Poster C

Controlling the self aggregation of active triblock Janus colloids — •Juri Schubert, Salman Fariz Navas, and Sabine H. L. Klapp — ITP, Technische Universität Berlin, Germany

Triblock Janus colloids belong to the family of patchy particles, interacting with hydrophobic attraction at opposite poles and electrostatic repulsion in the equatorial region. They are known to self assemble into a colloidal kagome crystal from experiments [1] and theory [2]. Such structures are of particular interest owing to their novel optical and mechanical properties. However, the self-assembly of open-cell lattices is a multistep process involving the formation of intermediate competing structures resulting in long time-scales. Recently, it has been shown that introducing activity can significantly accelerate the self assembly and enhance the kagome yield [3].

Here, we study the model introduced in [3] and build upon the results to compare with prior research on Janus particles [2]. Investigating the aggregation pathway, we show preliminary results on the use of time dependent activity protocols to gain better control of the aggregation process.

[1] Q. Chen, S. C. Bae, S. Granick, Nature 469, 7330 (2011).
[2] F. Romano, F. Sciortino, Soft Matter 7, 12 (2011).
[3] S. A. Mallory, A. Cacciuto, JACS 141, 6 (2019).

DY 32.15 Wed 15:00 Poster C

Thermodynamics and coarse graining of colloidal heat engines with active baths — •Roland Wiese[1], Klaus Kroy[1], and Viktor Holubec[2] — [1]Institute for Theoretical Physics, Leipzig University, 04103 Leipzig, Germany — [2]Faculty of Mathematics and Physics, Charles University, CZ-180 00 Prague, Czech Republic

We review the applicability of effective temperatures to describe the thermodynamics of a colloidal probe particle in a bath of active Brownian particles - a prototypical example of a non-equilibrium Brownian system. Using Brownian dynamics simulations, we realise a microscopic Stirling cycle by modulating the probe's trapping potential and the bath particles' swim speed. In contrast to claims for recent experimental studies of colloids in bacterial baths, we show that Carnot's limit for the thermodynamic efficiency cannot be broken, even for a strongly non-Gaussian active bath, by reproducing and rationalising the average performance reported for the experimental system. The probe-in-active-bath setup is coarse-grained to a single active Brownian particle (ABP) and to a single active Ornstein-Uhlenbeck particle (AOUP), with their respective noise correlations determined by the underlying probe-bath interactions. Not only thermodynamic averages but even the stochastic fluctuations of the exchanged work and heat are faithfully preserved for the AOUP.

DY 32.16 Wed 15:00 Poster C

Kinetic Event-Chain Algorithm: Exploring mixtures of hard active and passive particles — •Nico Schaffrath, Thevashangar Sathiyanesan, Tobias Kampmann, and Jan Kierfeld — Physics Department, TU Dortmund, 44221 Dortmund, Germany

The novel cluster kinetic Monte-Carlo algorithm for active matter systems, which is based on the event-chain Monte-Carlo method, efficiently simulates systems of self-propelled hard particles. We extend this algorithm to various mixtures of active and passive particles. In doing so, we uncover the microscopic mechanism behind the enhanced diffusion of a completely symmetric passive tracer disk in a bath of active hard disks. Furthermore, our study includes a systematic exploration of the effective interaction between two large passive disks in a bath of active hard disks, along with an examination of the phase behavior of binary mixtures of active and passive hard disks.

DY 32.17 Wed 15:00 Poster C

Harnessing synthetic active particles for physical reservoir computing — •Xiangzun Wang[1,2] and Frank Cichos[1] — [1]Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI) Dresden/Leipzig, 04105 Leipzig, Germany

The processing of information is an indispensable property of living systems realized by networks of active processes with enormous complexity. They have inspired many variants of modern machine learning, one of them being reservoir computing, in which stimulating a network of nodes with fading memory enables computations and complex predictions. Reservoirs are implemented on computer hardware, but also on unconventional physical substrates such as mechanical oscillators, spins, or bacteria often summarized as physical reservoir computing. Here we demonstrate physical reservoir computing with a synthetic active microparticle system that self-organizes from an active and passive component into inherently noisy nonlinear dynamical units. The self-organization and dynamical response of the unit are the results of a delayed propulsion of the microswimmer to a passive target. A reservoir of such units with a self-coupling via the delayed response can perform predictive tasks despite the strong noise resulting from the Brownian motion of the microswimmers. To achieve efficient noise suppression, we introduce a special architecture that uses historical reservoir states for output. Our results pave the way for the study of information processing in synthetic self-organized active particle systems.

DY 32.18 Wed 15:00 Poster C

Spontaneous Symmetry Breaking in Microdroplets Filled with Heat Releasing Particles — •Akshay Kallikkunnath, Arthur Markus Anton, and Frank Cichos — Molecular Nanophotonics, Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth System Sciences, Leipzig University, Linnéstraße 5, 04103 Leipzig, Germany

Self-propulsion of microscopic objects require symmetry breaking, which is often achieved by preparing geometrically asymmetric particles, e.g., Janus particles. Self-propulsion can, however, also be achieved with symmetric particles like droplets, where the symmetry is broken dynamically, e.g., by a chemical reaction that induces Marangoni fluxes at the interface to the surrounding medium. Here, we show the self-propulsion of water-in-oil microdroplets encapsulated with symmetric iron oxide particles upon widefield laser illumination. The heat released by the particles close to the boundary of the droplet induces strong Marangoni flows that reshape the distribution of particles inside the droplet. The dynamics of the particles and hydrodynamic flow fields also couple to other particles to create collective motion and cohesive behavior. Our results provide insight into complex collective behavior of micro-particles in confinements and provide new directions for future research in the engineering of such actively propelled micromachines.

DY 32.19 Wed 15:00 Poster C

Phase ordering kinetics in discretized flocking — •Sayam Bandyopadhyay[1], Aditya Kumar Dutta[1], Swarnajit Chatterjee[2], Mintu Karmakar[1], Heiko Rieger[2], and Raja Paul[1] — [1]School of Mathematical & Computational Sciences, Indian Association for the Cultivation of Science, Kolkata – 700032, India — [2]Center for Biophysics & Department for Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

We undertake a numerical study of the ordering kinetics in the two-dimensional (2d) active Ising model (AIM), a discrete flocking model with a non-conserved scalar order parameter. For a quench into the liquid-gas coexistence region and in the ordered liquid region, the char-

acteristic length scale of both the density and magnetization domains follows the Lifshitz-Cahn-Allen (LCA) growth law: $R(t) \sim t^{1/2}$, consistent with the growth law of passive systems with scalar order parameter and non-conserved dynamics. The system morphology is analyzed with the two-point correlation function and its Fourier transform, the structure factor, which conforms to the well-known Porod's law, a manifestation of the coarsening of compact domains with smooth boundaries. We also find the domain growth exponent unaffected by the noise and the self-propulsion velocity of the active particles. However, transverse diffusion is found to play the most significant role in the growth kinetics of the AIM.

DY 32.20 Wed 15:00 Poster C

Hydrodynamic Interaction of a Microswimmer with a Deformable Membrane — •Sagnik Garai, Akhil Varma, and Christina Kurzthaler — Max Planck Institute for the Physics of Complex Systems, Dresden

We study the dynamics of microswimmers, such as bacteria, when they encounter elastic surfaces, like biological membranes, in their environment. In an unbounded domain, the far-field flow signature of a microswimmer is described by a combination of a force and a rotlet dipole. The presence of the membrane creates a non-linear coupling of this flow with the elastic deformation, thereby modifying the microswimmer's velocity. Using the Lorentz reciprocal theorem, we obtain a leading-order correction to the swimming velocity for small membrane deformations. The elastic deformations produce microswimmer trajectories that differ from those observed near rigid surfaces. We characterize them by identifying scattering and bound swimming states near the membrane. Our far-field results are compared to the analytical solution of an axisymmetric squirmer near the membrane.

DY 32.21 Wed 15:00 Poster C

Force-Free and Autonomous Active Brownian Ratchets — •Constantin Rein[1], Klaus Kroy[1], and Viktor Holubec[2] — [1]Universität Leipzig, Institut für theoretische Physik, Brüderstraße 16, 04109 Leipzig — [2]Charles University Prague, Department of Macromolecular Physics, V Holešovičkách 747/2, Praha 8

We present the recently found force-free activity ratchet, that rectifies active Brownian motion using solely time-independent activity landscapes (Rein2023,doi.org/10.1209/0295-5075/accca5). In one dimension, spatially asymmetric activity does not suffice to induce directed transport, unless the activity is modulated in time or an additional potential is used, whereas, in higher dimensions, static activity landscapes alone can induce ratcheting. The underlying principle is similar to the ratcheting induced by asymmetric obstacles in microswimmer baths: swimmers with suitable orientations get channeled, while the others get trapped in low-activity regions until they lost their orientation. The poster presents a full exploration of the properties and working mechanism of the ratchet and its response to external forcing, with an outlook on similarities to transport phenomena in rarefied gases.

DY 32.22 Wed 15:00 Poster C

Investigation in microfiltration for water purification — •Tim R. Baumann, Dario Anselmetti, and Martina Viefhues — Experimental Biophysics, Bielefeld University, Bielefeld, Germany

Fresh water and oceans' pollution due to contamination by plastics is a global endangerment and a highly discussed topic in politics and socioeconomics. Over the last years many restrictions on handling plastics were made specific in the European Union focussing mainly on reducing plastic waste production. Nevertheless, due to mechanical and photo-/chemical wear and tear macroplastics degrade to microplastics or even smaller nanoplastics. Particles of that size are able to migrate in organic tissue and therefore becoming part of the food chain. Filtering plastics of this size is a difficult effort. Thus, this work aims to develop a microfluidic device to be used for removing microplastics from water. Clark et al. proposed a bioinspired mechanism for purification mimicking the feeding mechanism of ray species. The device consists of two rows of tilted posts, splitting the volume. At high Reynolds numbers, i.e. high flow rates, filtration occurs due to position dependent shear and wall induced lift forces. This led to filtration of spherical beads down to 10 μm. In our work, we aim on recreating those results and gaining better understanding of the underlining mechanisms to improve the filter system. Our measurements revealed that the ratio of filtered volume, increased with flow rate up to 50%. Additionally, we were able to filtrate 82% of microparticles. Further, we gain insides of the geometric impact on the systems filtration throughput and efficiency.

DY 32.23 Wed 15:00 Poster C

Deep geothermal fluid flow in complex confinements — •Carola M. Buness, Fabian Nitschke, and Thomas Kohl — Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Deep geothermal projects often reach into hard rocks with low permeability. In these rock formations, the geothermal fluid flows through fracture voids, whose surface roughness varies significantly depending on the type of rock. The complex geometry of the fracture void plays a crucial role in the fluid dynamics as well as the flow rate, which depends highly on the distance to the borehole. However, the detailed description of roughness and fluid dynamics within fractures remains an open research challenge. Since these fluid dynamics define the fracture pressure field, understanding them is one key for the safe operation of deep geothermal power plants in low-porous rock formations. To address this issue, we investigate the fluid dynamics experimentally and numerically in various rough confinements. We measure and analyze the rock surface roughness of different rocks to identify the most appropriate parameters to describe the roughness. Utilizing these parameters, we are recreating rough surfaces to investigate the fluid dynamics within flow-through experiments across a broad range of flow rates, spanning from laminar flow (Re $<<$ 1) to intermediate flow regimes (Re $>$ 1). The research aims to investigate the onset of non-laminar flow and its associated rapid increase in the pressure gradient depending on the wall roughness.

DY 32.24 Wed 15:00 Poster C

A variational approach to the gradient statistics of passive scalar turbulence — •David Aderbauer, Gabriel B. Apolinário, and Michael Wilczek — Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth

Intermittent non-Gaussian statistics are a common characteristic of turbulent flows. Various approaches exist that use a superposition of Gaussian PDFs (probability density functions) to model these statistics.

This raises the question of how to systematically construct such superpositions. Here, we address this at the example of the Kraichnan model for passive scalar turbulence, which features heavy-tailed gradient statistics.

We derive the Fokker-Planck equation for the gradient PDF and construct a solution based on a superposition of Gaussian PDFs. To this effect, we develop an optimization method to iteratively determine the weight of each Gaussian in the superposition. We compare the PDF resulting from this procedure to the one directly estimated from simulation data, as well as to the stationary solution of the Fokker-Planck equation. We briefly discuss possible extensions to statistical field theories of turbulence.

DY 32.25 Wed 15:00 Poster C

Spatio-temporal correlation in MHD turbulence — •Raquel Mäusle and Wolf-Christian Müller — Technische Universität Berlin, Berlin, Germany

Turbulent flows are ubiquitous on Earth and throughout the universe. They can be understood as the superposition of turbulent fluctuations on various spatial and temporal scales. Energy is transferred between these scales through non-linear interactions, a process known in 3D as the direct energy cascade. We study this energy transfer process by computing the spatio-temporal correlation between fluctuations in magnetohydrodynamic turbulence. To this end, we employ direct numerical simulations, in which the fluctuations are measured in a quasi-Lagrangian manner to avoid the sweeping effect. This framework was used in previous studies of Navier-Stokes turbulence [Physics of Fluids 23.8 (2011):085107], which we extended to account for the anisotropy introduced by the presence of the magnetic field. We present the resulting correlation time scale, strength and direction of the cross-scale energy transfer in the directions parallel and perpendicular to the local magnetic field and relate them to phenomenological models of MHD turbulence. Furthermore, the limitations of the quasi-Lagrangian framework are discussed.

DY 32.26 Wed 15:00 Poster C

High-order finite volume numerics to achieve low numerical diffusivity — •Jean-Mathieu Teissier[1], Raquel Mäusle[1], and Wolf-Christian Müller[1,2] — [1]Technische Universität, Berlin, Germany — [2]Max-Planck/Princeton Center for Plasma Physics

Natural systems typically present turbulent dynamics at Reynolds numbers not yet achievable with current computing facilities. The discretization of the governing equations leads to a loss of energy over time, which can be partially modelled by a so-called "numerical viscosity", which gives an upper bound to the achievable Reynolds number for a given solver at a given numerical grid-size. Hence, finding ways to (*i*) minimize this loss of energy and (*ii*) quantify the dissipation of numerical nature is crucial to perform more realistic simulations. We present high-order dimension-by-dimension finite-volume solvers for the Navier-Stokes and magnetohydrodynamics equations, with discretization orders up to ten. Although higher-order schemes are more costly at a given grid-size, they allow results of similar quality on significantly coarser grids as compared to, e.g. second-order schemes. This leads to an overall gain in computing efficiency, typically a factor of order 10–100. In order to quantify the improvement of the numerical viscosity and magnetic diffusivity of the solvers with discretization order, we present simulations of the tearing mode instability, whose growth rate is a function of (physical) viscosity and magnetic diffusivity.

DY 32.27 Wed 15:00 Poster C

Reduced order network model of incompressible magnetohydrodynamic turbulent flows — •Maria Mathew and Wolf-Christian Müller — ZAA, Technische Universität Berlin, Germany

Plasma turbulence is a widespread phenomenon in astrophysical systems. However, three-dimensional simulations of these systems with realistic parameter values present a significant challenge due to the extensive spectral bandwidth of nonlinearly interacting fluctuations within turbulent flows.

To address this, model reduction techniques have been employed to facilitate a more cost-effective approximative representation of the flow. We extend the network model ansatz newly proposed in a reduced scalar model for the energy dynamics in magnetohydrodynamic flows [Beck, Müller; arXiv:2203.11536 (physics.flu-dyn)], to encompass the dynamics of magnetic helicity, in order to obtain an easily modifiable, reduced representation of plasma turbulence. Our approach involves selecting an inherently minimal subsystem that conservatively transports energy and other quadratic invariants across wavenumber space. This network-based representation of energy-exchanging interconnected agents adeptly captures the intricate dynamics of the flow while simultaneously reducing computational complexity. Within this framework, the spectral scaling is studied, comparing it to the established phenomenological models. Additionally, the impact of various geometric constraints on our transfer function is investigated, particularly on the spectrum of magnetic helicity. We discuss our findings as well as the associated limitations.

DY 32.28 Wed 15:00 Poster C

Numerical simulations of subsonic magnetized plasma-jets — •Thomas Christian Vandamme[1], David Kube[1], Jean-Mathieu Teissier[1], and Wolf-Christian Müller[1,2] — [1]Technische Universität Berlin, ER 3-2, Hardenbergstr. 36a, 10623 Berlin, Germany — [2]Max-Planck/Princeton Center for Plasma Physics

In astrophysical processes such as star formation and accretion of material around compact objects free starting jets that travel huge distances, more than 10^5 or 10^7 times their initial radius, can be generated. This is in contrast to hydrodynamic jets, observed e.g. on earth, that suffer from Kelvin-Helmholtz-instabilities leading to disruption of their shear-layer and to turbulent mixing with the environment. Thus, astrophysical jets are subject to stability enhancing processes. Most of all the presence of a magnetic field has a significant impact on the jet's stability.

In order to study the stabilizing effects of magnetic fields, we perform fourth-order accurate numerical simulations of isothermal subsonic jets, both in the hydrodynamic and magnetohydrodynamic case, for different magnetic field configurations in the interior of the jet.

Setups with a helical field topology dominated by axial field components show the most stabilizing effects. Simulations with purely axial or purely azimuthal fields tend to destabilize the jet through current driven instabilities or can not suppress the Kelvin-Helmholtz-modes effectively.

DY 32.29 Wed 15:00 Poster C

A basic structure of 2D Boussinesq-Convection — •Lukas Moczarski and Wolf-Christian Müller — Plasma-Astrophysik, TU Berlin, Deutschland

In thermally driven turbulence, heat is mainly carried by buoyant structures, so called thermal plumes. We show that in DNS of 2D homogeneous Boussinesq-convection these plumes condensate on a characteristic scale, on which their mutual interaction induces a large-scale vorticity to the flow. This plume-induced vorticity is proposed as a basis for flow structuring. It is shown that the zero-vorticity level set takes shape as a grid of intersecting lines, whose structure changes slowly on the scale of the large-eddy buoyancy time. A Lagrangian tracer diffusion analysis indicates that the grid lines and their intersection points are paths of enhanced convective transport, whereas the centres of large-scale vortices in between them entrap tracers and lead to reduced transport. A subsequent investigation of the energy cascade in physical space, obtained by Gaussian filtering in spectral space, reveals a strong correlation of the cross-scale energy flux with the grid lines. We show that this is due to the (mis-)alignment of large-scale strain and small scales stress which is strongly modulated by the motion of individual thermal plumes on the grid.

DY 33: Poster: Nonlinear Dynamics, Pattern Formation and Networks

Time: Wednesday 15:00–18:00 Location: Poster C

DY 33.1 Wed 15:00 Poster C

Force networks in granular experiments: From topology to dynamics — •Lou Kondic — New Jersey Institute of Technology, Newark, NJ, USA

We will discuss force networks that spontaneously form in particulate-based systems. These networks, most commonly known as 'force chains' in granular systems, are dynamic structures of fundamental importance for revealing the underlying causes of many physical phenomena involved in the statics and dynamics of particulate-based systems. While the networks emerging from discrete element simulations have been analyzed extensively, the analysis of networks found in physical experiments is far less developed. The presentation will focus on applications of algebraic topology, particularly persistent homology (PH) to analysis of such networks. PH allows for a simplified representation of complex interaction fields in both two and three spatial dimensions in terms of persistent diagrams (PDs) that are essentially point clouds. These point clouds could be compared meaningfully, allowing for the analysis of the underlying systems' static and dynamic properties. The presentation will focus on applications of topological data analysis of such networks found in photoelastic experiments involving an intruder moving in a stick-slip fashion through a 2D granular domain. We will particularly focus on exploring the predictability potential of the considered topological measures.

DY 33.2 Wed 15:00 Poster C

Resonant Velocity Tuning of Solitary States in Complex Networks — •Jakob Niehues[1,2,3], Serhiy Yanchuk[1,2,4], Rico Berner[2], Jürgen Kurths[1,2], Frank Hellmann[1], and Mehrnaz Anvari[1,5] — [1]Potsdam Institute for Climate Impact Research (PIK), Member of the Leibniz Association, P.O. Box 60 12 03, D-14412 Potsdam, Germany — [2]Humboldt-Universität zu Berlin, Department of Physics, Newtonstraße 15, 12489 Berlin, Germany — [3]Technische Universität Berlin, ER 3-2, Hardenbergstrasse 36a, 10623 Berlin, Germany — [4]University College Cork, School of Mathematical Sciences, Western Road, Cork, T12 XF62, Ireland — [5]Fraunhofer Institute for Algorithms and Scientific Computing, 53757 Sankt Augustin, Germany

Partially synchronized solitary states occur frequently when a synchronous system of networked oscillators is perturbed locally. Remarkably, several asymptotic states of different frequencies can coexist at the same node. Here we uncover the mechanism underlying this multistability. The resonant back-reaction of the networks' modes on the solitary oscillator can lead to large energy transfer between them. The frequency adaptation of the oscillator can tune the system to this resonance. We provide a full analytic analysis of this mechanism, and show which network structures enable its presence.

DY 33.3 Wed 15:00 Poster C

Wave Digital Model of a Relaxation Oscillator with Optical Memsensor — •Sebastian Jenderny[1], Rohit Gupta[2], Roshani Madurawala[3], Maik-Ivo Terasa[3], Franz Faupel[2], Sören Kaps[3], Rainer Adelung[3], Alexander Vahl[2], and Karlheinz Ochs[1] — [1]Ruhr-University Bochum, Chair of Digital Communication Systems, Bochum, Germany — [2]Christian-Albrechts University Kiel, Chair for Multicomponent Materials, Kiel, Germany — [3]Christian-Albrechts University Kiel, Functional Nanomaterials Chair, Kiel, Germany

Biological neuronal networks, besides their increased energy-efficiency, are especially interesting due to their learning and adaption abilities. To come up with new designs for circuits adapting to new tasks in a self-organizing fashion, it is important to transfer findings on the biological wiring and rewiring mechanisms to electrical circuits. Up to now, the wiring mechanisms are typically associated with the change of synaptic weights and are often implemented by memristors. Growth in real neuronal networks, however, strongly depends on the integration of sensory information from their surroundings. For this purpose, in this work, we report on the use of memsensors. We specifically introduce a relaxation oscillator that includes an optical sensor as well as a memristor. The oscillator acts as an optical memsensor displaying basic neuronal behavior. To be able to evaluate the usage of this memsensor in larger circuit setups, we develop a corresponding wave digital model on the basis of experimental data of the memsensor.

DY 33.4 Wed 15:00 Poster C

Kirman's herding model with stochastic resetting — •Pece Trajanovski[1], Petar Jolakoski[1], Arnab Pal[2], Ljupco Kocarev[1,3], and Trifce Sandev[1,4] — [1]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [2]Institute of Mathematical Sciences, Chennai, India — [3]Ss. Cyril and Methodius University in Skopje, Macedonia — [4]University of Potsdam, Germany

Kirman's herding model with stochastic resetting extends the seminal Kirman*s ants model by incorporating stochastic resetting, which mimics sharp external influences on the system. The dynamics are characterized by two essential parameters b and a, the first representing the strength of agents influence to convert others, and other signifying the likelihood of spontaneous preference alteration by each agent. The resetting rate (r) introduces a pivotal interplay, yielding unexpected outcomes in the mean first passage time to a specific binary choice.

Our approach enhances Kirman's model by introducing exogenous factors, resulting in a more realistic herding/recruiting model adaptable to diverse behavioral scenarios. The analysis provides a comprehensive understanding, including the derivation of the probability distribution function solution, the distribution for the stationary case, and the mean first passage time distribution using the backward master equation. This exploration contributes valuable insights into the nuanced dynamics of collective decision-making and population configurations within complex systems, enriching our understanding of the Kirman's herding model.

DY 33.5 Wed 15:00 Poster C

Nature of the volcano transition in the fully disordered Kuramoto model — •Axel Prüser, Sebastian Rosmej, and Andreas Engel — Carl von Ossietzky University Oldenburg, Institut für Physik, D26111 Oldenburg, Germany

Randomly coupled phase oscillators may synchronize into disordered patterns of collective motion. We analyze this transition in a large, fully connected Kuramoto model with symmetric but otherwise independent random interactions. Using the dynamical cavity method we reduce the dynamics to a stochastic single oscillator problem with self-consistent correlation and response functions that we study analytically and numerically. We clarify the nature of the volcano transition and elucidate its relation to the existence of an oscillator glass phase.

DY 33.6 Wed 15:00 Poster C

A novel cutoff criterion for spectral derivatives in the context of ordinary differential equation model estimation — •Oliver Strebel — Angelstr. 17, 75392 Deckenpfronn

After the advent of SINDy-methods [1] estimation of ordinary differential equation models involves typically the numerical calculation of derivatives for noisy data. This contribution presents a novel determination method concerning the cutoff parameter for spectral derivatives. The method is benchmarked against 60 differential equations and estimation methods of reference [2].

It is compared to numerical differentiation methods like finite differences, derivatives using the Friedrichs mollifier and weak differentiation using this mollifier. The hyperparameters of all these methods are optimized against the test set of these equations at a fixed noise level. Then the resilence against larger noise or fewer data points per time interval is examined. It turns out that the novel method is overall superior to the other methods.

[1] Steve L. Brunton, PNAS 113 (2016): https://doi.org/10.1073/pnas.1517384113
[2] Oliver Strebel, Nonlinear Dynamics 111 (2023): https://doi.org/10.1007/s11071-023-08242-y

DY 33.7 Wed 15:00 Poster C

Reliability of Numerical Solutions in Transient Chaos — Ali Goodarzi[1], Maryam Rahimi[1], Mohammadjavad Valizadeh[2], and •Fakhteh Ghanbarnejad[3] — [1]Institute of Physics, EPFL, Lausanne, Switzerland — [2]Department of Mathematics, Simon Fraser University, Burnaby, Canada — [3]Chair of Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), Technical University of Dresden, 01062 Dresden, Germany

In dealing with nonlinear systems, it is common to use numerical solutions. Unlike the careful behavior towards the numerical results in chaotic regions, the validity of numerical results in regions of transient chaos might not always be taken into consideration. This article demonstrates that using numerical methods to solve systems undergoing transient chaos can be challenging and sometimes unreliable.

To illustrate this issue, we use the Lorenz system in the region of transient chaos as an example. We show how the result of the computation might completely change when using different mathematically equivalent expressions. This raises the question of which result should be relied on. To answer this question, we propose a method based on the Lyapunov exponent to determine the reliability of the numerical solution and apply it to the provided example. In fact, this method checks a necessary condition for the validity of the numerical solution. Then, by increasing the precision to the extent suggested by our method, we show that the result of our studied case passes this test. In the end, we briefly discuss the scope and limits of our method.

full article: arXiv:2310.13155

DY 33.8 Wed 15:00 Poster C

A Study of complex Kuramoto Agents in Small-World Networks — Toni Sollfrank[1], Sibylle Gemming[1], and •Jeffrey Kelling[1,2] — [1]Institut für Physik, TU Chemnitz, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany

Synchronization is a phenomenon frequently observed or employed in natural or engineered systems. Swarms of animals can show synchronized behavior which has been qualitatively modeled as dynamic networks of Kuramoto oscillators. We propose a model for networks of complex agents, where each agent is a small sub-network which is only very sparsely coupled to other agents via designated input-output nodes. The internal structure of each agent gives rise to complex response to stimuli from the external network. Here, we present a study of the dynamical synchronization behavior on these, by construction, hierarchical graphs. A range of defined agent sub-network types are considered connected by small-world networks Barabási–Albert, Erdös–Rényi or Watts–Strogatz types.

DY 33.9 Wed 15:00 Poster C

Minimal thermal and thermoelectric rectifiers — •José Balduque[1] and Rafael Sánchez[1,2] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain. — [2]Condensed Matter Physics Center (IFIMAC), and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Madrid, Spain.

Modern electronic devices are currently operated at the nanoscale regime, where overheating becomes a problem. Controlling the undesired heat flows in a useful manner is another less explored way of improving its performance. For this, efficient thermal diodes need to be designed [1]. Usual proposals rely in nonlinear scenarios [2]; here, we identify the minimal conditions for a nanoscale device to rectify the heat and thermoelectric currents, even in the absence nonlinearities. This is achieved for asymmetric coherent conductors that allow for some local thermalization of the heat carriers. We quantify the amount of rectification achieved by this mechanism in some proposed systems composed of resonant-tunneling quantum dots and compare (and combine) it with the nonlinear scenarios. Finally, we propose feasible experimental realizations of this idea in an elastic conductor where the interplay between thermalization and nonlinearities can be

controlled via quantum interference [3].

[1] G. Benenti et al., Springer International Publishing (Cham, Switzerland), 2016.

[2] B. Li et al., Phys. Rev. Lett., 93 (2004) 184301.

[3] R. Sánchez et al., Phys. Rev. B, 104 (2021) 115430.

DY 33.10 Wed 15:00 Poster C

Oscillations in SIRS model with block delay kernels — •Daniel Henrik Nevermann and Claudius Gros — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Deutschland

Oscillations are an omnipresent feature of epidemic dynamics, however, the classical SIRS model with exponentially distributed dwell-times in the compartments is unable to capture stable oscillations. Models with non-exponentially distributed dwell-times, on the other hand, may exhibit periodic outbreaks in its endemic state for certain parameter values. These oscillatory solutions are already present when considering a simple normalized step function kernel, what we call a block delay kernel, for the time of immunity of a recovered individual. We investigate the resulting attractor topology and study the characteristics of the periodic outbreaks, where we use the skewness of the time series as a measure for the shape of the periodic outbreaks.

A continuous approximation to the block delay kernel is given by the normalized sum of N Erlang distributions, where the block delay kernel is recovered in the limit $N \to \infty$. We show that this finite sum may be equally represented by an upper incomplete gamma function, which simplifies the derivation of its mathematical properties. We apply the kernel series framework to recast the system with continuous block delay kernel to a set of ordinary differential equations. Using this, we study the onset of periodic outbreaks when systematically decreasing the slope of the block delay kernel. Comparing the skewness of the time series to limiting case of a fixed time in the recovered compartment, we find that the relative deviation scales as a power-law in N.

DY 33.11 Wed 15:00 Poster C

Square waves and Bykov T-points in a delay algebraic model for the Kerr-Gires-Tournois interferometer — Mina Stöhr[1], •Elias Koch[2], Julien Javaloyes[3], Svetlana Gurevich[2,4], and Matthias Wolfrum[1] — [1]Weierstrass Institute, Mohrenstrasse 39, 10117 Berlin, Germany — [2]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany — [3]Departament de Física & IAC-3, Universitat de les Illes Balears, C/ Valldemossa km 7.5, 07122 Mallorca, Spain — [4]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, 48149 Münster, Germany

We study theoretically the mechanisms of square wave formation in an injected vertically emitting micro-cavity, containing a nonlinear Kerr medium and subjected to strong time-delayed optical feedback. We show that for large delays, square wave solutions of the time-delayed system can be treated as relative homoclinic solutions of an advanced argument equation. This allows the use of classical homoclinic bifurcation theory to study different types of square wave solutions. In particular, we unveil the mechanisms behind the collapsed snaking scenario of square waves and explain the formation of complex-shaped multistable square wave solutions through a Bykov T-point. Finally, we relate the position of the T-point to the position of the Maxwell point in the original time-delayed system.

DY 33.12 Wed 15:00 Poster C

Dynamics and bifurcation analysis of active mode-locked semiconductor lasers — •Elias Koch[1], Svetlana Gurevich[1,3], and Julien Javaloyes[2] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany — [2]Departament de Física, Universitat de les Illes Balears & IAC-3, Cra. de Valldemossa, km 7.5, E-07122 Palma de Mallorca, Spain — [3]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstraße 2, 48149 Münster, Germany

We study theoretically the dynamics and bifurcations of an actively mode-locked laser by employing a delay differential equation model. This allows us to consider regimes of high gain and losses typical of semiconductor lasers. Using a combination of numerical path continuation and direct numerical simulation we find that the solution branches corresponding to higher order Hermite-Gauss modes in a modulated potential can interact leading to a complex scenario. By performing a multiple time-scale analysis close to the lasing threshold, we derive a Haus master equation which shows a good agreement with the original time-delayed model. Finally, we study the regime of multiple pulses in a cavity. There, we identify different dynamical regimes and the underlying bifurcation structure, discovering a global bifurcation scenario.

DY 33.13 Wed 15:00 Poster C

Chaotic Diffusion in Delay Systems: Transition to Anomalous Diffusion and Weak Ergodicity Breaking by Time Lag Modulation — •Tony Albers[1], Lukas Hille[1], David Müller-Bender[1], and Günter Radons[1,2] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Institute for Mechanical and Industrial Engineering, Chemnitz, Germany

In this contribution, we show that in a typical class of time-delayed systems with linear instantaneous and nonlinear delayed term a transition from normal diffusion to anomalous diffusion and weak ergodicity breaking can be induced by a modulation of the delay time. This change is related to a transition from turbulent chaos to laminar chaos [1] and reveals a new kind of dynamical behavior consisting of a coexistence of turbulent and laminar phases alternating within one single time series. We investigate this transition in detail and its influence on the diffusive and ergodic properties of the system and the related occurrence of infinite densities. We show that some of the observed features in the system can be explained by low-dimensional iterated maps and appropriate stochastic models.

[1] David Müller, Andreas Otto, and Günter Radons, Phys. Rev. Lett. **120**, 084102 (2018)

DY 33.14 Wed 15:00 Poster C

Dynamic patterns in active particles with delayed all-to-all attractions — •Pin-Chuan Chen[1], Klaus Kroy[1], and Viktor Holubec[2] — [1]Institute for Theoretical Physics, Universität Leipzig - 04103 Leipzig, Germany — [2]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University 18000 Prague, Czech Republic

Time delayed effective interactions are ubiquitous in coarse-grained models of complex systems. Using Brownian dynamics simulations, we study a collection of active particles attracting each other with a time delay. In two dimensions, we find patterns similar to those reported previously [1,2] for a delayed attraction to a common center. For long delays, a more symmetric configuration arises. In three dimensions, the situation is somewhat similar, but due to the extra degree of freedom, the phenomenology is much richer. Beyond rotating crystallites, shear bands and co-orbiting satellites, conveyor belts with shapes of a tennis ball seam appear.

[1] Wang, X., Chen, P. C., Kroy, K., Holubec, V., & Cichos, F. (2023). Spontaneous vortex formation by microswimmers with retarded attractions. Nature Communications, 14(1), 56.

[2] Chen, P. C., Kroy, K. D., Cichos, F., Wang, X., & Holubec, V. (2023). Active particles with delayed attractions form quaking crystallites. Europhysics Letters.

DY 33.15 Wed 15:00 Poster C

The route to mesoscale turbulence in a model of active fluids — •Henning Reinken[1,2], Sebastian Heidenreich[3], Markus Bär[3], and Sabine H. L. Klapp[2] — [1]Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany — [2]Technische Universität Berlin, Straße des 17. Juni 135, 10623, Berlin, Germany — [3]Physikalisch-Technische Bundesanstalt Braunschweig und Berlin, Abbestr. 2-12, 10587 Berlin, Germany

Suspensions of microswimmers are a paradigmatic example of active fluids and are known to develop mesoscale turbulence, a state of dynamic vortex structures characterized by the presence of a characteristic length scale. Here, we employ a minimal model for the effective microswimmer velocity field [1,2] to explore how the turbulent state develops from regular, stationary vortex patterns when the strength of nonlinear advection is increased. To this end, we perform an extended stability analysis and uncover a linear instability, which follows from the mutual excitement and simultaneous growth of multiple perturbative modes. The extended analysis allows us to calculate a critical advection strength signifying the onset of mesoscale turbulence in the active fluid model, in very good agreement with numerical results. By this we establish an analogy to a critical Reynolds number in driven flow exhibiting inertial turbulence.

[1] Wensink, Dunkel, Heidenreich, Drescher, Goldstein, Löwen, Yeomans, Proc. Natl. Acad. Sci. U.S.A. **109**, 14308 (2012)

[2] Reinken, Klapp, Bär, Heidenreich, Phys. Rev. E **97**, 022613 (2018)

DY 33.16 Wed 15:00 Poster C

Towards bacterial growth laws for shape-conserving cell wall growth: a linear stability analysis — •Paul Nemec and Ulrich Gerland — Physics Department, Technical University of Munich

Inspired by the question of how bacteria maintain their shapes during growth, we study how pressurised elastic shells may grow robustly. Specifically, we ask how cell envelope growth could depend on local observables like curvature or stress, such that perturbed spherical or spherocylindrical cells recover their shape. Within a simplistic continuum model of a growing elastic shell, general requirements like locality, isotropy and material-frame indifference provide strong constraints on local growth laws. By linearising around a growing and pressurised reference trajectory, we obtain linear stability results for different ways that growth may couple to local observables. By requiring that growth depends on local observables isotropically, the space of possible linear couplings dramatically reduces. For a sphere, we are left with a six-dimensional space of couplings, which we investigate to find that naive isotropic growth is generally unstable, but can be stabilised by additional coupling.

DY 33.17 Wed 15:00 Poster C

Experimental study of stress in force chains in granular matter — •Lukas Reiter[1], Amelie Mayländer[1], Raphael Blumenfeld[3], Clara Wanjura[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, D-89069 Ulm — [2]Max Planck Institute for the Science of Light, Staudststr. 7, D-91058 Erlangen — [3]Gonville & Caius College, University of Cambridge, Trinity St., Cambridge CB2 1TA, UK

The properties of dense granular media are largely determined by the contact forces between particles. Experimentally, these forces become visible as interference patterns in photo-elastic particles, but, so far, their quantitative analysis from experimental data has been challenging. Using a dark field polariscope, we explore the stress dynamics of a sheared, two-dimensional granular system of photo-elastic discs forming a self-organizing many-particle contact network and observe the formation of force chains. We use a convolutional neural network (CNN) approach based on [1] to analyse the interference fringes arising in the photo-elastic particles due to strain. We train and compare different pre-trained state-of-the-art CNN models on synthetically generated 2D images of particles. The CNNs provide quantitative information on the number of forces, their magnitudes and angles at which the forces are applied.

[1] R. Sergazinov, M. Kramár. Mach. Learn.: Sci. Technol. 2 045030 (2021).

DY 34: Poster: Machine Learning, Data Science, and Reservoir Computing

Time: Wednesday 15:00–18:00 Location: Poster C

DY 34.1 Wed 15:00 Poster C

A First Approach to Dynamically Solving Quadratic Unconstrained Optimization Problems with Memristive Oscillator Networks — •Bakr Al Beattie and Karlheinz Ochs — Chair of Digital Communication Systems, Ruhr University Bochum, 44801 Bochum, Germany

In recent years, a new computational paradigm based on a network of resistively coupled oscillators has emerged. These devices are referred to as oscillator-based optimizers. They are built, so they have the natural tendency of minimizing an energy function to which quadratic unconstrained binary optimization problems (QUBOs) can be mapped. A challenge of oscillator-based optimization is that the structure of the oscillator network must be changed every time a new QUBO is mapped. This is because the connectivity of the network encodes the coefficients of the optimization problem. To deal with this issue, we propose making use of memristors (memory resistors), which can switch between multiple resistance states. To utilize these devices, it is usually required to have a dedicated programming circuit to set the desired resistance state. In this work, we aim to show that we can omit on using such programming circuits by working with suitable oscillators. To demonstrate this approach, we iteratively solve multiple optimization problems, where we alternate between a programming phase and a solution phase.

DY 34.2 Wed 15:00 Poster C

Optical Ising model simulations with caesium vapor cells — •Kilian Junicke[1], Elizabeth Robertson[1,2], Mingwei Yang[1,2], Inna Kwiatkowski[2,3], and Janik Wolters[1,2] — [1]Technische Universität Berlin, Institute for Optics and Atomic Physics, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Rutherfordstr. 2, 12489 Berlin, Germany — [3]TU Berlin, Institut für Luft und Raumfahrt

Several computationally hard optimization problems can be mapped to finding the ground state of an Ising model [1]. Simulating Ising models optically promises speed increases [2]. Building an optical Ising machine then raises the question of how to simulate the spin states [3].

Here we present a scheme for simulating an Ising model using the ground states of cesium vapor at room temperature. We present methods for implementing positive and negative interactions using a measurement and feedback strategy. In the system electromagnetically induced transparency acts as a frequency transducer. We initialize the system and allow it to evolve by executing a series of pump probe operations on spatially multiplexed regions of an atomic vapor cell until a ground state solution is found.

[1] Lucas, A. Ising formulations of NP problems. Front. Phys. 2, 5 (2014).

[2] McMahon, P.L. Physics of optical computing. Nat Rev Phys 5, 717-734 (2023).

[3] Böhm et al. Poor man's coherent Ising machine for optimization. Nat Commun 10, 3538 (2019).

DY 34.3 Wed 15:00 Poster C

Exploring neural criticality through the structure of input-induced attractors in random neural networks under external perturbations — •Hiromichi Suetani[1,2] and Ulrich Parlitz[3,4] — [1]Faculty of Science and Technology, Oita Univerisyty, Oita, Japan — [2]International Research Center for Neurointelligence, The University of Tokyo, Tokyo, Japan — [3]Max Planck Research Group Biomedical Physics, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [4]Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany.

In recent years, a focus has turned to the neural criticality hypothesis, suggesting that the neural system optimizes information processing by maintaining activity near a critical point between order and disorder. Reservoir computing (RC) provides a theory for the neural criticality. For example, the hyperparameter region with the maximum Lyapunov exponent (LE) near zero, termed the "edge of chaos," claims the optimality of the performance of RC. Yet, reservoirs are non-autonomous dynamical systems with external perturbations. The maximal LE is defined for autonomous systems and if applied to non-autonomous systems, it is the conditional LE where its positivity and negativity doesn't generally indicate the existence of chaos.

This study explores input-induced attractors in random neural networks under external inputs. Examining them through generalized synchronization and embeddings, we aim at developing a new theoretical foundation for neural criticality by elucidating the relationship with performances of RC such as information processing capacity.

DY 34.4 Wed 15:00 Poster C

Physical interpretation of learning dynamics in neural networks — •Yannick Mühlhäuser[1,2], Max Weinmann[2,3], and Miriam Klopotek[2] — [1]University of Tübingen, Tübingen, Germany — [2]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [3]University of Stuttgart, Interchange Forum for Reflecting on Intelligent Systems, IRIS3D, Stuttgart, Germany

Neural network-based machine learning methods are becoming ubiquitous for applications to physics and science. A key challenge for their seamless integration into science is their opacity, or "black-box-ness". How they learn, i.e. their learning dynamics, can shed some light into their "reasoning" process. We look at the learning dynamics of autencoder-type neural networks trained via different optimization techniques [1]. We use statistical model systems for finding specific analogies to well-known phenomena from physics like phase transitions [2], offering a route towards interpretation.

[1] Borysenko, O., and Byshkin, M. (2021). CoolMomentum: A method for stochastic optimization by Langevin dynamics with simulated annealing. Scientific Reports, 11(1), 10705.
[2] Liu, Z., Kitouni, O., Nolte, N. S., Michaud, E., Tegmark, M., and Williams, M. (2022). Towards understanding grokking: An effective theory of representation learning. Advances in Neural Information Processing Systems, 35, 34651-34663.

DY 34.5 Wed 15:00 Poster C

Understanding Neural Network Models for Phase Recognition — •Shashank Kallappara, Janett Prehl, and Martin Weigel — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

The Ising model is one of the best-known models in statistical physics, undergoing a phase transition in dimensions $d > 2$, described by a simple order parameter: its magnetisation. Machine learning techniques have been successfully used in physics for classifying phases of different physical systems. Fully connected neural networks have been shown to learn the translational invariance of the Ising model when learning its phases using only a single hidden layer; analytic solutions for the same exist for highly compact networks that are constructed to obey the translational invariance automatically. Here, we show this learning of the invariance in single-layer networks of different widths and compare the networks' performance in classifying the phases. We also consider a highly compact network but focus on the gradient descent learning dynamics over its loss landscape; we suggest a few changes to this that greatly improve its performance while preserving interpretability.

DY 34.6 Wed 15:00 Poster C

Sand Grain Generation through Deep Learning and Lower Dimensional Representations — •Lira Yelemessova[1] and Matthias Schröter[1,2] — [1]Georg-August-Universität Göttingen, Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

How would one create artificial realistic sand grains? This project explores this question by representing sand grains as point clouds and then employing the denoising diffusion probabilistic model. The first step is to use an autoencoder to transform the complex three-dimensional structures of synthetic sand grains into a lower-dimensional space. Then, the model generates additional samples using denoising diffusion, which is also the algorithm behind programs such as Stable Diffusion and DALL-E. We study how variations in the number of points and dimensions of additional features impact the generated samples.

DY 34.7 Wed 15:00 Poster C

Squeezing Sand Grains through a Bottleneck: Can Deep Learning Find a Minimal Description for Granular Particles? — •Azhar Akhmetova[1] and Matthias Schröter[1,2] — [1]Georg-August-Universität Göttingen, Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The optimal number of parameters required for reliably describing a specific class of shapes is an open question. We test the possibility of retrieving the minimum number of parameters needed using the autoencoder architecture. Autoencoders are neural networks consisting of two parts: the encoder that compresses input data into a lower-dimensional representation, creating an information bottleneck. Then, the decoder reconstructs the original input from this compact representation. We start by applying autoencoders to shapes generated with a known parameter count based on their Fourier descriptors. The focus is on testing if the autoencoder's bottleneck dimension can measure the required number of parameters. Another open question is how the resolution influences particle shape description. The final aim of the project is to apply autoencoders on X-ray tomography data of real-world particles.

DY 34.8 Wed 15:00 Poster C

Mutual information estimation in the learning process of neural networks — •Lea Melina Faber, Ibrahim Talha Ersoy, and Karoline Wiesner — Universität Potsdam, Institut für Astronomie und Physik, Potsdam, Deutschland

Deep neural networks play an increasingly important role to predict the dynamics of highly complex systems. The most prominent example is that of climate models. Nonetheless it is still unknown how the actual learning process works. To better understand such models it is crucial to open the black box of neural nets. It has been conjectured, that mutual information is a good measure of learning in neural networks. Often times the simplest of estimation techniques, like binning, are used. However, it has been shown that in some settings they are only very crude estimators. We have analyzed the MSE, bias and variance for standard mutual information estimators, using the specific settings relevant for neural network analysis. Our results show that most estimators have problems with high dimensions and high mutual information, specifically in combination, which is a standard situation in the context of neural networks. Furthermore, it has been shown, that generally estimators show the best results for Gaussian distributions. However, our numerical experiments show that non-Gaussian distributions are likely to play a significant role in the learning processes in neural networks. Hence, we require suitable estimators for these cases. We illustrate our results with the MNIST dataset.

DY 34.9 Wed 15:00 Poster C

Cumulative entropy as a bridge between statistical physics and statistical machine learning — •Hans Reimann and Karoline Wiesner — University of Potsdam, Germany

Cumulative entropies, such as cumulative Shannon entropies or Phi-entropies, have been of growing interest to tackle shortcomings of classical notions of entropy while keeping as many of the desired properties as possible. Some context driven intuitions and overarching frameworks managed to provide some independent insights, yet they are not fully understood or incorporated in well established physical or statistical contexts is still work in progress. We investigate towards statistical and physical properties as well as understanding of the cumulative paired Shannon entropy (CPE) as a promising special case. Utilizing tools from mathematical statistics in combination with information theory our work paves the way toward a thorough understanding along the lines of well established notions of entropy. Next to some first results on parametric and non-parametric estamation and asymptotic properties, we managed to relate the CPE in its most striking properties to both concpets of equilibrium statistics and thermodynamics as well as statistical data analysis. Moreover, we work on expanding these ideas to recent results in physics informed machine learning for binary classification tasks via arguing for the CPE to be a measure of a natural degree of seperability under considerations of Jaynes' understanding of maximum Shannon entropy.

DY 34.10 Wed 15:00 Poster C

Phase Transitions and Information Flow in Deep Neural Networks — •Ibrahim Talha Ersoy[1] and Karoline Wiesner[2] — [1]Universität Potsdam, Institut für Astronomie und Physik, Potsdam, Deutschland — [2]Universität Potsdam, Institut für Astronomie und Physik, Potsdam, Deutschland

The learning process of neural networks (NNs) can be characterized as an optimization toward specific balance between complexity of the representa- tion and precision, both of which can be measured by the mutual informa- tion. This observation as well as the so called information bottleneck (IB) approach where one restricts complexity goes back Tishby et al. [1,2]. In the IB approach two mutual information terms are built into the loss function, with some trade-off parameter giving their balance. It was observed that the system undergoes a number of second order phase transitions when varying this parameter [3]. We utilize this feature to better understand the change between different model representations. A close connection to schemes like the variational autoencoder and other networks with variable regularizes has been suggested [5]. We investigated these claims and make a number of trials and theoretical considerations to make this claim manifest. In particular we probed the dependencies of hidden representations and the features they represent. We also compared the compression behaviour of the NN-input to other methods like PCA, Diffusion maps and t-SNE. For gaussian data we see a strong connection between the VAE, IB as well as PCA, as expected.

DY 34.11 Wed 15:00 Poster C

Ab-initio-based interatomic potential for laser-excited Bismuth — •Jimiben Patel, Bernd Bauerhenne, and Martin Garcia — Institute for Physics, University of Kassel, Kassel, Germany

The intricate processes involving atomic motions, occurring on a subpicosecond timescale, influence phenomena like chemical reactions, bond formation, and breaking. To get deep insights into these processes, femtosecond laser pulses have proven indispensable. The ultrashort interaction time in this context ensures that the laser field strongly influences electrons. A precise description of the structural

relaxation of materials after femtosecond laser excitation is achieved through Te dependent Density Functional Theory (DFT). However, employing Te dependent DFT for simulations involving a large number of atoms is computationally expensive or even impossible. To address this challenge, our work introduces a polynomial Te dependent interatomic potential (Φ(Bi)(Te)) for Bismuth, which is trained using a database constructed from DFT simulations. Bismuth is an experimentally widely used material, for which so far no theory to describe ultrafast processes has been developed. In our analysis, we compared the physical properties of our polynomial potential Φ(Bi)(Te), with those obtained from ab initio simulations. Additionally, we conducted an examination of the thermophysical properties of the polynomial potential, including the determination of the melting temperature. This innovative approach allows for efficient and accurate exploration of complex material behaviors, offering a valuable alternative to computationally demanding Te dependent DFT simulations.

DY 34.12 Wed 15:00 Poster C

Long-Range Electrostatic Descriptors for Machine Learning Force Fields — •Carolin Faller[1,2], Bernhard Schmiedmayer[1], and Georg Kresse[1,3] — [1]Computational Materials Physics, University of Vienna, Austria — [2]Vienna Doctoral School in Physics, University of Vienna, Austria — [3]VASP Software GmbH, Vienna, Austria

We present flexible and physically meaningful descriptors for modeling long-range electrostatic interactions in machine learning force fields (MLFFs).

While local, atom-centered descriptors can accurately describe properties of several materials, they completely disregard long-range effects. For example long-range electrostatics are a crucial aspect of ionic materials, which makes it necessary to develop new techniques that account for them in order to ensure the predictive capability of MLFFs.

Our novel descriptors account for long-range interactions without resorting to a global description. They characterize the atomic density, similar to commonly used short-range methods. Periodic images of all atoms are accounted for by calculating the atomic density in reciprocal space.

This new long-range model is comparable to the long-distance equivariant (LODE) framework [1] for system with purely electrostatic interactions. Our model outperforms LODE in predicting energies and forces for real materials, where local approaches fall short.

[1] A. Grisafi, The Journal of Chemical Physics, **151**, 204105 (2019).

DY 34.13 Wed 15:00 Poster C

Feedback Controlled Microscopy Using Machine Learning — •M Asif Hasan and Frank Cichos — Faculty of Physics and Earth System Sciences, Leipzig University, Linnéstraße 5, Leipzig, Germany

Feedback control is crucial in stabilizing unstable states, evident in living organisms to regulate system functions and in technological applications like quantum state control. The combination with machine learning offers novel approaches to probe and manipulate complex physical or chemical processes, where machine learning algorithms determine the control strategy for inducing specific physical or chemical perturbations in a microscopic system. Our project investigates a more cohesive approach to feedback-controlled microscopy, particularly in steering active microparticles amidst complex, noisy environments. To this end, we integrate a microscope and laser steering system with real-time particle detection and machine learning enabled feedback algorithm, specifically, the Actor-Critic Reinforcement Learning (ACRL) approach. We show that the AI agent can navigate the active particles and complex mixtures of passive particles to a target state with high precision, amidst environmental uncertainties such as Brownian motion and flow fields. With a multi-agent real-time learning design, we focus on navigating, adapting, and optimizing behaviors under fluctuating conditions, enabling the agents to proficiently interpret sensory data and learn optimal response policies in continuous action spaces. This study therefore paves the way to develop a universal Actor-Critic Reinforcement Learning multi-agent system enabling high-precision control in noisy settings of various fluidic scenarios.

DY 34.14 Wed 15:00 Poster C

Atomistic Simulations of Laser-Excited Carbon with Convolutional Neural Network Interatomic Potentials — •Luc Wieners, Bernd Bauerhenne, Malwin Xibraku, and Martin E. Garcia — University of Kassel

Atomistic simulations in solid state physics are usually done with density functional theory (DFT). While DFT has a great accuracy, its computation time scales cubical with the size of the system due to the high computational cost of solving the Kohn-Sham equations. Therefore we look at a faster approach which uses machine learning with neural networks to replicate DFT results. We build a machine learning interatomic potential and train it to predict atomic forces based on DFT calculations. This neural network interatomic potential can be used for MD simulations of laser-excited carbon due to the high accuracy of its force predictions. At the same time, the computational cost of this potential scales linear with the system size, enabling simulations of large systems and long time spans which cannot be simulated with DFT. In this work we focus on convolutional neural networks which allow the direct processing of the atomic structure as an image which speeds up the calculation of the network input.

DY 34.15 Wed 15:00 Poster C

Machine Learning the Anderson model of localization — Djénabou Bayo[1,2] and •Rudolf A. Römer[1] — [1]Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Laboratoire de Physique Théorique et Modélisation (LPTM) (CNRS UMR8089), CY Cergy Paris Université, 95302 Cergy-Pontoise, France

In recent years, we witnessed the emergence of DNN techniques in several fields of physics as a new tool for data analysis. In condensed matter physics in particular, DNN and CNN proved to be performing well in identifying and classifying the phases of matter or learning order parameters. The Anderson model of localization is characterised by a phase transition from a metal state (with an extended wave function) to an insulator (with a localised wave function) in the presence of high disorder. This model was previously studied by T. Ohtsuki et al. and it was shown that ML techniques were able to distinguish the two phases. In our study, we employ a ResNet18 to reconstruct the full disorder resolution from normalised eigenstates ψ. We find that given large enough system sizes $L^3 > 40^3$, classification methods are able to make acceptable predictions on the disorder. Furthermore, we show that by using a reduced number of trained disorder values, regression methods are able to make good predictions on a larger set of disorders. Our implementation was made by using the PyTorch library.

DY 34.16 Wed 15:00 Poster C

Bridging the Gap: From EIS to Real-World Battery Performance with Stochastic Pulse Design — •Limei Jin[1,2], Franz Bereck[2], Josef Granwehr[2], Rüdiger-A. Eichel[2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]IEK-9, Forschungszentrum Jülich

While Electrochemical Impedance Spectroscopy (EIS) offers valuable insights into a battery's state, real-world battery operation during driving scenarios involves dynamic state changes, where current and voltage signals are far from ideally sinusoidal. To bridge the gap between EIS and real-world driving cycle analysis, we introduce the concept of a stochastic pulse design compatible with the load profile. This approach starts with frequency-based impedance data as a reference and transitions into time-based noisy permuted sinusoidal signals, eventually yielding stochastic pulse signals that more accurately reflect the complexities of real-world operation. The analysis of this multifaceted data is conducted in the latent space of an autoencoder, which comprises essential features extracted from the input data. Through latent space segmentation and its correlation with battery aging, we ensure the validity of the generated pulse signals compared to traditional EIS. Detailed point-to-point evaluations in the feature space enable the identification of the best and worst pulse load profiles, which can then be utilized to facilitate battery fast-charging and lifetime optimization.

DY 35: Poster: Quantum Dynamics and Many-body Systems

Time: Wednesday 15:00–18:00 Location: Poster D

DY 35.1 Wed 15:00 Poster D

Krylov Complexity in generic and flat band spinsystems — •Max Pieper, Jannis Eckseler, and Jürgen Schnack — Universität Bielefeld

Krylov Complexity [1] is a measure of the operator growth in quantum many-body-systems. It describes how an initial operator spreads in the Krylov-space under unitary Heisenberg time evolution. The behavior of Krylov complexity has been linked to a difference between integrability and chaos [2]. We are investigating the evolution of the Krylov complexity in generic and flat-band-systems.

[1] Daniel E. Parker et. al. Phys. Rev. X 9, 041017 (2019)
[2] E. Rabinovici et. al. JHEP07(2022)151

DY 35.2 Wed 15:00 Poster D

Impact of noise on localized solutions in the discrete nonlinear Schrödinger equation — •Mahdieh Ebrahimi[1], Wolfram Just[2], and Barbara Drossel[1] — [1]Institute of Condensed Matter Physics, Technical University of Darmstadt, Hochschulstr. 6, 64289 Darmstadt, Germany — [2]Institute of Mathematics, University of Rostock, D-18057 Rostock Germany

The Discrete Nonlinear Schrodinger equation (DNLS) serves as a prominent model across various scientific domains, ranging from physics and chemistry to biology. Within the realm of Hamiltonian systems, the nonlinear Schrodinger equation emerges as a fundamental representation for pattern formation, with a particular focus on examining localized solutions known as breather states. Understanding the underlying processes of the discrete systems is important for many physical phenomena such as excitations in crystal lattices and molecular chains, the light propagation in waveguide arrays, and the dynamics of Bose-condensate droplets. Here, we consider the DNLS as an effective macroscopic equation for a quantum mechanical many-particle system. We explore how localized solutions are affected by adding damping and noise to the Hamiltonian equations of motion.

DY 35.3 Wed 15:00 Poster D

Probing many-body localization via compression of Floquet random circuits — •Francesca De Franco[1,6], David J. Luitz[2], Dante M. Kennes[3,4], Matteo Rizzi[1,5], and Markus Schmitt[1,6] — [1]FZ Jülich, Institute of Quantum Control (PGI-8), Jülich, Germany — [2]University of Bonn, Bonn, Germany — [3]RWTH Aachen University, Aachen, Germany — [4]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [5]University of Cologne, Cologne, Germany — [6]University of Regensburg, Regensburg, Germany

We investigate many-body localization (MBL) in Floquet random circuits and methods for their compression into shallow circuits. In particular, we address the question how the different characteristics of entanglement spreading in the localized and ergodic regimes affect the compressibility of the circuits. Besides serving as a possible probe for localization, compressed Floquet random circuits might open a practical route to observe dynamical signatures of localization in digital quantum simulations on near-term quantum processors.

DY 35.4 Wed 15:00 Poster D

Allosteric impurity effects in long spin chains — •Christian Eidecker-Dunkel and Peter Reimann — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Allosterism traditionally refers to local changes in an extended object, for instance the binding of a ligand to a macromolecule, leading to a localized response at some other, possibly quite remote position. Here, we show that such fascinating effects may already occur in very simple and common quantum many-body systems, such as an anisotropic Heisenberg spin chain: Introducing an impurity at one end of a sufficiently long chain may lead to quite significant changes of the observable behavior near the other end, but not in the much larger region in between. Specifically, spin autocorrelation functions at thermal equilibrium are found to exhibit a pronounced allosterism of this type.

DY 35.5 Wed 15:00 Poster D

Aspects of the dynamics of the Kagome Heisenberg Antiferromagnet in the one magnon space — •Henrik Schlüter, Jannis Eckseler, and Jürgen Schnack — Bielefeld University. Bielefeld, Germany

We present aspects of the one-magnon dynamics of the antiferromagnetic kagome lattice as an example of flat-band-dynamics, extending the work of [1] to two dimensional systems. We illustrate how localized eigenstates also called localized magnons influence the dynamics of excitations and possibly prevent the system from thermalization.

[1] Florian Johannesmann et al. Phys. Rev. B 108, 064304

DY 35.6 Wed 15:00 Poster D

Probing Many-Body Dynamics in Dense Nitrogen Vacancy Ensembles — •David O'Shea, Soham Pal, Toby Mitchell, and Helena Knowles — University of Cambridge

Dense ensembles of nitrogen-vacancy centres (NVs) in diamond offer a promising platform for investigating the intricate dynamics of disordered, strongly interacting spin systems and the interplay between different thermalizing processes in them. Floquet engineering can then be used to tune the interactions and on site disorder in the sample, allowing for exploration of predicted phenomena such as many-body-localisation and quantum many-body-scars.

The study of many-body phenomena in NV centres holds several advantages like (a) High Fidelity Control: NV centres provide a platform for global control of spins enabling manipulation of spin states and interactions, (b) Scalability: Dense NV ensembles offer a scalable platform for studying large-scale many-body systems, (c) Coupling to different spin baths: NV ensembles can be coupled to other spin baths, enabling exploration of non-equilibrium dynamics in open systems. Our research aims to elucidate the thermalization dynamics of these complex coupled systems by systematically tuning the disorder and dimensionality of the NV ensemble using a state-of-the-art homebuild AFM setup integrated in a confocal setup.

DY 35.7 Wed 15:00 Poster D

revealing quantum effects in bosonic Josephson junctions: a multi-configuration atomic coherent state approach — •Yulong Qiao[1] and Frank Grossman[2] — [1]Institute for theoretical physics, TU Dresden, 01062 Dresden, Germany — [2]Institute for theoretical physics, TU Dresden, 01062 Dresden, Germany

The bosonic Josephson junction can be effectively described by a two-site Bose-Hubbard model. Many quantum phenomena in this model result from the dynamic interplay between the particle imbalance and the relative phase between two sites, which are treated as a pair of conjugated variables in mean-field theory. However, some nontrivial quantum effects such as the self-trapping effect and spontaneous symmetry breaking are described incorrectly by mean-field results [1].

We have developed a new variational approach utilizing a set of generalized coherent states to study the non-equilibrium dynamics of the Bose-Hubbard model [2]. Here, we apply this method to the bosonic Josephson junction and demonstrate that quantum effects beyond the mean-field approximation are easily uncovered by only a few basis functions [3]. Specifically, for the case of plasma oscillations, just two basis states already gives a good qualitative agreement with numerically exact quantum solutions. In order to correctly account for macroscopic quantum self-trapping, moderately more basis states are needed.

[1] Y. Qiao and F. Grossmann, Phys. Rev. A 103, 042209 (2021). [2] S. Wimberger, G Manganelli, A Brollo, L Salasnich, Phys. Rev. A 103, 023326 (2021) [3] Y. Qiao and F. Grossmann, Front. in Phys., 11:1221614 (2023)

DY 35.8 Wed 15:00 Poster D

Thermalization of locally perturbed many-body quantum systems — Peter Reimann[1], •Patrick Vorndamme[1], and Lennart Dabelow[2] — [1]Universität Bielefeld — [2]Queen Mary University, London

Deriving conditions under which a macroscopic system thermalizes directly from the underlying quantum many-body dynamics of its microscopic constituents is a long-standing challenge in theoretical physics. The well-known eigenstate thermalization hypothesis (ETH) is presumed to be a key mechanism, but has defied rigorous verification for generic systems thus far. A weaker variant (weak ETH), by contrast, is provably true for a large variety of systems, including even many integrable models, but its implications with respect to the problem

of thermalization are still largely unexplored. Here we analytically demonstrate that systems satisfying the weak ETH exhibit thermalization for two very natural classes of far-from-equilibrium initial conditions: the overwhelming majority of all pure states with a preset nonequilibrium expectation value of some given local observable, and the Gibbs states of a Hamiltonian which subsequently is subject to a quantum quench in the form of a sudden change of some local system properties. As numerical example we show our findings for the (integrable) transverse-field Ising model (TFIM).

DY 35.9 Wed 15:00 Poster D

perfect solitary waves in flat band systems — •Jannis Eckseler and Jürgen Schnack — Bielefeld University

Solitary waves appear in many-body systems if the initial state is a superposition of eigenstates of the Hamiltonian and the translation operator which fulfill a generalised linear dispersion relation [1]. In general a system only has approximate solitary waves, due to the finite size and discreteness of the energy spectrum which does not allow for an exact linear dispersion relation. However, in flat band systems, such as the delta-chain, an exact linear dispersion relation can be fulfilled. We investigate such perfect solitary waves in the delta chain and their robustness to small perturbations.

[1] Jürgen Schnack et al. Journal of Magnetism and Magnetic Materials 306 (2006), 79-84

DY 35.10 Wed 15:00 Poster D

Nonequilibrium Green functions simulations of 2D hexagonal monolayers with the G1-G2 scheme — •Tim Kalsberger, Christopher Makait, Jan-Philip Joost, and Michael Bonitz — CAU Kiel, Germany

Since their discovery, 2D quantum materials such as graphene and TMDCs have been of great importance in solid state physics due to their unique properties. However, the numerical treatment of these quantum systems with satisfactory accuracy has been severely limited due to their complexity. Previous methods, for instance, utilize density matrix formalism to describe the behavior of electrons in nonequilibrium conditions [1]. Nonequilibrium Green functions (NEGF) provide an alternative method capable of capturing electronic correlations within the material. However, the scaling of NEGF is highly unfavorable due to its two-time nature. The G1-G2 scheme [2] has facilitated significant improvements in this scaling and was already successfully applied to finite graphene systems [3]. Now, this approach is extended to macroscopic systems and we present first results for the electronic relaxation following optical excitations.

[1] T. Winzer *et al.*, *Nano letters*, 10(12), 4839-4843 (2010)
[2] N. Schlünzen *et al.*, *Phys. Rev. Lett.*, 124, 076601 (2020)
[3] Anna Niggas *et al.*, *Phys. Rev. Lett.*, 129, 086802 (2022)

DY 35.11 Wed 15:00 Poster D

Disorder-Averaged Effective Time Evolution — •Mirco Erpelding[1], Adrian Braemer[1], and Martin Gärttner[1,2] — [1]Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany — [2]Institute of Condensed Matter Theory and Optics, Friedrich-Schiller-University Jena, Max-Wien-Platz 1, 07743 Jena, Germany

In his seminal work, Anderson demonstrated that a disordered quantum system may localize, i.e. escape thermalization, thereby initiating a whole new area of research. More recently, localization has also been studied for quantum many-body systems. Here information is usually gathered via the exact solution of many disorder realizations making the studies computationally very expensive. In this work, we approach this challenge by taking the disorder average first and explore what can be learned from the resulting effective description. Often additional symmetries arise in the average picture: For example while disorder typically breaks spatial symmetries within each shot, most of the time every site/spin experiences the same disorder distribution restoring the symmetry in the averaged time-evolution.

Concretely, we derive an effective Lindbladian for disordered Ising models with independent couplings, such as the Sherrington-Kirkpatrick model. Subsequently, we compare our findings to interacting models sharing the same effective symmetries, aiming for a simplified description.

DY 35.12 Wed 15:00 Poster D

Quantum engineering for compactly localized states in disordered Lieb lattices — Carlo Danieli[1], Jie Lie[2,3], and •Rudolf A. Römer[2,4] — [1]Institute for Complex Systems, CNR, Rome, Italy — [2]School of Physics and Optoelectronics, Xiangtan University, Xiangtan, China — [3]Institute of Mathematics and Physics, Central South University of Forestry and Technology, Changsha, China — [4]Department of Physics, University of Warwick, Coventry, UK

Blending ordering within an uncorrelated disorder potential in families of 3D Lieb lattices preserves the macroscopic degeneracy of compact localized states and yields unconventional combinations of localized and delocalized phases. We proceed to reintroduce translation invariance in the system by further ordering the disorder. We discuss the spectral structure and eigenstates features of the resulting perturbed lattices. We restore order in steps by first (i) rendering the disorder binary, i.e. yielding a randomized checkerboard potential, then (ii) reordering the randomized checkerboard into an ordered one, and at last (iii) realigning all the checkerboard values yielding a constant potential shift, but only on a sub-lattice. Along this path, we test the influence of additional random impurities on the order restoration. We find that in each of these steps, sub-families of states are projected upon the location of the degenerate compact states, while the complementary ones are localized in the perturbed sites with energy determined by the strength of the checkerboard. This highlights order restoration as an experimental pathway to engineer features in disordered lattice structures in the pursuit of quantum storage and memory applications.

DY 35.13 Wed 15:00 Poster D

Non-abelian invariants in periodically-driven quantum rotors — •Volker Karle, Areg Ghazaryan, and Mikhail Lemeshko — Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg

This poster explores the role of topological invariants in the nonequilibrium dynamics of periodically-driven quantum rotors, inspired by experiments on closed-shell diatomic molecules driven by periodic, far-off-resonant laser pulses. This approach uncovers a complex phase space with both localized and delocalized Floquet states. We demonstrate that the localized states are topological in nature, originating from Dirac cones protected by reflection and time-reversal symmetry. These states can be modified through laser strength adjustments, making them observable in current experiments through molecular alignment and observation of rotational level populations. Notably, in scenarios involving higher-order quantum resonances leading to multiple Floquet bands, the topological charges become non-Abelian. This results in the remarkable finding that the exchange of Dirac cones across different bands is non-commutative, enabling non-Abelian braiding, paving the way for the study of controllable multi-band topological physics in gas-phase experiments with small molecules, as well as for classifying dynamical molecular states by their topological invariants.

DY 35.14 Wed 15:00 Poster D

Semiclassical structure of resonance states of the three-disk scattering system — Roland Ketzmerick, Florian Lorenz, and •Jan Robert Schmidt — TU Dresden, Institute of Theoretical Physics, Dresden, Germany

For the paradigmatic three-disk scattering system, the structure of resonance states in the semiclassical limit is investigated. We introduce a classical multifractal measure that describes resonance states with decay rate γ in this limit. This measure (i) maximizes an entropy-like quantity and (ii) is conditionally invariant with the same decay rate γ. It is derived from a local random vector model and replaces previous approximate approaches. This supports the recently proposed factorization conjecture, that resonance states are a product of a classical measure and universal fluctuations [1, 2]. Here, these results are applied to the three-disk scattering system. Furthermore, we confirm the fractal Weyl law, counting the number of states, over an unprecedented large range.

[1] R. Ketzmerick, K. Clauß, F. Fritzsch, and A. Bäcker,
Chaotic resonance modes in dielectric cavities: Product of conditionally invariant measure and universal fluctuations,
Phys. Rev. Lett. **129**, 193901 (2022).

[2] J. R. Schmidt and R. Ketzmerick,
Resonance states of the three-disk scattering system,
arXiv:2308.12783 (2023).

DY 35.15 Wed 15:00 Poster D

Ray-segment scars in the random wave model — •Jakob Lindermeir, Jan Robert Schmidt, and Roland Ketzmerick — TU Dresden, Institute of Theoretical Physics, Dresden, Germany

A new type of scars along ray segments, unrelated to periodic-orbit scars, was recently observed in optical microcavities [1] and in the 3-disk scattering system. We introduce a method for their numerical analysis and apply it, as a first step, to the random wave model. This method involves calculating a new representation of the wave function that distinctly highlights scars. Subsequent steps enable the determination of length, width, and wavenumber of these scars. We compare the result of the numerical analysis to analytical predictions.

[1] R. Ketzmerick, K. Clauß, F. Fritzsch, and A. Bäcker, Chaotic resonance modes in dielectric cavities: Product of conditionally invariant measure and universal fluctuations, Phys. Rev. Lett. **129**, 193901 (2022).

DY 35.16 Wed 15:00 Poster D

Phase-space representations of three-dimensional optical microcavities — •Tom Rodemund[1], Shilong Li[2], Síle Nic Chormaic[3], and Martina Hentschel[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]College of Information Science and Electronic Engineering, Zhejiang University, Hangzhou, China — [3]Okinawa Institute of Science and Technology Graduate University, Okinawa, Japan

Analyzing the phase-space of a given dynamical system is a well-established and versatile tool towards their profound understanding. Prominent methods include the Poincaré surface of section for particle dynamics and the Husimi function for their wave counterpart. Often these are two-dimensional (2D) systems that allow for a convenient phase-space representation along a surface of section.

Three-dimensonal (3D) cavities such as bottles or microtoroids are typical samples investigated in mesoscopic optics. They are interesting objects of study, as they may behave qualitatively different to their 2D counterparts, e.g. due to Arnold diffusion. The existence of four phase-space coordinates hinders a compact representation of all their properties [1], making it impossible including all information in a single representation. Here we discuss possibilities and demonstrate how to extend the well-established concept of Husimi functions [2] to 3D optical microcavities of arbitrary shape, thereby focussing on experimentally accessible characterisitcs of 3D resonance modes.

[1] Firmbach et al., *Phys. Rev. E* **98** 022214 (2018)
[2] Hentschel et al., *Europhys. Lett.* **62** 636 (2003)

DY 35.17 Wed 15:00 Poster D

Analytical expressions for stationary solutions of the Lindblad equation — •Bernd Michael Fernengel — HIFMB, Oldenburg

The Lindblad equation is a quantum master equation describing the time evolution of quantum mechanical states. It is used to model open quantum systems. We give an analytical expressions of stationary solutions of the Lindblad equation in the case of a finite state space, using the concept of state transition networks of Markov chains. Our treatment is based on the so-called quantum-jump unravelling, which is an ensembles of stochastic quantum trajectories, compatible with the Lindblad equation. A single such trajectory is a piecewise deterministic process, which is interrupted by stochastic jumps. We discuss differences to the classical case and conditions, under which the Lindblad equation is asymptotically stable.

DY 35.18 Wed 15:00 Poster D

Topological phases in measurement-only quantum circuits and their transitions — •Pugazharasu Anancia Devaneyan[1,2], Michael Buchhold[2], and Kai Klocke[3] — [1]Department of Physics, Rheinische Friedrich-Wilhelms-Universität Bonn, D-53113 Bonn, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, D-50937 Cologne, Germany — [3]Department of Physics, University of California, Berkeley, California 94720, USA

Random quantum circuits serve as a fertile domain for uncovering far from equillibrium phenomena, with measurements providing directionality to dynamics. Recent advances emphasize the utility of statistical mechanics of d-dimensional loop models as a framework for understanding specific classes of measurement-only random quantum circuits in $d+1$ dimensions. This work explores quantum phase transitions between different topological states in measurement-only random circuits, featuring a competition among several classes of non-commuting measurement operators precisely described by a loop model. Numerical simulations of the loop model yield information-theoretic observables entanglement entropy, mutual information, and the entanglement scaling pre-factor discerned from the distribution of loop lengths at the boundary. Our findings reveal a novel topological phase transition between well-defined winding number phases and those with fluctuating winding numbers, intricately linked to the annihilation of Majorana zero modes.

DY 35.19 Wed 15:00 Poster D

Scarred circuits - implementing integer subspaces within digital chaotic quantum dynamics — •Tobias Dörstel and Michael Buchhold — Institut für Theoretische Physik, Universität zu Köln, D-50937 Cologne, Germany

Weak ergodicity breaking describes scenarios where a subpart of the Hilbert space does not thermalise under generic time evolution. In Hamiltonian systems, this corresponds to so-called quantum many-body scar states, which are eigenstates of the Hamiltonian but disobey the eigenstate thermalisation hypothesis. Here, we extend the concept to chaotic quantum circuits by implementing conditioned unitary gates and measurements with feedback. The unitary gates implement the projector-based Shiraishi-Mori construction that leaves the scarred-subspace invariant. Measurements and feedback are designed such that they preserve this subspace and, in addition, guide the dynamics towards the scarred subspace. We study the robustness of the scarred subspace by categorizing the evolution into the scars and their stability against external perturbations. To do so, we combine efficient numerical simulations of so-called conditioned Haar random gates and feedback with analytical arguments.

DY 35.20 Wed 15:00 Poster D

A margin of stability in the propagation of open quantum systems — •Malte Krug and Jürgen Stockburger — Institute for Complex Quantum Systems, Ulm University

The Hierarchical Equations of Motion (HEOM) method has become one of the cornerstones in the simulation of open quantum systems and their dynamics. It is a non-perturbative method, suitable also for strong coupling and sluggish environments with long-time correlations [1]. In spite of the wide range of successful applications of HEOM, there are certain instances where the necessary finite truncation of the hierarchy of auxiliary density operators leads to divergent solutions. We present results on the nature and causes of this type of critical error based on analytic results and numerical experiments [2]. Both the case of pure decoherence, where exact results are available for comparison, and divergences in certain parameter regions of the spin-boson model are investigated. We find that truncating the hierarchy to any finite size can be problematic for strong coupling to a dissipative reservoir, in particular when combined with an appreciable reservoir memory time.

[1] Xu, M., Yan, Y., Shi, Q., Ankerhold, J. and Stockburger, J.T. Taming quantum noise for efficient low temperature simulations of open quantum systems Phys. Rev. Lett. **129**, 230601 (2022). https://doi.org/10.1103/PhysRevLett.129.230601.

[2] Krug, M., Stockburger, J. On stability issues of the HEOM method. Eur. Phys. J. Spec. Top. (2023). https://doi.org/10.1140/epjs/s11734-023-00972-9.

DY 35.21 Wed 15:00 Poster D

Giant DC Residual Current Generated by Subcycle Laser Pulses — •Adrian Seith, Ferdinand Evers, and Jan Wilhelm — Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, 93053 Regensburg

On an ultrashort timescale, experimental indications have been reported suggesting that laser pulses can produce currents that survive long after the illumination has died out. Such residual currents (remnants) may have applications in petahertz logical gates. The amplitude of remnants strongly depends on the pulse shape. We develop an analytical formula that allows to optimize the pulse shape; we predict remnants that exceed the values observed so far by orders of magnitude. In fact, remnants can become almost as strong as the peak current under irradiation.

DY 35.22 Wed 15:00 Poster D

Attempts towards a quantum coherent extension of the "macroscopic fluctuation theory": Are there universal fluctuations of quantum coherences in noisy mesoscopic systems? — •Ludwig Hruza — Laboratoire de Physique de l'École Normale Supérieure, Université Paris Cité, 75005 Paris, France

The "macroscopic fluctuation theory" has been major achievement in the understanding of classical non-equilibrium over the past 20 years. Notably, it has been realized that the fluctuation of density and cur-

rent profiles in classical current-carrying many-body systems with diffusive transport (e.g. a conductor between two reservoirs at different potentials) are non-local and universal, in the sense that they only depend on two system specific constants (the diffusion constant and the mobility) and the "macroscopic fluctuation theory" provides analytic formulae to compute these fluctuations. The question I will explore in this talk, is how one could incorporate quantum coherent effects into such a theory and why this would be an interesting thing to do? While experimentally, the measurement of coherences (and their fluctuations) between two points of a diffusive metallic conductor is still out of reach, the study of an analytically solvable toy model, the so-called QSSEP (Quantum Simple Symmetric Exclusion Principle), has provided us with first ideas for the mathematical structure of such a theory – with surprising connections to the free probability theory. I will also comment on our most recent finding, that the predictions of the QSSEP seems to agree with numerical simulations of the more realistic 3D Anderson model, which emphasizes the importance of QSSEP as a potential paradigmatic toy model in the study of the fluctuation of quantum coherences.

Reference: "Coherent Fluctuations in Noisy Mesoscopic Systems, the Open Quantum SSEP, and Free Probability", Ludwig Hruza and Denis Bernard, Phys. Rev. X 13, 011045, 2023.

DY 36: Focus Session: Wetting on Adaptive Substrates I (joint session CPP/DY/O)

The focus session aims to discuss recent developments in the wetting dynamics of adaptive, deformable, and switchable surfaces.

Time: Thursday 9:30–11:00 Location: H 0107

Invited Talk DY 36.1 Thu 9:30 H 0107

Extraordinarily slippery liquid-repellent surfaces using self-assembled monolayers — •Robin Ras — Aalto University, Espoo, Finland

Water-repellent surfaces have the attractive property of staying dry, and find applications in self-cleaning, anti-icing, anti-fogging and much more. Liquid-repellent surfaces, especially smooth solid surfaces with covalently grafted flexible brushes or alkyl monolayers, are the focus of an expanding research area.[1] Surface-tethered flexible species are highly mobile at room temperature, giving solid surfaces a unique liquid-like quality and unprecedented dynamical repellency.

We challenge two common assumptions on liquid-repellency.[2] It is generally assumed that water-repellent surfaces requires hydrophobicity. We demonstrate a hydrophilic surface with the unusual combination of low sliding angle and low contact angle. Surface heterogeneity is generally acknowledged as the major cause of increased contact angle hysteresis and friction of droplets. Here we challenge this long-standing premise for chemical heterogeneity at the molecular length scale.

Furthermore, we demonstrate world's most slippery surface, by combining self-assembled monolayers and surface structuring. Finally, by a suitable surface texture, we can trap a thin air layer for months, opening new strategies for underwater applications.[3]

[1] Nature Chemistry Reviews (2023) https://doi.org/10.1038/s41570-022-00455-w[2] Nature Chemistry (2023) https://doi.org/10.1038/s41557-023-01346-3 [3] Nature Materials (2023) https://doi.org/10.1038/s41563-023-01670-6

DY 36.2 Thu 10:00 H 0107

Volatile binary mixtures on polymer brushes — •Jan Diekmann und Uwe Thiele — Institut für Theoretische Physik, Universität Münster, 48149 Münster, Germany

We present a mesoscopic thin-film model in gradient dynamics form for binary liquid mixtures on brush-covered substrates incorporating volatility in a narrow gap. Thereby, we expand models established in [1, 4-6] by incorporating two substances present in each of three bulk phases - liquid, brush and gas. We discuss the different contributions to the free energy, thereby employing Flory-Huggins theory of mixing for the condensed phases and assuming ideal gases for the vapor phase. Interface energies are modeled as linear interpolations of known limiting cases. The resulting six-field model is then analyzed with numerical time simulations showing results with a focus on lateral concentration gradients, notably at the contact line.

[1] S. Hartmann, C. Diddens, M. Jalaal, and U. Thiele. JFM 960, 2023. doi: 10.1017/jfm.2023.176. [2] S. Hartmann, J. Diekmann, D. Greve, and U. Thiele. 2023. doi: 10.48550/ARXIV.2311.07307. [3] S. Schubotz, Q. A. Besford, S. Nazari, P. Uhlmann, E. Bittrich, J.-U. Sommer, and G. K. Auernhammer. Langmuir, 39, 2023. doi: 10.1021/acs.langmuir.2c03009. [4] L. A. Smook, G. C. R. van Eck, and S. de Beer. Macromolecules, 53, 2020. doi: 10.1021/acs.macromol.0c02228. [5] U. Thiele and S. Hartmann. EPJ-ST 229, 2020. doi:10.1140/epjst/e2020-900231-2. [6] Özlem Kap, S. Hartmann, H. Hoek, S. de Beer, I. Siretanu, U. Thiele, and F. Mugele. JFM 158, 2023. doi: 10.1063/5.0146779.

DY 36.3 Thu 10:15 H 0107

Wetting Phenomena in Hierarchically Porous Silicon: How Experiments and 2D Fluid-Dynamic Simulations Complement Each Other — •Stella Gries[1,2], Stefan Schulz[1], Marc Thelen[1,2], Silja Flenner[3], Imke Greving[3], and Patrick Huber[1,2] — [1]Institute for Materials and X-ray Physics, Hamburg University of Technology, Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Institute of Materials Physics, Helmholtz Zentrum Hereon, Geesthacht, Germany

Nature is an expert in designing highly efficient, multi-functional (hybride-)materials such as hierarchically capillary systems in respiratory systems or plants. These systems achieve large internal surfaces while allowing an optimized mass transport. This is used in plants to perform capillarity- induced motions, transport substances to reaction sites and remove educts from chemical processes. We are aiming to mimic such systems with artificially produced hierarchically porous silicon. The bimodal, hierarchical structure leads to a different imbibition behavior than porous systems with a monomodal pore-size distribution. Therefore, we used 2D finite element fluid dynamic simulations to achieve deeper insights into single-pore events and competing Laplace pressures in pore sections with distinct pore sizes. The simulations are related to the experimental results from dilatometry, mass-uptake and synchrotron-based, in-situ X-ray radiography imbibition experiments. This allows a complete description of the transport phenomena and will help us to tailor the material for applications in capillarity-driven pumps or energy harvesting from natural processes.

DY 36.4 Thu 10:30 H 0107

Percolation in Networks of Liquid Diodes — Camilla Sammartino, Yair Shokef, and •Bat-El Pinchasik — Tel Aviv University, School of Mechanical Engineering, Israel

Liquid diodes are surface structures that facilitate the spontaneous flow of liquids in a specific direction. In nature, they are used to increase water collection and uptake, reproduction, and feeding. However, pump-free large networks with directional properties are exceptional and are typically limited up to a few centimeters. Here, we simulate, design, and 3D print networks consisting of hundreds of liquid diodes. We provide structural and wettability guidelines for directional transport of liquids through these networks and introduce percolation theory in order to identify the threshold between a connected network, which allows fluid to reach specific points, and a disconnected network. By constructing well-defined networks with uni- and bidirectional pathways, we experimentally demonstrate the applicability of models describing isotropically directed percolation. We accurately predict the network permeability and the liquid final state. These guidelines are highly promising for the development of structures for spontaneous, yet predictable, directional liquid transport. In addition, they comprise an initial realization of complex liquid circuits, analogoues to electric circuits.

DY 36.5 Thu 10:45 H 0107

Wetting underneath droplets on an oily surface — •Shiva Moradimehr and Kirsten Harth — Fachbereich Technik, TH Brandenburg, Brandenburg a. d. Havel

When a liquid drop impacts on a smooth surface, a thin layer of air evolves between the drop and the surface. The drop deforms under the

influence of the ambient air that needs to be squeezed out before the drop can touch the substrate. The actual air layer profile depends on the impact velocity, ambient gas, drop liquid as well as the deformability of the substrate. For small impact Weber number, the air film ruptures before drop rebound. The wetting front connecting the drop and layer liquids propagates at velocities of few meters per second.

We study the wetting front velocity for droplets impacting on hard substrates covered by thin oil layers using high-speed interferometry at oblique incidence. The impact velocity, viz. the thickness of the entrained air layer, and the oil layer properties are varied. Both a model for contact spreading on a thin film or an film-rupture based model are initial candidates to describe the wetting front propagation.

DY 37: Statistical Physics of Biological Systems II (joint session BP/DY)

Time: Thursday 9:30–12:00 Location: H 1028

DY 37.1 Thu 9:30 H 1028

Coarsening model explains cross-species universality of crossover interference — •Marcel Ernst[1], Raphael Mercier[2], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]Max Planck Institute for Plant Breeding Research, Carl-von-Linné-Weg 10, 50829 Cologne, Germany

During meiosis, crossovers between female and male chromosomes mix genetic information. Experimental observations consistently produce two important results: First, the number of crossovers per chromosome is at least one and usually small, ranging from one to three. Second, there is crossover interference, which prevents nearby crossovers on a single chromosome. In this talk, I will present a novel quantification of crossover interference, which reveals a universal behavior across multiple species. This behavior is consistent with a recently proposed model, where biomolecular condensates that coarsen by exchanging material along chromosomes determine crossover positions. This process is disrupted in mutants lacking the axial structure connecting chromosome pairs, leading to strongly reduced interference. To explain that behavior, I will also present an extension of the coarsening model, which includes material exchange with the surrounding nucleoplasm. The modified coarsening dynamics provide a more detailed description of all experimental data and unveil the physical mechanism of crossover interference.

DY 37.2 Thu 9:45 H 1028

Designing phase coexistence in multicomponent mixtures: surface tensions and the Gibbs' rule — •Filipe Thewes and Peter Sollich — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

Gibbs' phase rule constrains the maximum number of phases that can coexist in multicomponent mixtures. It relates the maximum number of phases to the number of components and the degrees of freedom. The phases formed in equilibrium depend directly on the interactions between the different components, opening the possibility for the inverse problem of designing a set of interactions that recover a desired phase behavior. This perspective has been explored recently in relation to phase separation in biological systems as a mechanism for cells to control their internal structure and function. Interestingly, recent approaches for such interactions design are able to retrieve in the grand-canonical setting a number of phases that is larger than predicted by a naive application of Gibbs' phase rule. In this talk, I will first revisit Gibbs' rule in the *grandcanonical* ensemble and show that designed interactions act as new degrees of freedom that do increase the number of possible phases. I then show that in a canonical setting the number of phases is determined by interfacial tensions; above the naive Gibbs limit we find long-lived metastable states in numerical simulations. In the second part, I will discuss which conditions on the interfacial tensions result in "super-Gibbs" canonical phase splits. These conditions lead to a second step in the design problem of multicomponent mixtures, namely that of controlling the interfacial properties.

DY 37.3 Thu 10:00 H 1028

Microscopic model for aging of RNA condensates — •Hugo Le Roy — EPFL, Lausanne, Switzerland

Biomolecular condensates are membrane-less comparments in the cell that are involved in a wide diversity of biological processes. These liquid-liquid phase-separated droplets exhibit a viscoelastic mechanical response. This behavior is rationalized by modeling the complex molecules that make up a condensate as stickers and spacers that can assemble into a network-like structure. The proper functioning of biocondensates requires precise control over their composition, size, and mechanical response. For example, several neurodegenerative diseases are associated with dysfunctional condensates that solidify over a long period of time (days) until they become solid. A phenomenon usually described as aging. The emergence of such a long timescale of evolution from microscopic events, as well as the structural reorganization that leads to aging remains mostly an open question. To explore the connection between the mechanical properties of the condensates and their structure, we use a simplified description of the condensates. In our framework, a condensate is considered as an associative gel made of polymers (RNA) and linkers (DEAD-box proteins), whose response time is related to the interaction time between the constituents. We show that the interaction between linkers and long polymers results in an attractive Casimir force between linkers. As a consequence, linkers tend to cluster over equilibration of the network. Such a clustering does not make the material stiffer but leads to an exponential increase of the relaxation timescale in agreement with experimental observations.

DY 37.4 Thu 10:15 H 1028

Are phases an appropriate description for cells? — •Martin Girard — Max-Planck-Institute für Polymerforschung

Phase separation has emerged as an important topic for cellular function. From lipid rafts to liquid-liquid phase separation, our current understanding is that it is crucial for organization. We putatively expect that rules extracted from simple systems, two component mixtures, extend to multicomponent systems. While this is true in the thermodynamic limit, I will discuss here the thermodynamic limit for multicomponent systems. Using a toy model, I will show that what we consider "large systems" is largely subjective and dependent on details in multicomponent systems. For "small" systems, rules are very different, and the system is dominated by fluctuations. Usual assumptions, such as equivalence of thermodynamic ensembles, are broken. Still, the system can be driven to exhibit behavior that is similar to a phase transition, for instance by changing the statistical ensemble. Practically, this means that observed phase behavior may be largely dependent on system preparation. This naturally leads to a fundamental question: is the traditional phase behavior an appropriate description for cellular behavior?

15 min. break

DY 37.5 Thu 10:45 H 1028

Complex and 3-dimensional RNA random walks: comparison and application to sequence data across biological taxa — •Jack Mortimer and Jens Christian Claussen — School of Computer Science, University of Birmingham, UK

The DNA random walk is a classical attempt to grasp long-range features of DNA (or RNA) sequences by mapping pairs of amino acids to ± 1 steps of a random walk, and interpret the resulting "time series" by scaling analysis [1]. But as four letters C,G,A,T comprise the DNA alphabet it is a straightforward idea to utilize complex numbers to exploit this information (rather than ignoring it). This direction has been investigated also elsewhere [2] but different definitions were used, and it is not yet conclusive how far biological data can be differentiated.

In this contribution, we attempt a comparison of different complex RW definitions together with a 3D RW, discuss their relations between each other, and apply them to a wide range of DNA sequences. While the various DNA RW's seem not to be directly disciminatory for each species, we find that they provide a wide spread across the datasets. In conclusion, complex and higher-dimensional DNA random walks are a promising tool to extract long-range features from DNA, although the biological interpretation of this method remains to be investigated.

[1] Peng, Buldyrev, Goldberger et al., Nature 356,168 (1992)
[2] Cattani, in: Bioinf Res Dev, Springer, p. 528 (2008)

DY 37.6 Thu 11:00 H 1028

Trajectory mutual information in biochemical systems: Gaussian vs. Poissonian fluctuations — •Anne-Lena Moor[1,2], Christoph Zechner[1,2], and Pieter Rein ten Wolde[3] — [1]Max Planck Institute of Molecular Cell Biology and Genetics — [2]Center for Systems Biology Dresden — [3]AMOLF Amsterdam

Signal processing in biochemical networks relies on dynamic information transmission between time-trajectories of the respective molecular components. From a mathematical point of view, the transferred information can be described via the mutual information. Traditionally, this has been calculated using a Gaussian approximation. Our recent work suggests that this method is not always suitable for every biochemical networks which can lead to quantitative and qualitative mismatches to the exact solution. In this work, we explain the origin of these discrepancies and present a modified version of the Gaussian framework that aligns better with the characteristics of stochastic biochemical networks.

DY 37.7 Thu 11:15 H 1028

Geometry and epigenetic memory during ageing — •Matteo Ciarchi[1], Steffen Rulands[2], and Benjamin Simons[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Ludwig-Maximilians-Universität, München — [3]Department of Applied Mathematics and Theoretical Physics, Cambridge

Ageing is the decline of the physiological function of an organism over time. This process has been shown to be tightly correlated to changes in epigenetic modifications of the DNA. But how does the slow process of ageing over decades emerge from the fast molecular changes in the epigenome? Here, we show that the interplay between fluctuations and DNA geometry gives rise to memory that translates short-term molecular changes to a slow drift on the time-scales of aging. We draw on sequencing experiments that compare DNA methylation on the time scales of few cell divisions to longitudinal measurements over the much longer time scales of aging. We find that the drift of DNA methylation over time in both cases is highly nonlinear and cannot be explained by known biochemical processes. In order to understand these observations, we derive a field-theoretic framework that couples epigenetic processes along the DNA sequence with dynamic geometrical changes of the DNA in three-dimensional space. Using this theory, we show that the conformational changes in three-dimensional space allow for memory to form along the DNA sequence. Taken together, our work shows that epigenetic ageing is the accumulation of fast, intrinsic molecular processes over long time scales.

DY 37.8 Thu 11:30 H 1028

Exploring tumor karyotype evolution using the Macro-Karyotype concept — •Lucija Tomašić[1], Thomas van Ravesteyn[2,3], Geert J. P. L. Kops[2,3], and Nenad Pavin[1] — [1]Faculty of Science, University of Zagreb, Croatia — [2]Hubrecht Institute and University Medical Centre Utrecht, Utrecht, The Netherlands — [3]Oncode Institute, Utrecht, The Netherlands

Most tumors exhibit abnormal chromosome content (karyotype) resulting from errors in mitotic division. While tumors tend to manifest diverse karyotype aberrations, typically with gains of specific chromosomes, understanding the dynamics leading to these configurations is challenging due to the dimensionality of the karyotype space. To address this complexity, we introduce the 'Macro-Karyotype' concept,a novel framework for comprehensively exploring tumor chromosomal evolution. Combining in vitro organoid evolution with mathematical modeling, our study demonstrates that premalignant human organoids spontaneously undergo chromosome copy number alterations related to cancer. A gradual gain of specific chromosomes over time is observed, propelled by the enhanced fitness of these karyotypes. Additionally, some karyotypes undergo dramatic changes through whole-genome duplication and multipolar divisions, followed by normalization over time through the selection of karyotypes with lower mitotic error rates. Our findings uncover the selection of homogeneous karyotypes driven by cellular fitness, significantly constraining the available karyotype space. Our study deepens understanding of tumor karyotype evolution and informs factors influencing cancer related chromosomal changes.

DY 37.9 Thu 11:45 H 1028

How do particles with complex interactions self-assemble ? — •Lara Koehler[1], Martin Lenz[2], and Pierre Ronceray[3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Université Paris Saclay — [3]Aix Marseille Université

In living cells, proteins self-assemble into large functional structures based on specific interactions between molecularly complex patches. Due to this complexity, protein self-assembly results from a competition between a large number of distinct interaction energies, of the order of one per pair of patches. Current self-assembly models however typically ignore this aspect, and the principles by which it determines the large-scale structure of protein assemblies are largely unknown. Here, we use Monte-Carlo simulations and machine learning to start to unravel these principles. We observe that despite widespread geometrical frustration, aggregates of particles with complex interactions fall within only a few categories that often display high degrees of spatial order, including crystals, fibers, and micelles. We then successfully identify the most relevant aspect of the interaction complexity in predicting these outcomes, namely the particles' ability to form periodic structures. Our results provide a first characterization of the rich design space associated with identical particles with complex interactions, and could inspire engineered self-assembling nanoobjects as well as help understand the emergence of robust functional protein structures.

DY 38: Nonequilibrium Quantum Systems 2 (joint session TT/DY)

Time: Thursday 9:30–13:00 Location: H 3025

DY 38.1 Thu 9:30 H 3025

Nontrivial damping of quantum many-body dynamics in the spin-1/2 XXZ chain — •Mariel Kempa and Robin Steinigeweg — U Osnabrück, Germany

Understanding how the dynamics of a given quantum system with many degrees of freedom is altered by the presence of a generic perturbation is a notoriously difficult question. Recent works predict that, in the overwhelming majority of cases, the unperturbed dynamics is just damped by a simple function, e.g., exponentially as expected from Fermi's golden rule. While these predictions rely on random-matrix arguments and typicality, they can only be verified for a specific physical situation. It also remains unclear how frequent and under which conditions counterexamples to the typical behavior occur. We address this question from the perspective of projection-operator techniques, where exponential damping of a density matrix occurs in the interaction picture but not necessarily in the Schrödinger picture. We show that a nontrivial damping in the Schrödinger picture can emerge if the dynamics in the unperturbed system possesses rich features, for instance due to the presence of strong interactions. We substantiate our theoretical arguments by large-scale numerical simulations of spin transport in a perturbed spin-1/2 XXZ chain.

[1] T. Heitmann et al., Phys. Rev. E 104 (2021) 054145

[2] M. Kempa et al., in preparation

DY 38.2 Thu 9:45 H 3025

Cluster Truncated Wigner Approximation: Long-range bond disordered interacting spin-1/2 models — Adrian Braemer[1], •Javad Vahedi[1,2], and Martin Gärttner[1,2] — [1]Physikalisches Institut, Heidelberg, Germany — [2]Friedrich-Schiller-University, Jena, Germany

Phase-space methods, like Truncated Wigner Approximation (TWA), effectively simulate quantum system dynamics near classical limits by simplifying complexity and preserving initial noise information. However, TWA has limitations in finite times and classical/non-interacting scenarios. For strongly interacting systems far from the classical limit, conventional methods may provide unreliable approximations. The Cluster Truncated Wigner Approximation (cTWA) is an alternative approach introducing additional degrees of freedom to represent correlations independently, using classical equations of motion with initial conditions sampled from Gaussian distributions [1].

Our investigation focuses on quench dynamics in a spin chain with long-range interactions and disordered couplings[2]. Initializing the system in a Néel state, we compute dynamical observables, such as the staggered magnetization and Renyi entropy S_2 for a two-spin

subsystem, using cTWA with different choices for the clustering and compare these to results from exact diagonalization. We find that a clustering strategy inspired by real-space renormalisation group argument matches the exact dynamics almost perfectly for a wide range of both interaction range and disorder strength.

DY 38.3 Thu 10:00 H 3025

Current-Voltage Characteristics of the Normal Metal-Insulator-PT-Symmetric Non-Hermitian Superconductor Junction as a Probe of Non-Hermitian Formalisms — •Viktoriia Kornich — Universität Würzburg

We study theoretically a junction consisting of a normal metal, PT-symmetric non-Hermitian superconductor, and an insulating thin layer between them. We calculate current-voltage characteristics for this junction using left-right and right-right bases and compare the results. We find that in the left-right basis, the Andreev-scattered particles move in the opposite direction compared with the right-right basis and conventional Andreev scattering. This leads to profound differences in current-voltage characteristics. Based on this and other signatures, we argue that the left-right basis is not applicable in this case. Remarkably, we find that the growth and decay with time of the states with imaginary energies in the right-right basis are equilibrated.

DY 38.4 Thu 10:15 H 3025

A Conjecture Regarding Ground State Overlaps — •Sarah Damerow and Stefan Kehrein — Institut für Theoretiche Physik, Friedrich-Hund-Platz 1, 37077 Göttingen, Georg-August Universität Göttingen, Germany

A conjectured extension of the adiabatic theorem to quantum quenches, i.e. non-adiabatic changes, is presented. Using Exact Diagonalisation and the Lanczos method, we study the Axial Next Nearest Neighbour Ising Model (ANNNI). We numerically test the following conjecture: A system is prepared in its ground state. Under adiabatic time evolution of the Hamiltonian this initial ground state evolves under the time-dependent Schrödinger equation. The overlap between the initial and the final ground state will be larger than any other overlap, if both states are in the same magnetic phase.

DY 38.5 Thu 10:30 H 3025

Constructing nonequilibrium steady states from equilibrium correlation functions in generic nonintegrable systems — •Markus Kraft[1], Jonas Richter[2,3], Fengping Jin[4], Sourav Nandy[5], Zala Lenarčič[5], Jacek Herbrych[6], Kristel Michielsen[4], Hans De Raedt[7], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]U Osnabrück — [2]U Stanford — [3]U Hannover — [4]FZ Jülich — [5]U Ljubljana — [6]U Wroclaw — [7]U Groningen

State-of-the-art approaches to extract transport coefficients of many-body quantum systems broadly fall into two categories: (i) they target the linear-response regime in terms of equilibrium correlation functions of the closed system; or (ii) they consider an open-system situation typically modeled by a Lindblad equation, where a nonequilibrium steady state emerges from driving the system at its boundaries. While quantitative agreement between (i) and (ii) has been found for selected model and parameter choices, also disagreement has been pointed out in the literature. Studying magnetization transport in the spin-1/2 XXZ chain, we here demonstrate that at weak driving the nonequilibrium steady state in an open system, including its buildup in time, can remarkably be constructed just on the basis of correlation functions in the closed system. We numerically illustrate this direct correspondence of closed-system and open-system dynamics.

[1] T. Heitmann et al., arXiv:2303.00430
[2] T. Heitmann et al., Phys. Rev. E 108 (2023) 024102
[3] M. Kraft et al., in preparation

DY 38.6 Thu 10:45 H 3025

A Mixed Quantum-Classical Approach to Nonequilibrium Charge Transport in Strongly Interacting Molecular Junctions — •Samuel Rudge, Christoph Kaspar, and Michael Thoss — University Freiburg, Freiburg im Breisgau, Deutschland

Electronic friction and Langevin dynamics (EF-LD) is a popular mixed quantum-classical approach to modeling the dynamics of molecules near metal surfaces [1]. We have recently shown that, using the numerically exact hierarchical equations of motion (HEOM) transport method, one can calculate the electronic friction of systems containing electron-electron correlations or high-frequency quantum vibrational modes [2].

In this contribution, we use, for the first time, the combined EF-LD and HEOM approach to explore nonequilibrium charge transport in molecular junctions containing strong interactions. The analysis is performed for a broad parameter regime and uncovers interesting transport behavior arising from the strong interactions. The method opens the door for the analysis of realistic multimode molecular models containing anharmonic vibrational modes and nonlinear electronic-vibrational interactions, which fully quantum methods currently struggle to treat [3].

[1] J. T. Lü *et al.*, Prog. Surf. Sci. **94** (2019) 21
[2] S. L. Rudge *et al.*, Phys. Rev. B **107**, (2023) 115416
[3] C. Schinabeck *et al.*, Phys. Rev. B **97**(2018) 235429

DY 38.7 Thu 11:00 H 3025

Transport resonances in systems with time periodic impurities — •Jan Mathis Giesen and Sebastian Eggert — Department of Physics and Research Center Optimas, University of Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Periodically driven impurities in tight binding chains can lead to the complete breakdown of transport even at infinitesimal small driving amplitudes due to a Fano-like resonance [1]. We now go beyond the simple model to analyse effects of time-periodic impurities in general setups like electronic systems, magnons in thin ferromagnetic films, photonic waveguides and the scattering of cold atoms. More specifically we examine single particle transport resonances in models featuring long range coupling and generally more complicated band structures as well as multiple channels, modes or bands.
We extend the Floquet scattering ansatz using plane waves to include multiple modes and also apply a generalization in form of a Floquet-S-matrix scattering approach. We find that transport resonances are highly susceptible to changes in the band structure. Depending on the driving parameters and energy of incoming states new transport resonances can appear while others might become completely suppressed.

[1] S. A. Reyes *et al.*. New J. Phys. **19** (2017) 043029

15 min. break

DY 38.8 Thu 11:30 H 3025

Numerically exact simulation of photo-doped Mott insulators — •Fabian Künzel[1], André Erpenbeck[2], Daniel Werner[3], Enrico Arrigoni[3], Emanuel Gull[2], Guy Cohen[4], and Martin Eckstein[1] — [1]University of Hamburg, 20355 Hamburg, Germany — [2]University of Michigan, Ann Arbor, Michigan 48109, USA — [3]Graz University of Technology, 8010 Graz, Austria — [4]Tel Aviv University, Tel Aviv 6997801, Israel

A description of long-lived photo-doped states in Mott insulators is challenging, as it needs to address exponentially separated timescales. These photo-doped states simultaneously host strongly correlated electron-like and hole-like carriers and can show instabilities into various non-thermal orders. In our recent work (arXiv:2311.13933 [cond-mat.str-el]) we demonstrate how properties of such quasi-steady states can be accessed using numerically exact techniques, in particular the steady state Quantum Monte Carlo inchworm framework, by establishing a time-local ansatz for the distribution function with separate Fermi functions for the electron and hole quasiparticles. We compare the results to non-perturbative steady state solvers and validate the consistency of this approach upon comparison with real-time simulations in a quenched Hubbard model. The simulations show that the Mott gap remains robust to large photo-doping, and the photo-doped state has hole and electron quasiparticles with strongly renormalized properties. By combining the steady state ansatz with Quantum Boltzmann Equation schemes, they open up new avenues for characterizing the slow dynamics of Mott insulators.

DY 38.9 Thu 11:45 H 3025

Fractonic Dynamics in Breathing Quantum-Spin Ice — •Gloria Isbrandt[1,2], Frank Pollmann[1,2], and Michael Knap[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Fracton quantum matter is characterized by excitations with constrained mobility. It remains an open challenge to identify suitable material candidates for such systems. Recently, breathing pyrochlore lattices have been argued as potential candidates for realizing fractonic constraints. Here, we study the dynamics of excitations in such

a breathing pyrochlore lattice. We derive an effective Hamiltonian for excitations in the fractonic ground state manifold, by resorting to the rank-2 U(1) gauge theory formulation and the rank-2 Gauss law of fractons. We show both by analytical considerations and by numerical simulations based on cellular automaton circuit dynamics, that excitations in these systems are confined to two-dimensional planes within the three-dimensional breathing pyrochlore lattice. We derive a height-field theory for the effective two-dimensional dynamics, which exhibits diffusive dynamics with slow modes at finite momenta, resulting from effective subsystem symmetries. Coined as "Fractonic Quantum-Spin Ice," this system offers a physically realizable platform for fractonic excitations predicted by higher-rank gauge theories

DY 38.10 Thu 12:00 H 3025

Dynamical Spectral Response of Fractonic Quantum Matter — •Philip Zechmann[1,2], Julian Boesl[1,2], Johannes Feldmeier[3], and Michael Knap[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Department of Physics, Harvard University, Cambridge, MA 02138, USA

Quantum many-body systems with fractonic excitations can realize fascinating phases of matter. Here, we study the low-energy excitations of a constrained Bose-Hubbard model in one dimension, which conserves the center of mass or, equivalently, the dipole moment in addition to the particle number. This model is known to realize fractonic phases, including a dipole Mott insulator, a dipole Luttinger liquid, and a metastable dipole supersolid. We use tensor network methods to compute spectral functions from the dynamical response of the system and verify predictions from low-energy field theories of the corresponding ground state phases. We demonstrate the existence of gapped excitations compatible with strong coupling results in a dipole Mott insulator, linear sound modes characteristic of a Luttinger liquid of dipoles, and soft quadratic modes at both zero and finite momenta in a supersolid state with charge density wave order and phase coherence at non-integer filling.

DY 38.11 Thu 12:15 H 3025

Deconfinement Dynamics of Fractons in Tilted Bose-Hubbard Chains — •Julian Boesl[1,2], Philip Zechmann[1,2], Johannes Feldmeier[3], and Michael Knap[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Department of Physics, Harvard University, Cambridge, MA 02138, USA

Fractonic constraints can lead to exotic properties of quantum many-body systems. Here, we investigate the dynamics of fracton excitations on top of the ground states of a one-dimensional, dipole-conserving Bose- Hubbard model. We show that nearby fractons undergo a collective motion mediated by exchanging virtual dipole excitations, which provides a powerful dynamical tool to characterize the underlying ground state phases. We find that in the gapped Mott insulating phase, fractons are confined to each other as motion requires the exchange of massive dipoles. When crossing the phase transition into a gapless Luttinger liquid of dipoles, fractons deconfine. Their transient deconfinement dynamics scales diffusively and exhibits strong but subleading contributions described by a quantum Lifshitz model. We examine prospects for the experimental realization in tilted Bose-Hubbard chains by numerically simulating the adiabatic state preparation and subsequent time evolution, and find clear signatures of the low-energy fracton dynamics.

DY 38.12 Thu 12:30 H 3025

Current-induced excitonic condensation in bilayer systems — •Alexander Osterkorn and Denis Golež — Institut "Jožef Stefan", Jamova cesta 39, 1000 Ljubljana, Slovenia

Excitons are correlated electron-hole pairs in multi-band electron systems, which can condense and form ordered phases of matter called excitonic insulators. These are expected to display novel and interesting features like superfluid energy transport and perfect Coulomb drag. While it is experimentally challenging to identify real materials hosting equilibrium excitonic order, out-of-equilibrium protocols open up an independent route to stabilize excitonic condensates. Ma et.al. [1] proposed a gated semiconductor bilayer architecture, in which an applied voltage bias allows for the continuous creation of interlayer excitons by means of an induced electrical current. We model the setup starting from the quasi-stationary situation [2] within the Hartree-Fock and second order Born approximations and discuss the strong impact of dimensionality on the formation of the excitonic state. In order to go beyond the static picture, we demonstrate the dynamical formation of a steady-state subsequent to a switch-on of the voltage bias within real-time DMFT. We discuss how the formation of an excitonic condensate depends on steady-state temperature and doped carrier concentration.

[1] L. Ma et al., Nature 598 (2021) 585
[2] M. Xie, A.H. MacDonald, Phys. Rev. Lett. 121 (2018) 067702

DY 38.13 Thu 12:45 H 3025

Semi-classical analysis of HHG in pseudo-relativistic materials — •Wolfgang Hogger[1], Vanessa Junk[1], Alexander Riedel[1], Cosimo Gorini[2], Angelika Knothe[1], Juan-Diego Urbina[1], and Klaus Richter[1] — [1]Institute for theoretical physics, University of Regensburg, Germany — [2]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

The study of high-order harmonic generation (HHG) in solids by virtue of intense laser pulses provides a fascinating platform to study ultrafast electron dynamics as well as material properties. We theoretically investigate HHG on the basis of massive Dirac Fermions, serving as a prototypical model for topologically non-trivial matter and other systems with pseudo-relativistic dispersion. A successful and intuitive picture for HHG in gases is the three-step model[1], which was also generalized and brought to the realm of semiconductors and 2D materials[2]. We study the emergence of this semi-classical model from a LZS-transfer-matrix method[3] which can account for the characteristic transition dynamics of Dirac Fermions and thus may provide a way to understand the physical mechanism of HHG in these systems.

[1] M. Lewenstein, P. Balcou, M. Y. Ivanov, A. L. Huillier, P. B. Corkum, Phys. Rev. A 49 (1994) 2117
[2] G. Vampa, C. R. Mcdonald, G. Orlando, D. D. Klug, P. B. Corkum, T. Brabec, Phys. Rev. Lett. 113 (2014) 073901
[3] S. N. Shevchenko, S. Ashhab, F. Nori, Phys. Rep. 492 (2010) 1

DY 39: Focus Session: Nanomechanical Systems for Classical and Quantum Sensing III (joint session HL/DY/TT/QI)

Nanomechanical and cavity-optomechanical systems have been recently established as a controllable and configurable platform that can be engineered to tackle outstanding sensing challenges both in the classical and in the quantum regime. With this focus session, experts from different but synergetically overlapping fields of nanomechanical sensing pursuing classical, non-linear and quantum approaches are brought together. The session shall provide an overview over the recent exciting developments of the techniques explored in micro- and nanomechanical systems and sensing concepts exploring quantum measurement schemes.

Organized by Eva Weig, Hubert Krenner, and Hans Hübl.

Time: Thursday 9:30–13:00 Location: EW 202

Invited Talk DY 39.1 Thu 9:30 EW 202
Quantum sensors and memories based on soft-clamped phononic membrane resonators — •Albert Schliesser — Niels Bohr Institute, Copenhagen University, Denmark

Soft-clamping of membrane resonators using a phononic pattern enables Q-factors above 1 billion and coherence times exceeding 100 ms at low temperature. We monitor the motion of such membranes with optical interferometry. This allows us to measure force and displacement at and beyond the standard quantum limit, and control the motional quantum state, even at room temperature. This platform lends itself for sensing applications; as an example, we image individual viruses and nanoparticles using the membrane as a force sensor. In a different set of experiments, we demonstrate mechanical storage and subsequent retrieval of optical pulses with an efficiency of 40%, suggesting applications as quantum memory for light.

Invited Talk DY 39.2 Thu 10:00 EW 202
Quantum mechanics-free subsystem with mechanical oscillators — •Laure Mercier de Lepinay[1], Caspar Ockeloen-Korppi[1], Matthew Woolley[2], and Mika Sillanpää[1] — [1]Department of Applied Physics, Aalto University, P.O. Box 15100, FI-00076 Aalto, Finland — [2]School of Engineering and Information Technology, UNSW Canberra, ACT, 2600, Australia

Quantum mechanics sets a limit on the precision of the continuous measurement of an oscillator's position. However, with an adequate coupling configuration of two oscillators, it is possible to build an oscillator-like subsystem of quadratures isolated from quantum and classical backaction which therefore does not suffer from this limit. We realize such a quantum mechanics-free subsystem using two micromechanical drumheads coupled to microwave cavities. Multitone phase-stable microwave pumping of the system allows to implement the necessary effective coupling configuration. We first demonstrate the measurement of two collective quadratures, evading backaction simultaneously on both of them, obtaining a total noise within a factor of 2 of the full quantum limit. Secondly, this measurement technique is directly adapted to the detection of continuous variable entanglement which is based, according to the Duan criterion, on variance estimates of two collective quadratures. We therefore verify the stabilized quantum entanglement of the two oscillators deeper than had been possible before for macroscopic mechanical oscillators.

Invited Talk DY 39.3 Thu 10:30 EW 202
Electrothermally tunable metal-graphene-siliconnitride membrane mechanical device — •Elke Scheer, Mengqi Fu, and Fan Yang — Department of Physics, University of Konstanz, 78457 Konstanz

Controlling the properties of mechanical devices over a wide range is important for applications as well as for fundamental research. In this work, we demonstrate an on-chip tunable device composed of a suspended siliconnitride (SiN) membrane with a graphene (G) layer on top which is connected to Au electrodes. Taking advantage of the electrical and thermal conductance properties of G and the difference in the thermal expansion coefficients of SiN and Au, we developed a device in which the G-Au interface serves as local heater by injecting a dc current. The force induced by the thermal expansion difference tunes the residual stress in the SiN membrane and deflects the membrane when the loading power overcomes the threshold to the buckling transition. With this device we realize an extreme large eigenfrequency tuning (more than 50 %) of the vibration mode. By injecting an ac voltage instead, and thus applying a periodic force to the membrane, we achieve strong excitation of the membrane resonator into the nonlinear vibration. This device may act as proof-of-principle for a compact on-chip excitation scheme for multidimensional and composite nanomechanical resonators.

15 min. break

Invited Talk DY 39.4 Thu 11:15 EW 202
From Nanomechanics to Spins — •Christian Degen — ETH Zurich, Switzerland

Nanomechanical resonators are exquisite sensors for weak magnetic forces, with exciting prospects in nanoscale detection and imaging of nuclear and electronic spins. In this talk, I will give an overview of our laboratory's activities in this field, including force detection with optomechanical membranes and strings, and nuclear spin imaging with the technique of magnetic resonance force microscopy.

Invited Talk DY 39.5 Thu 11:45 EW 202
Enhanced cooling efficiency in nonlinear cavity optomechanics — •Anja Metelmann[1], Nicolas Diaz-Naufal[2], David Zoepfl[3], Lukas Deeg[3], Christian Schneider[3], Mathieu Juan[4], and Gerhard Kirchmaier[3] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Free University Berlin, Berlin, Germany — [3]University of Innsbruck, Innsbruck, Austria — [4]Universite de Sherbrooke, Sherbrooke, Canada

Unlocking the quantum potential of mechanical resonators hinges on achieving ground state cooling, a key milestone for quantum information processing and ultra-precise quantum measurements. In the vibrant field of cavity optomechanics, dynamical backaction cooling and feedback protocols have successfully nudged macroscopic mechanical elements toward the quantum ground state. While linear regime cooling is well-explored, recent theoretical insights suggest that a nonlinear cavity could amplify cooling efficiency. We explore this intriguing nonlinear regime, focusing on the cooling dynamics of a mechanical resonator coupled to a nonlinear cavity, embodying the characteristics of a high-Q Duffing oscillator. In this talk we present a comparative analysis between theoretical predictions and experimental results from a magnetomechanical platform. The findings unveil a captivating enhancement in cooling efficiency attributed to the Duffing nonlinearity. This breakthrough not only enriches our understanding of optomechanical interactions but also holds promise for advancing cooling strategies in quantum technologies.

DY 39.6 Thu 12:15 EW 202
Brillouin scattering selection rules in elliptical optophononic resonators — •Anne Rodriguez[1,2], Priya Priya[1], Edson Cardozo de Oliveira[1], Abdelmounaim Harouri[1], Isabelle Sagnes[1], Florian Pastier[3], Martina Morassi[1], Aristide Lemaître[1], Loic Lanco[1], Martin Esmann[1], and Daniel Lanzillotti-Kimura[1,4] — [1]Centre de Nanosciences et de Nanotechnologies, Université Paris-Saclay, CNRS, Palaiseau, France — [2]present address: Chair for Nano and Quantum Sensors, Technische Universität München, Garching, Germany — [3]Quandela SAS, Palaiseau, France — [4]Institut für Physik, Universität Oldenburg, Germany

The selection rules of spontaneous Brillouin scattering in bulk crystalline solids are intrinsic material properties that formally constrain the energy, direction and polarization of the scattered photons for a given input state. In this work, we manipulate the polarization states of the input laser and Brillouin signal independently using polarization-sensitive optical micropillar cavities. The ellipticity of the micropil-

lars lifts the degeneracy of the optical cavity modes, and induces a wavelength-dependent rotation of polarization [1,2], altering the Brillouin scattering selection rules. We developed a Brillouin spectroscopy scheme based on polarization filtering, allowing to measure acoustic phonon resonances with frequencies in the range of 20-100 GHz [3], with background-free spontaneous Brillouin scattering spectra.

[1] H. Wang et al., Nat. Phot. 13, 770 (2019). [2] B. Gayral et al., APL 72, 1421 (1998). [3] A. Rodriguez et al., ACS Photonics 10, 1687 (2023).

DY 39.7 Thu 12:30 EW 202

3D Microwave Cavity-Assisted Detection of High-Q Silicon Nitride Nanomechanical String Resonators — •Run Fa Jonny Qiu, Anh Tuan Le, Avishek Chowdhury, and Eva Weig — Technical University of Munich, Chair of Nano- and Quantum Sensors, Hans-Piloty Str. 1, 87548 Munich, Germany

Amorphous, low-pressure chemical vapor deposition (LPCVD)-grown silicon nitride (Si3N4) is a highly pre-stressed material due to its thermal-coefficient mismatch and is exploited in our fabrication of doubly-clamped freely suspended nanomechanical string resonators with superjacent electrodes for dielectric drive and detection. High-quality factor (Q-factor) nanomechanical string resonators with a Q-factor of roughly 300000 were fabricated. Two large gold-coated antennas connected to the electrodes are deposited on-chip which permits for a direct coupling of the mechanical displacement-induced change of the capacitance between the electrodes to the electric field of the three-dimensional (3D) rectangular cavity. Research on the quarter-wave coaxial cavity together with a capacitive loop and disk coupling revealed the possibility of both coupling schemes for the detection of mechanical modes. Applying direct current (DC) voltage to the electrodes allows for a frequency tuning of the mechanical flexural modes in the opposite direction, which due to the inherent coupling of the two in-plane (ip) and out-of-plane (oop) modes leads to an avoided crossing.

DY 39.8 Thu 12:45 EW 202

Optomechanical acceleration beats in confined polariton condensates — Alexander Kuznetsov, Klaus Biermann, and •Paulo Ventura Santos — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

High-frequency optomechanics involving optoelectronic systems with long temporal coherences enable access to the regime of non-adiabatic modulation, where the optomechanical modulation quantum $\hbar\Omega_M$ exceeds the typical energy decoherence rate of the optoelectronic resonances. Characteristic for this regime is the appearance of modulation sidebands around the optoelectronic resonance line displaced by energy multiples $m\Omega_M$,$(m = 0, \pm 1, \dots)$ with amplitude and number determined by the energy modulation amplitude ΔE_M. Here, we experimentally demonstrate a novel regime of temporal coherence invoked by the harmonic modulation of an optomechanical resonance at extreme energy modulation amplitudes $\Delta E_M/(\hbar\Omega_M) > 150$. We show that the resonance energy of a confined exciton-polariton Bose-Einstein condensate harmonically driven at these high relative modulation amplitudes exhibit temporal correlations with timescales much shorter than the modulation period [Kuznetsov et al., DOI:10.21203/rs.3.rs-3197243/v1]. These correlations manifest themselves as comb of spectral resonances with energy scale determined by the ratio $\Delta E_M/(\hbar\Omega_M)$. We show that they arise from accelerated rates of energy change during the harmonic cycle and are, thus, termed the acceleration beats.

DY 40: Many-body Quantum Dynamics I (joint session DY/TT)

Time: Thursday 9:30–13:00 Location: A 151

DY 40.1 Thu 9:30 A 151

Topological synchronization of fractionalized spins — •Christopher Wächtler[1] and Joel Moore[1,2] — [1]University of California, Berkeley, USA — [2]Lawrence Berkeley National Laboratory, Berkeley, USA

The gapped symmetric phase of the Affleck-Kennedy-Lieb-Tasaki (AKLT) model exhibits fractionalized spins at the ends of an open chain. We show that breaking SU(2) symmetry and applying a global spin-lowering dissipator achieves synchronization of these fractionalized spins. Additional local dissipators ensure convergence to the ground state manifold. In order to understand which aspects of this synchronization are robust within the entire Haldane-gap phase, we reduce the biquadratic term which eliminates the need for an external field but destabilizes synchronization. Within the ground state subspace, stability is regained using only the global lowering dissipator. These results demonstrate that fractionalized degrees of freedom can be synchronized in extended systems with a significant degree of robustness arising from topological protection.

DY 40.2 Thu 9:45 A 151

Understanding NMR signals by cluster dynamic mean-field theory — •Timo Gräßer[1], Thomas Hahn[2], and Götz S. Uhrig[1] — [1]Condensed Matter Theory, TU Dortmund University, Otto-Hahn Straße 4, 44221 Dortmund, Germany — [2]School of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, United Kingdom

A recently developed dynamic mean-field theory for spins at infinite temperature (spinDMFT)[1] is used to understand NMR signals quantitatively. The underlying idea is to couple a spin to a dynamic Gaussian mean-field with second moments that are self-consistently linked to the spin's autocorrelations. We improve the approach by considering clusters of spins quantum-mechanically (CspinDMFT)[2]. The extended model is more accurate and it allows for computing multi-spin correlations. We show that generic NMR signals comprise contributions of such multi-spin correlations. The applicability and validity of this approach is shown by describing NMR data for calcium fluoride (Ca F2) and adamantane (C10 H16).

[1] T. Gräßer et al., Phys. Rev. Research 3, 043168 (2021).

[2] T. Gräßer et al., arXiv:2307.14188 (2023).

DY 40.3 Thu 10:00 A 151

Domain wall dynamics of a two dimensional quantum Ising model using tree tensor networks — •Wladislaw Krinitsin[1], Niklas Tausendpfund[1,2], Matteo Rizzi[1,2], and Markus Schmitt[1,3] — [1]Forschungszentrum, Jülich, Deutschland — [2]Institut für Theoretische Physik, Köln, Deutschland — [3]Fakultät für Informatik und Data Science, Regensburg, Deutschland

Many body systems out of equilibrium are notoriously difficult to solve due to the rapid growth of entanglement with time. In particular the expanding possibilities to address two-dimensional systems in quantum simulations turn a spotlight on the lack of reliable numerical methods in this regime. We explore an approach to solve the time evolution of two-dimensional quantum systems by applying the time-dependent variational principle to Tree Tensor Networks. As an application, we consider the relaxation of domain wall initial conditions in a quantum Ising model, where pre-thermal behavior leads to a slow relaxation of domain wall initial conditions.

DY 40.4 Thu 10:15 A 151

Edge modes of the random-field Floquet quantum Ising model — •Harald Schmid[1], Alexander-Georg Penner[1], Kang Yang[1], Leonid Glazman[2], and Felix von Oppen[1] — [1]Dahlem Center for Complex Quantum, Freie Universität Berlin, 14195 Berlin, Germany — [2]Department of Physics, Yale University, New Haven, Connecticut 06520, USA

Motivated by a recent experiment on a superconducting quantum processor [Mi et al., Science 378, 785 (2022)], we study edge modes in the random-field Floquet quantum Ising model. The edge modes induce pairings in the many-body Floquet spectrum with splittings exponentially close to zero or π. We find that random transverse fields induce a log-normal distribution for both types of splittings. In contrast, random longitudinal fields affect the zero and π splittings in drastically different ways. While zero pairings are rapidly lifted, the π pairings are remarkably robust, or even strengthen, up to vastly larger disorder strengths. We explain our result within a self-consistent Floquet perturbation theory and study implications for boundary spin-spin correlations. The robustness of π pairings against longitudinal disorder

may be useful for quantum information processing.

DY 40.5 Thu 10:30 A 151

A metronome spin stabilizes time-crystalline dynamics — •Niklas Euler[1,2], Adrian Braemer[2], and Martin Gärttner[1,2] — [1]Institute of Condensed Matter Theory and Optics, Friedrich-Schiller-University Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany

We investigate a disorder-free quantum Ising chain subject to a time-periodic drive that rotates each spin by an angle $\pi(1-\epsilon_i)$. In case all spins experience the same deviation ϵ and the system starts from a fully magnetized state, the dynamics is known to be time crystalline: The magnetization exhibits stable, period-doubled oscillations for timescales that grow exponentially with system size. In this work, we study the effect of ϵ differing between the spins. We find that reducing ϵ for a single spin drastically enhances the lifetime of spatial-temporal order, suggesting the name "metronome" spin. Employing perturbative arguments, we explain this observation for initial states with macroscopic bulk magnetization. Furthermore, in the case of random bitstring initial states, we report enhancement of the lifetime of a topological edge mode. Here, we relate the presence of the metronome spin to the suppression of resonant processes. Finally, we discuss an altered geometry in which the metronome spin is not directly part of the chain, making the two described mechanisms clearly distinguishable. Our results illuminate the rich nature of spatially-varying Floquet driving, establishing it as a promising technique for fields like Floquet engineering.

DY 40.6 Thu 10:45 A 151

Non-equilibrium dynamics of bosons with dipole symmetry: Emergence of new symmetry broken steady states — •Md Mursalin Islam[1,3], Krishnendu Sengupta[2], and Rajdeep Sensarma[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Indian Association for the Cultivation of Science, Kolkata, India — [3]Tata Institute of Fundamental Research, Mumbai, India

We study equilibrium and dynamical phase diagrams of an interacting system of N-component charged bosons with dipole symmetry. In the large N limit, the equilibrium phase diagram of these bosons shows a first-order transition between two phases. The first one is a localized normal phase where both the global U(N) and the dipole symmetries are conserved and the second one is a delocalized condensed phase where both the symmetries are broken. In contrast, the steady state after an instantaneous quantum quench from the condensed phase shows an additional, delocalized normal phase, where the global U(N) symmetry is conserved but the dipole symmetry is broken, for a range of the quench parameters. A study of the ramp dynamics of the model shows that the above-mentioned steady state exists only above a critical ramp rate.

DY 40.7 Thu 11:00 A 151

Symmetries as Ground States of Local Operators — •Sanjay Moudgalya[1,2] and Olexei Motrunich[3] — [1]Technical University of Munich, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [3]Department of Physics, California Institute of Technology, Pasadena, California 91125, USA

Symmetry algebras of quantum many-body systems with locality can be understood using commutant algebras, which are defined as algebras of operators that commute with a given set of local operators. In this work, we show that these symmetry algebras can be expressed as frustration-free ground states of a local superoperator, which we refer to as a "super-Hamiltonian". We demonstrate that for conventional on-site unitary symmetries, the symmetry algebras map to various kinds of ferromagnetic ground states. We obtain a physical interpretation of this super-Hamiltonian as the superoperator that governs the operator relaxation in noisy symmetric Brownian circuits, which relates its low-energy excitations to approximate symmetries that determine slowly relaxing modes in symmetric systems. We find examples of gapped/gapless super-Hamiltonians indicating the absence/presence of slow-modes, which happens in the presence of discrete/continuous symmetries. In the gapless cases, we recover slow-modes such as diffusion in the presence of U(1) symmetry. We also demonstrate this framework for unconventional symmetries that lead to Hilbert space fragmentation and quantum many-body scars, which lead to novel kinds of slow-modes such as tracer diffusion and asymptotic quantum scars.

15 min. break

DY 40.8 Thu 11:30 A 151

Active quantum flocks — •Reyhaneh Khasseh[1], Sascha Wald[2], Roderich Moessner[3], Christoph A. Weber[1], and Markus Heyl[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Statistical Physics Group, Centre for Fluid and Complex Systems, Coventry University, Coventry, England — [3]Max-Planck-Institut fur Physik komplexer Systeme, 01187 Dresden, Germany

In the captivating overlap of quantum physics and biophysics, our research seeks to reveal how characteristics intrinsic to living systems can manifest within quantum matter. Flocks of animals in the macroscopic classical world are iconic representations of collective behavior, where constituents move in harmony as though a singular entity. The intriguing intersection between quantum physics and biophysics prompts the exploration of whether such flocks can manifest in the microscopic quantum realm. Introducing the concept of active quantum matter through a series of models on a one-dimensional lattice, we present analytical and numerical evidence pointing to the emergence of quantum flocks.

DY 40.9 Thu 11:45 A 151

Quantum motility-induced phase separation — •Laurin Brunner[1], Reyhaneh Khasseh[1], Federico Carollo[2], Igor Lesanovsky[2], Juan Garrahan[3], and Markus Heyl[1] — [1]University of Augsburg, Augsburg, Germany — [2]Universität Tübingen, Tübingen, Germany — [3]University of Nottingham, Nottingham, United Kingdom

Active matter is a central concept in biophysics explaining key mechanisms of living organisms. Very recently, a quantum analogue in open quantum systems has been introduced for the first time. Here, we study a theoretical model showing evidence of a quantum counterpart of motility-induced phase separation. We solve the dynamics by means of neural quantum states and we furthermore discuss the quantum features of our model.

DY 40.10 Thu 12:00 A 151

Fluctuations Approach to Quantum Many-Body Systems and its Application to Density Correlations and the Dynamic Structure Factor — •Erik Schroedter, Jan-Philip Joost, and Michael Bonitz — CAU Kiel, Germany

The dynamics of quantum many-body systems following external excitation are of great interest in many areas, such as correlated solids or dense plasmas. Standard approaches used for the description of the dynamics of such systems include the formalisms of reduced density matrices (RDM) and nonequilibrium Green functions (NEGF). However, both approaches are limited in their applicability due to the numerical scaling of simulations with respect to the system size or propagation time. Here, an alternative approach to the dynamics of quantum systems is presented, which is based on fluctuations and their correlation functions [1]. While this new approach is closely related to NEGF and RDM theory [2], it has interesting complementary features, such as the capability to simulate many-body effects using stochastic methods [3,4], which reduce the computational complexity and additionally increase numerical stability for stronger coupling. Moreover, this approach provides direct access to spectral two-particle quantities, such as the density response function or dynamic structure factor, for systems in and far from equilibrium.

[1] E. Schroedter, *et al.*, Cond. Matt. Phys. **25**, 23401 (2022)
[2] E. Schroedter, and M. Bonitz, phys. stat. sol. (b) (2024)
[3] D. Lacroix, *et al.*, Phys. Rev. B **90**, 125112 (2014)
[4] E. Schroedter, *et al.*, Phys. Rev. B **108**, 205109 (2023)

DY 40.11 Thu 12:15 A 151

Conserved Superoperators and Non-Universality in Unitary Circuits — •Marco Lastres[1,2], Frank Pollmann[1,2], and Sanjay Moudgalya[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

An important result in the theory of quantum control is the "universality" of 2-local unitary gates, i.e. the fact that any global unitary evolution of a system of L qudits can be implemented by composition of 2-local unitary gates. Surprisingly, recent results show that uni-

versality can break down in the presence of symmetries: in general, not all globally symmetric unitaries can be constructed using k-local symmetric unitary gates. This also restricts the dynamics that can be implemented by symmetric local Hamiltonians.

In this study, we show that these obstructions to universality can in general be understood in terms of unconventional superoperator symmetries associated with unitary evolution by k-local gates. We demonstrate this explicitly in several examples by systematically deriving the superoperator symmetries using the framework of commutant algebras, which has recently been applied to derive the unconventional symmetries responsible for weak ergodicity breaking phenomena, such as quantum many body scars and Hilbert space fragmentation. In all, our work establishes a new comprehensive approach to explore the universality of unitary circuits and derive physical consequences of its absence.

DY 40.12 Thu 12:30 A 151

Exploring Quantum Dynamics of hard disks on a lattice — •Vighnesh Dattatraya Naik, Fabian Ballar Trigueros, and Markus Heyl — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Recent strides in quantum simulators have propelled the investigation of quantum matter with local constraints to the forefront of research. This study delves into the hard-disk problem, a paradigmatic class of constrained matter, by introducing its quantum version on lattices, which exhibits a natural realization in Rydberg atom arrays due to the Rydberg blockade mechanism. While static properties align with classical cases, dynamical properties are fundamentally different. In one dimension, we identify genuine quantum features in the melting process of a finite-size crystal displaying ballistic behavior, whereas the classical scenario exhibits sub-diffusion governed by the Kardar-Parisi-Zhang universality class. On two-dimensional square lattices, we show that in the quantum domain, crystals remain intact against most defects, whereas classically the initial crystal structure is washed out completely. We link this peculiar quantum behavior to the presence of quantum many-body scars, breaking conventional expectations of ergodicity. Our study highlights the potential of constrained two-dimensional quantum matter to display unique dynamical behaviors.

DY 40.13 Thu 12:45 A 151

Non-ergodic dynamical phenomena in lattice gauge theories — •Nilotpal Chakraborty[1], Markus Heyl[2], and Roderich Moessner[1] — [1]Max Planck Institute for physics of complex systems, Dresden — [2]University of Augsburg

Lattice gauge theories are paradigmatic examples of constrained many-body interacting systems. Such theories, while ubiquitous in nature, emerge in condensed matter settings as effective low-energy theories for certain classes of topological magnets. More recently such theories have also been at the forefront of a large quantum simulation effort using ultra cold atoms. With the advent of such simulation efforts and novel dynamical methods for solid state systems, the dynamics of such constrained interacting theories becomes an important theoretical question with physical relevance. In this talk I shall present lattice gauge theories as an ideal testbed for exploring a plethora of non-ergodic dynamical phenomena - ranging from fragmentation to scars as well as many-body localization. In particular, I shall focus on the occurrence of an interference induced many-body localization transition in two dimensional U(1) lattice gauge theories. Such a transition occurs for the problem of a single matter field hopping on a disordered background of interacting gauge fields. I will explore the problem both at the classical and quantum level and highlight interesting dynamical phenomena for both - such as sub-diffusion for the classical and many-body localization for the quantum problem.

DY 41: Statistical Physics: General

Time: Thursday 9:30–12:45 Location: BH-N 128

DY 41.1 Thu 9:30 BH-N 128

Survival probability of stochastic processes beyond persistence exponents — •Maxim Dolgushev — Laboratoire de Physique Théorique de la Matière Condensée, Sorbonne Université, 4 Place Jussieu, 75005 Paris, France

How long does it take a random walker to find a "target"? This time, called the first-passage time (FPT), appears in various domains: time taken by a predator to find its prey or by a transcription factor to find a specific sequence on the DNA, time taken by a virus to infect a cell or by a financial asset to exceed a certain threshold, time taken for the cyclization of a polymeric chain, etc.

From a theoretical point of view, a crucial parameter to evaluate FPTs is the possible presence of a geometrical confinement. For a symmetric random walk in a confined domain, the mean FPT $\langle T \rangle$ is in general finite. The opposite case of unconfined random walks is radically different. In this case, either the walker has a finite probability of never finding the target (transient random walks), or he reaches it with probability one (recurrent random walks) and the probability of survival of the target decreases algebraically with time, $S(t) \sim S_0/t^\theta$.

Our main result is a general exact relation for a process with stationary increments (more generally, for a process whose increments become stationary at long time only), Markovian or not, between the full asymptotic behavior (defined in the absence of confinement) and the mean FPT $\langle T \rangle$ for the same process in a large confinement volume.

DY 41.2 Thu 9:45 BH-N 128

Perturbative approach to non-linear non-Markovian vibrational spectroscopy — •Hélène Colinet — AG Netz, FU Berlin

Using perturbation theory, we investigate how non-harmonic potential contributions and non-Markovian friction influence vibrational absorption spectra, in particular the OH stretch band in liquid water. Non-Markovian friction gives rise to homogeneous and inhomogeneous line broadening of vibrational bands and is accurately accounted for using the generalized Langevin equation.

Our analytical results are validated by numerical simulations of the generalized Langevin equation, by which we demonstrate that our perturbation theory successfully reproduces changes in line shape and position. In particular, we show that the non-harmonic bond potential is crucial for resolving the inhomogeneous line broadening of the OH stretch band in the infrared absorption spectrum of liquid water. For this, anharmonic bond potentials and time-dependent friction kernels are extracted from ab initio molecular dynamics simulations.

DY 41.3 Thu 10:00 BH-N 128

Stochastically driven motion under nonlinear, Coulomb-tanh friction — a basic representation of the consequences of shear thinning — Theo Lequy[1] and •Andreas M. Menzel[2] — [1]Eidgenössische Technische Hochschule Zürich, Rämistrasse 101, 8092 Zürich, Switzerland — [2]Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Nonlinear friction is abundant in nearly all kinds of scenarios of relative motion. We here consider the stochastically driven dynamics of an object that is subject to the so-called Coulomb-tanh friction force [1]. This force increases linearly with speed at small magnitudes of the velocity and levels off at a constant value at large speeds. In this way, it interpolates between linear and solid (dry, Coulomb) friction. Under such conditions, in the case of one-dimensional motion, we find that the velocity spectrum can be found by formally linking the mathematical description to a Schrödinger equation including a Pöschl-Teller potential. Thus, an analytical approach is possible. We consider the velocity and displacement statistics of individual objects and find intermediate non-Gaussian tails in the spatial distribution function that are pushed outward over time. Both limits of linear and solid (dry, Coulomb) friction are well reproduced. For instance, our description should apply to the case of an object driven on a vibrated substrate covered by a layer of shear-thinning material that leads to the mentioned nonlinear friction.

[1] Theo Lequy, Andreas M. Menzel (submitted).

DY 41.4 Thu 10:15 BH-N 128

Oscillating autocorrelation functions and their physical implications in equilibrium odd-diffusive systems — •Erik Kalz[1], Hidde D. Vuijk[2], Jens-Uwe Sommer[3,4,5], Ralf Metzler[1,6], and Abhinav Sharma[2,3] — [1]University of Potsdam, Germany — [2]University of Augsburg, Germany — [3]Leibniz-Institute for Polymer

Research, Dresden, Germany — [4]Technical University Dresden, Germany — [5]Technical University Dresden, Cluster of Excellence Physics of Life, Germany — [6]Asia Pacific Centre for Theoretical Physics, Pohang, Republic of Korea

Autocorrelation functions (ACF) can be shown to decay monotonically in equilibrium systems. Despite being in equilibrium, this strict monotonicity condition of ACFs is broken in so-called odd-diffusive systems, which are characterized by probability fluxes perpendicular to density gradients. In fact, the velocity-ACF of a tracer-colloid can even be shown to be oscillatory. In normal systems, the monotonic decay of the velocity-ACF translates into an interaction-induced reduction of the diffusion coefficient of the colloid (Green-Kubo relation). We show that in odd systems, the non-monotonicity of the ACF instead results in an enhancement of the tracer diffusion with interparticle interactions.

Ref: E. Kalz, H. Vuijk, J.-U. Sommer, R. Metzler and A. Sharma: Oscillatory force autocorrelations in equilibrium odd-diffusive systems (PRL accepted manuscript)

DY 41.5 Thu 10:30 BH-N 128

Finite-size excess-entropy scaling for simple liquids — •Mauricio Sevilla, Atreyee Banerje, and Robinson Cortes-Huerto — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Integral equations in statistical mechanics play a crucial role in connecting thermodynamics to microscopic properties of simple liquids. In computer simulations, these integral equations manifest explicit and implicit size effects that arise from systems with a fixed number of particles and periodic boundary conditions, respectively. The excess entropy is of particular interest in the theory of liquids and glasses. However, often, in the computation of the two-body excess-entropy s_2 finite-size effects are overlooked and simulations are treated as if they were in the Grand Canonical ensemble. In this talk, we introduce and validate a finite-size two-body excess-entropy integral equation. Through analytical arguments and computer simulations of prototypical simple liquids, we demonstrate that the excess entropy s_2 displays a finite-size scaling with the inverse of the linear size of the simulation box. To valid our expression and given that the self-diffusivity coefficient D^* also exhibits a similar finite-size scaling, we establish that the empirical relation $D^* = A\exp(\alpha s_2)$ also depends on the simulation box size. Extrapolating this relation to the thermodynamic limit, we report values for A and α with excellent agreement with the literature. Finally, we find a power law relation between the scaling coefficients for $D^*(L)$ and $s_2(L)$, suggesting a constant viscosity-to-entropy ratio.

DY 41.6 Thu 10:45 BH-N 128

Finite-size diffusion coefficients and excess entropy for binary mixtures — •Maria C. Duenas-Herrera, Mauricio Sevilla, Luis A. Baptista, and Robinson Cortes-Huerto — Max Planck Institute for Polymer Research, Mainz, Germany

A universal relation between transport properties and excess entropy - the difference between a simple liquid's entropy and its ideal gas counterpart at equal density and temperature - has been widely investigated in theoretical, experimental and simulation studies. Similar connections between self-diffusion per component and excess entropy have been proposed for binary mixtures. However, excess-entropy scaling with multi-component diffusion coefficients such as Maxwell-Stefan (MS) or Fick (F) is mainly missing. To contribute to filling this gap, we perform molecular dynamics simulations of prototypical Lennard-Jones binary mixtures from which the excess entropy can be safely approximated to two-body terms. Multi-component diffusion coefficients and two-body excess entropy exhibit explicit and implicit finite-size effects present in conventional computer simulations. By considering finite-size versions of integral equations in statistical mechanics, a robust extrapolation to the thermodynamic limit allows one to establish a consistent scaling behavior of MS and F diffusivities with excess entropy.

15 min. break

DY 41.7 Thu 11:15 BH-N 128

A grand canonical hybrid approach to sample explicit solvent in small solvation shells — •Mohammad Rahbar and Christopher J. Stein — Technical University of Munich; TUM School of Natural Sciences, Department of Chemistry, Lichtenbergstr. 4, D-85748 Garching, Germany

Solvation effects significantly influence reactions in solution by modifying potential energy surfaces. Treating the solvent with an implicit model often lacks the depth to provide detailed insights into the structure and statistical fluctuations of the solvent. Explicit solvation models are an alternative approach, where both solute and solvent degrees of freedom are explicitly included. However, this method is limited by computational cost already for simulations with a small number of solvent molecules. Therefore, a hybrid approach that combines implicit and explicit methods may offer a more comprehensive understanding. A recurrent challenge in various hybrid methodologies is the lack of inclusion of statistical solvent fluctuation and heavy reliance on chemical intuition for the structure of the solute-solvent microsolvation shell. In our proposed approach, the grand canonical model plays a crucial role in facilitating the transfer of energy and particles between explicit and implicit domains, ensuring agreement with thermodynamic constraints for the simulated system. Free from ad hoc assumptions, our methodology aims to eliminate any nonphysical biases tied to the explicit set of solvent molecules included in the simulation. We construct a framework for accurately sampling solute and solvent configurations at the QM, QM-MM, or purely MM level in a small solvation shell.

DY 41.8 Thu 11:30 BH-N 128

Analysis of the effects of the entropy source on Monte Carlo simulations — •Anton Lebedev[1], Olha Ivanyshyn Yaman[1], Annika Möslein[2], Zhanet Zaharieva[2], and Charles Bryant[2] — [1]UKRI-STFC Hartree Centre, Keckwick Ln, Warrington, United Kingdom — [2]Quantum Dice Ltd, Oxford Centre for Innovation, Oxford, United Kingdom

In this contribution we present the benefits of quantum random number generators (QRNGs) for Monte Carlo simulations using select examples from mathematics and physics. We further present the set of statistical tests performed to arrive at this conclusion when comparing QRNGs to (industry-standard) pseudo-random and radio-based random number generators.

From simple Pi estimation to Bayesian model fitting: Monte Carlo applications are ubiquitous. All rely on randomness to sample the solution space, yet analysis of the quality of random number generators is limited. Understanding the effects of the randomness source on MC simulations and leveraging verifiable quantum randomness will yield a reasonable reduction in the number of simulations required to achieve a prescribed uncertainty bound and thereby the amount of compute resources consumed.

Using examples from mathematics and physics, we have analysed the statistically significant differences in simulation outcomes between quantum RNGs, classical hardware RNGs and (parallel) pseudo-random number generators. Tests for statistical significance have been selected based on the amount of underlying assumptions.

DY 41.9 Thu 11:45 BH-N 128

Population annealing on massively-parallel and distributed compute hardware — •Denis Gessert[1,2], Wolfhard Janke[1], and Martin Weigel[3] — [1]Institut für Theoretische Physik, Universität Leipzig, 04081 Leipzig — [2]Centre for Fluid and Complex Systems, Coventry University, Coventry CV1 5FB, UK — [3]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

Population annealing (PA) is a Monte Carlo (MC) method well suited for problems with a rough free energy landscape such as glassy systems. A PA simulation starts by equilibrating R replicas at an easy-to-sample high temperature. Akin to simulated annealing (SA) of a single system, the replicas are collectively cooled down to an otherwise hard-to-sample low temperature. Unlike in SA, before MC updates at the next lower temperature a selection process is carried out in PA, which makes the algorithm less prone to trapping in metastable states. The population size required to reach equilibrium strongly depends on the "difficulty" of the studied system, with some spin-glass simulations requiring populations of several million replicas. Despite the immediate technical challenge, this opens up an opportunity of achieving a level of parallelism that grows with the difficulty of the task.

Here, we present a simple replica-redistribution protocol for a distributed compute architecture that significantly reduces network traffic as compared to previous approaches, thus improving performance. For small instances, our protocol is only slightly worse than the optimal redistribution protocol found by brute-force. Finally, in some cases a form of speculative execution can be used to hide the network latency.

DY 41.10 Thu 12:00 BH-N 128

Extrapolation of Rate Functions from Finite-Size Numerical

Large-Deviation Simulations — •Peter Werner and Alexander K. Hartmann — Institute of Physics, University of Oldenburg, Germany

When performing large-deviation simulations, a typical question is whether the system at hand follows a *large-deviation principle* [1]. This can be done by checking if the probability distribution of an intensiv system quantity converges for increasing system sizes to a form that possesses a corresponding rate-function. Analytical solutions exist for certain models that allow for comparisons with numerical results [2]. Some special-purpose algorithms, as the *cloning* approach [3], can be used for a direct estimate. However, by using data from arbitrary simulation procedures, the results usually depend heavily on the specific finite-size scaling behaviour of the probability distributions. Here, a numerical procedure is presented that relies on samples obtained from general biased Monte-Carlo simulations [4]. Instead of working with the probability distributions directly, the scaled cumulant-generating function is approximated. From this approximation the *Gärtner-Ellis theorem* is applied to obtain the rate function. Example results are shown for a simple binomial distributed variable and the largest connected component in Erdös-Rényi random graphs.

[1] H. Touchette, Phys. Rep. **478**, 1-69 (2012)
[2] A. K. Hartmann, Eur. Phys. J. Special Topics **226**,567-579 (2017)
[3] E. Hidalgo, JSTAT **2018**, 083211 (2018)
[4] A. K. Hartmann, Phys. Rev. E **89**, 052103 (2014)

DY 41.11 Thu 12:15 BH-N 128

Calculation of second virial coefficients of convex bodies in *D*-dimensional Euclidean spaces via Brunn-Minkowski theory — •Markus Kulossa and Joachim Wagner — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

The virial series expands the compressibility factor of imperfect gases in a power series of the particle number density ϱ, where the virial coefficient of order i accounts for the contribution of interactions in an i-particle cluster to the non-ideal behavior. In the low-density limit, the second virial coefficient is the leading contribution to the departure from ideal gas behavior. For hard particles, the second virial coefficient is the orientationally-averaged mutual excluded volume per particle which is within the Brunn-Minkowski theory analytically accessible via quermassintegrals.

In this talk we present analytical formulations for the second virial coefficient of hard, convex bodies in D-dimensional Euclidean spaces $\mathbb{R}^D$ with emphasis on so far unknown expressions for second virial coefficients of uni-axial solids of revolution in $\mathbb{R}^4$. In addition to the effect of the aspect ratio, the detailed influence of the particle shape is analyzed. The effect of the dimensionality D is shown by comparing virial coefficients of 4D objects with their sections in lower-dimensional spaces.

DY 41.12 Thu 12:30 BH-N 128

Dimensional Phase Transitions in Quantum Gases — •Philipp Schöneberg[1], Hans-Otto Carmesin[1,2,3], Phil Immanuel Gustke[1], and Jannes Ruder[1] — [1]Gymnasium Athenaeum, Harsefelder Straße 40, 21680 Stade — [2]Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — [3]Universität Bremen, Fachbereich 1, Postfach 330440, 28334 Bremen

In the early universe, there occurred a rapid increase of distances usually called 'cosmic inflation'.

We model the objects in the early universe by a quantum gas. We show that there occurred dimensional phase transitions at high density in the early universe. We derive the critical densities. With it we explain the rapid increase of distances usually called 'cosmic inflation'.

Literature: Carmesin, H.-O. (2023): Geometrical and Exact Unification of Spacetime, Gravity and Quanta, Berlin: Verlag Dr. Köster.

DY 42: Focus Session: Computing with Dynamical Systems: New Perspectives on Reservoirs and Applications I – Fundamentals

Reservoir Computing uses the dynamic response of driven dynamical systems to predict and analyze temporal signals. The best-known example is the Echo State Networks proposed by H. Jaeger in 2001, where the reservoir consists of a recurrent neural network. However, in recent years, other realizations have been proposed, in particular those in which the reservoir system can be implemented in hardware in a fast and energy-efficient manner (e.g., using optical components). Other recent developments concern the specific incorporation of prior (physical) knowledge about the source of the input signal (physics aware/informed Reservoir Computing) as well as various application examples in different disciplines. Therefore, the goal of this focus session is to highlight the rapidly advancing current developments in the field of Reservoir Computing in order to enable a direct scientific exchange between new methodological approaches and innovative applications.

Organized by Ulrich Parlitz (Göttingen), Kathy Lüdge (Ilmenau), and Christoph Räth (München)

Time: Thursday 9:30–12:15 Location: BH-N 243

Invited Talk DY 42.1 Thu 9:30 BH-N 243

Is predicting chaos and extreme dynamics possible? An overview of (some) scientific machine learning approaches — •Luca Magri — Imperial College London, London, United Kingdom

The ability of modelling reality to predict the evolution of complex systems is enabled by principles and empirical approaches. Physical principles, for example conservation laws, are extrapolative (until the assumptions upon which they hinge break down): they provide predictions on phenomena that have not been observed. Human beings are excellent at extrapolating knowledge because we are excellent at finding physical principles. On the other hand, empirical modelling provides correlation functions within data, which are useful when principles are difficult to deduce. Artificial intelligence and machine learning are excellent at empirical modelling. In this talk, the complementary capabilities of both approaches will be merged (scientific machine learning). The approaches will achieve real-time modelling and optimization of nonlinear, unsteady and uncertain dynamical systems with chaotic and turbulent dynamics, which exhibit extreme events. The focus of the talk is on computational methodologies for modelling and optimization of chaotic flows with data-driven strategies that involve reservoir computing. I will conclude the talk with some lessons that we have learnt, and a discussion on future directions including quantum reservoir computing.

DY 42.2 Thu 10:00 BH-N 243

Harnessing multistability: Expanding the capabilities of reservoir computers via multifunctionality — •Andrew Flynn[1], Vassilios Tsachouridis[2], and Andreas Amann[1] — [1]School of Mathematical Sciences, University College Cork, Cork, IrelandIreland — [2]Collins Aerospace Applied Research & Technology, Cork, Ireland

Multifunctionality describes a neural network's ability to harness multistability in order to perform various tasks without altering its network properties. In this talk we demonstrate the advantages of extending multifunctionality to the domain of artificial neural networks (ANNs). Multifunctionality unlocks several new machine learning application for ANNs such as: data-driven modelling of multistability, generating chaotic itinerancy, novel memory recall techniques, and reconstructing transitions present in the epileptic brain. We outline how multifunctionality has so far been realised in an artificial setting with a reservoir computer (RC), a dynamical system in the form of an ANN. We employ generalised synchronisation to describe how to train a RC to

achieve multifunctionality and also explore some of the challenges involved in realising multifunctionality. Our results not only illuminate the exotic dynamics and exciting applications of multifunctional RCs but also highlight the importance of a dynamics-driven approach when training ANNs to display a broader level of intelligence by performing multiple tasks without compromising on explainability.

DY 42.3 Thu 10:15 BH-N 243

Generation of persistent memory using stable chaos in random neural networks — •Hiromichi Suetani — Faculty of Science and Technology, Oita University, Oita, Japan — International Research Center for Neurointelligence, The University of Tokyo, Tokyo, Japan

In high-dimensional nonlinear dynamical systems, it is well established that even when fixed points or (quasi) periodic orbits serve as stable attractors, the system often undergoes prolonged irregular transient states before settling into the attractor. This phenomenon is known as super transient chaos. Particularly within coupled dynamical systems comprising elements characterized by strong nonlinearities such as discontinuous changes, they may display unstable transient states concerning finite perturbations, despite their linear stability to infinitely small perturbations. This phenomenon is termed stable chaos.

In this study, we explore a version of random neural networks. We begin by quantifying trajectory instability using the finite-size Lyapunov exponent (FSLE) and presenting the corresponding phase diagram. Our findings confirm the presence of stable chaos in the critical region between periodic attractors and super-transient chaos. Additionally, introducing external input shows that stable chaos achieves generalized synchronization at a lower amplitude than super-transient chaos. Employing the reservoir computing framework, we reveal the utility of stable chaos in information processing tasks such as the delayed classification of nonlinear signals.

DY 42.4 Thu 10:30 BH-N 243

Enhancing reservoir predictions of chaotic time series by incorporating delayed values of input and reservoir variables — •Luk Fleddermann[1,2] and Ulrich Parlitz[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Chaotic time series can be predicted using linear readouts of driven reservoir dynamics. In the applied case, typically only time series of incomplete measurements, i.e. partial observations of the dynamical state, are available. We compare the performance of reservoir computing for time series predictions with complete and partial system state knowledge. By combining delayed values of input and reservoir variables, we increase the mean time length of valid predictions for partial observations of the dynamical state.

15 min. break

DY 42.5 Thu 11:00 BH-N 243

Prediction of spatio-temporal chaos using parallel reservoir computing in combination with dimensionality reduction — Kai-Uwe Hollborn[1], Luk Fleddermann[1,2], •Gerrit Wellecke[1], and Ulrich Parlitz[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Reservoir computers can be used to predict time series of spatio-temporal chaotic systems. Using multiple reservoirs in parallel has shown improved performances for these predictions. Similarly, enhancements can be achieved by reducing the dimensionality of the input data. To utilise both options for better predictions, we combine parallel reservoirs with a dimensionality reduction of the input data by Fourier transformation or principal component analysis. The performance of this hybrid approach will be illustrated and evaluated for data generated by a one-dimensional Kuramoto-Sivashinsky equation and a two-dimensional Aliev-Panfilov model describing chaotic spiral wave dynamics.

DY 42.6 Thu 11:15 BH-N 243

High Dimensional Hybrid Reservoir Computing — •Tamon Nakano[1], Sebastian Baur[1], and Christoph Räth[1,2] — [1]Institutfür KI-Sicherheit, Deutsches Zentrum für Luft-und Raumfahrt, Sankt Augustin/Ulm, Germany — [2]Fakultät für Physik, Ludwig-Maximilians-Universität, Munich, Germany

Reservoir Computing (RC) is getting popularity as an alternative solution for complex dynamical systems, where physically derived models reach their limitation. RC is by default fully data-driven method and is expected to learn the underlying system in the dataset. However RC can't do so for a lack of data quantity, for example. The hybrid approach is now recognized as a powerful option for it. The idea is to combine a knowledge-based model as a support (e.g. an imperfect governing equation) to the fully data-driven method. This combination can be done at the input, output layer of RC or both of them (respectively called, input-, output-, full-hybrid). Some studies have been already done, for example, input- and full-hybrid by Pathak et al.(2018), output-hybrid by Doan et al.(2019). Duncan et al.(2023) compared the performance of the three approaches and showed the superiority of output-hybrid compared to the others. The prior studies above have developed the hybrid approach in lower dimensional problems (e.g. 3 dimension). In this work, we will extend the hybrid approach to higher dimensional systems. This will allow to treat highly nonlinear and time evolutionary systems with system knowledge, such as fluid dynamics simulations and time evolutionary phenomena captured in 2 dimensional images.

DY 42.7 Thu 11:30 BH-N 243

Exploiting the Brownian motion of quasi-particles for unconventional computing — •Alessandro Pignedoli, Björn Dörschel, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen

The Brownian motion of quasi-particles offer a natural way of exploring the configuration space of a system. By mapping computational problems into this phenomenon, an ensemble of these particles can effectively solve them in an energy-efficient manner [1]. In this regard, magnetic skyrmions, which are topologically stable magnetic whirls that have been shown to behave like interacting Brownian particles, are promising candidates [2]. In this work, we show that the natural stochastic movement of such quasi-particles, in a given environment, provides a tool to solve different optimisation problems [3,4]. This type of computation could open up a new paradigm of low-power, in-materio implementation of swarm intelligence algorithms.

[1] C. H. Bennett, Int. J. Theor. Phys. 21, 905 (1982); [2] J. Zázvorka, et al. Nat. Nanotechnol. 14, 658 (2019); [3] German Patent Application DE 10 2023 131 171, K. Everschor-Sitte, A. Pignedoli, B. Dörschel (2023); [4] German Patent Application DE 10 2023 131 706, K. Everschor-Sitte, A. Pignedoli, B. Dörschel (2023).

DY 42.8 Thu 11:45 BH-N 243

Designing Active Matter Systems for Reservoir Computing — •Mario U. Gaimann and Miriam Klopotek — Stuttgart Center for Simulation Science (SimTech), Cluster of Excellence EXC 2075, University of Stuttgart, Germany

Reservoir computing with physical systems is a candidate for next-generation computing [1,2]. It is a powerful method to solve challenging tasks such as chaotic time-series prediction. However, tuning an arbitrary reservoir – which may be *physical* – for optimal properties like its dynamical regime remains an open question. To approach this problem we use a novel flavour of reservoir commuting based on simple active matter models [3]. We systematically study how the predictive performance of our driven active matter reservoir depends on a variety of physical hyper-parameters – the number of agents, the extent of driver-reservoir interaction, as well as different noise types and forces. For each set, we characterize the spatio-temporal, heterogeneous, yet also collective dynamics of the swarm. We aim to understand optimal conditions for learning and inspire new forms of physical, natural, and bio-inspired computing.

[1] Tanaka, G. *et al.* (2019), *Neural Networks* **115**, 100-123.
[2] Nakajima, K. and Fischer, I. (2021). *Reservoir Computing.* Springer Singapore.
[3] Lymburn, T. *et al.* (2021), *Chaos* **31(3)**, 033121.

DY 42.9 Thu 12:00 BH-N 243

Contextual Alignment for Robust Learning in Dynamical Systems — •Max Weinmann[1,2] and Miriam Klopotek[1] — [1]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [2]University of Stuttgart, Interchange Forum for Reflecting on Intelligent Systems, IRIS3D, Stuttgart, Germany

Dynamical systems have exhibited remarkable computational prowess, particularly in prediction tasks like reservoir computing [1]. Achieving efficient computational offloading to the reservoir demands precise alignment of system dynamics with computational requisites. This entails parameter tuning and input transformation to facilitate a natural representation within the system. While the significance of dynamical diversity and system memory is evident, tailoring systems for specific tasks remains challenging [2]; context plays a key role. Our study investigates cellular automaton and other complex model systems. We explore probabilistic and deterministic perturbations to alter system dynamics, offering contextual cues that optimize task-specific information processing capabilities. Our focus extends to identifying fundamental properties enabling a predictable, adaptable alignment, akin to a learning process, fostering robust model creation.

[1] Maass, W., Natschläger, T., and Markram, H. (2002). Real-time computing without stable states: A new framework for neural computation based on perturbations. Neural computation, 14(11), 2531-2560.
[2] Stepney, S. (2012). Nonclassical Computation-A Dynamical Systems Perspective. Handbook of natural computing, 2.

DY 43: Active Matter IV (joint session DY/BP/CPP)

Time: Thursday 9:30–13:00 Location: BH-N 334

Invited Talk DY 43.1 Thu 9:30 BH-N 334

Flocking by turning away — •Ricard Alert — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Flocking, as paradigmatically exemplified by birds, is the coherent collective motion of active agents. As originally conceived, flocking emerges through alignment interactions between the agents. Here, I will show a new mechanism of flocking based on interactions that reorient agents away from each other. Combining simulations, kinetic theory, and experiments, we demonstrate this mechanism of flocking in self-propelled Janus colloids with stronger repulsion on the front than on the rear. We show that, unlike for alignment interactions, the emergence of polar order from turn-away interactions requires particle repulsion. The polar flocking state is stable because particles achieve a compromise between turning away from left and right neighbors. These findings could help to reconcile the observations that cells can flock despite turning away from each other via contact inhibition of locomotion. Overall, our work shows that flocking is a very robust behavior that arises even when the orientational interactions seem to prevent it.

DY 43.2 Thu 10:00 BH-N 334

Metastability of ordered phase in discretized flocking — •Swarnajit Chatterjee[1], Mintu Karmakar[2], Matthieu Mangeat[1], Raja Paul[2], and Heiko Rieger[1] — [1]Center for Biophysics & Department for Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany. — [2]School of Mathematical & Computational Sciences, IACS, Kolkata – 700032, India.

Polar flocks are observed in a large class of active matter systems and have been considered robust to fluctuations. However, recent studies have argued that liquid polar flocks are metastable to the presence of small obstacles [1] or to the nucleation of opposite-phase droplets [2]. In this work, we study the stability of the ordered phase in flocking models with q-fold symmetry under the influence of counter- or transversely-propagating droplets. We observe that the liquid phase is more susceptible to a transversely-propagating droplet than a counter-propagating droplet. Also, for droplet counter-propagation, system morphology is dominated by a novel *"sandwich state"* of the liquid state and the droplet state rather than a reversal of the liquid phase. Here spatial anisotropy plays a crucial role. Metastability of the liquid phase in a discretized Vicsek model shows a strong dependency on the noise strength where the anisotropy parameter q does not significantly affect the reversal dynamics. Our study further investigates the influence of droplet size, density, and other control parameters on liquid stability.

[1] Codina et al., PRL 128, 218001 (2022).
[2] Benvegnen et al., arXiv:2306.01156 (2023).

DY 43.3 Thu 10:15 BH-N 334

Emergent Metric-like States of Active Particles with Metric-free Polar Alignment — Yinong Zhao[1], Cristian L. Huepe[2], and •Pawel Romanczuk[3,4] — [1]Shanghai Jiao Tong University, Shanghai, PR China — [2]Northwestern University, Chicago, USA — [3]Department of Biology, Humboldt Universität zu Berlin, Germany — [4]Excellence cluster "Science of Intelligence", Berlin

We study a model of self-propelled particles interacting with their k-nearest neighbors through polar alignment. By exploring its phase space as a function of two nondimensional parameters (scaled alignment strength g and Peclet number Pe), we identify two distinct order-disorder transitions. One appears to be continuous, occurs at a low critical g value independent of Pe, and resembles a mean-field transition with no density-order coupling. The other is discontinuous, depends on a combined control parameter involving g and Pe, and results from the formation of small, dense, highly persistent clusters of particles that follow metric-like dynamics. These dense clusters form at a critical value of the combined control parameter Pe/g^{α} , with $\alpha \approx 1.5$, which appears to be valid for different alignment-based models. Our study shows that models of active particles with metric-free interactions can produce characteristic length-scales and self-organize into metric-like collective states that undergo metric-like transitions.

DY 43.4 Thu 10:30 BH-N 334

Strong Casimir-like Forces in Flocking Active Matter — •Giuseppe Fava[1,2], Andrea Gambassi[3], and Francesco Ginelli[1,2] — [1]Dipartimento di Scienza e Alta Tecnologia and Center for Nonlinear and Complex Systems, Università degli Studi dell'Insubria, Como, Italy — [2]INFN sezione di Milano, Milano, Italy — [3]SISSA International School for Advanced Studies and INFN, via Bonomea 265, 34136 Trieste, Italy

Confining in space the equilibrium fluctuations of statistical systems with long-range correlations is known to result into effective forces on the boundaries.

In this work we demonstrate the occurrence of Casimir-like forces in the non-equilibrium context provided by flocking active matter. In particular, we consider a system of aligning self-propelled particles in two spatial dimensions, which are transversally confined by reflecting or partially reflecting walls. We show that in the ordered flocking phase this confined active vectorial fluid is characterized by extensive boundary layers, as opposed to the finite ones usually observed in confined scalar active matter. A finite-size, fluctuation-induced contribution to the pressure on the wall emerges, which decays slowly and algebraically upon increasing the distance between the walls.

We explain our findings which display a certain degree of universality within a hydrodynamic description of the density and velocity fields.

Ref: "Strong Casimir-like Forces in Flocking Active Matter", arXiv:2211.02644

DY 43.5 Thu 10:45 BH-N 334

Collective Dynamics in Dense Systems of Active Polar Disks — •yating zheng[1,2], weizhen tang[3], amir shee[4], pawel romanczuk[1,2], and cristian huepe[4] — [1]Humboldt-Universität zu Berlin — [2]Research Cluster of Excellence 'Science of Intelligence' — [3]Beijing Normal University — [4]Northwestern University

We study a general model of a dense system of active polar disks with repulsive linear interactions, confined by a circular boundary. Each disk advances with a preferred self-propulsion speed and changes heading by turning around an axis of rotation located at a distance R behind its barycenter. We characterize the emerging phases and collective states as a function of R, density, and noise, for disks with isotropic and anisotropic damping disks, and a smooth or rough boundary. We find a rich phase space that combines transitions from solid to fluid states with novel R-dependent transitions from a collective state displaying localized disk rotation to a milling state around a common centre of rotation. These transitions are related to the formation of vortices that follow simple or complex dynamics depending on the boundary properties and system size. Our results demonstrate generic collective states that are expected to be observed in experimental dense systems of natural or artificial active agents in confined spaces.

DY 43.6 Thu 11:00 BH-N 334

Cooperative resetting exhibits a delocalisation phase transition — •Felix J. Meigel and Steffen Rulands — Arnold Sommerfeld Center for Theoretical Physics, Department of Physics, Ludwig-Maximilians-Universität, München, Germany

In the realm of biology, many non-equilibrium systems are inherently noisy, while their proper functioning relies on the adept control of fluctuations. Stochastic resetting processes, where the state of a system is reset to its initial condition at random times, provide a framework for the control of the accumulation of fluctuations over time. Yet, in this framework, resetting is externally imposed. Here, we demonstrate that a constraint of fluctuations can also be achieved in a self-organized manner by cooperative resetting in many-particle systems. Specifically, we demonstrate that many-particle systems, wherein pairs of particles are reset to their respective average positions, exhibit a second-order phase transition as a function of the resetting rate. This transition delineates a regime where particles localize, thereby controlling fluctuations, and another regime where particle positions become unbounded. Our research showcases that cooperative resetting enables adaptation to external perturbations and enhances the optimization of search tasks compared to extrinsic resetting. We showcase the versatility of self-organized fluctuation control through cooperative resetting, with applications ranging from biological systems, such as intracellular vesicle dynamics and the fitness advantages of genetic recombination, to technical domains like the optimization of shared mobility services.

15 min. break

Invited Talk DY 43.7 Thu 11:30 BH-N 334

Growth and division as drivers of complex dynamics in dense cellular matter — •Philip Bittihn — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Cells in systems such as tissues, bacterial aggregates, embryonic development or tumors self-organize on large scales to fulfil their biological functions. Many such collective behaviors have been studied in the broader context of active matter, where they emerge from the intrinsic non-equilibrium activity of the constituent particles. Growth and division as drivers of activity have received less attention, although they are defining features of life and often play indispensable roles.

Here, I will describe some of our recent theoretical efforts in characterizing their effects in dense cellular matter. Using minimal models of mechanically interacting particles, we investigate scenarios in which growth and division either lead to large-scale flows and volume expansion or total volume is conserved. By developing statistical descriptions suited for non-conserved particle numbers, we find that certain components of particle motion follow simple scaling laws that can be related to macroscopic flows or to classical active particle models. Other features of the dynamics reveal new phenomena and transitions due to growth-induced pressure, confinement and anisotropic particle shapes. If time permits, I will outline interactions with motility or chemical activity. Overall, our results aim to establish universal physical principles as a baseline for experimental observations and provide design strategies for bio(technological) applications or artificial systems.

DY 43.8 Thu 12:00 BH-N 334

Motility-induced clustering of active particles under soft confinement — •Timo Knippenberg[1], Ashreya Jayaram[2], Thomas Speck[2], and Clemens Bechinger[1] — [1]FB Physik, Universität Konstanz, Deutschand — [2]Institute for theoretical physics IV, Universität Stuttgart, Deutschland

In the field of active matter, motility-induced phase separation (MIPS) is one of the most widely studied subjects. This phenomenon, characterized by a phase transition from a homogeneous phase into a densely clustered state with a gaseous surrounding, occurs at sufficiently high density and active particle (AP) velocity. However, most of these studies focus on APs in bulk or near hard walls, while research on APs in soft confinement is scarce. The latter promises insights into the dimensionality-dependent aspects of MIPS, as gradually increasing the confinement strength provides a way to approach the 1-dimensional limit, where MIPS is known to be absent.

To address this topic, here we experimentally investigate the structural and dynamical properties of APs confined in a soft annulus-shaped channel. Depending on the strength of the confinement and the AP velocity, we observe a novel re-entrant phase behavior. We can explain our measurements by the strong coupling between velocity and the effective confining dimensionality in such soft systems.

In addition to highlighting the important influence of soft boundaries on APs, our research has implications for future applications in micro-robotics.

DY 43.9 Thu 12:15 BH-N 334

Emergent memory from tapping collisions in active granular matter — •Lorenzo Caprini, Anton Ldov, René Wittmann, Christian Scholz, and Hartmut Löwen — Heinrich-Heine University of Düsseldorf

In an equilibrium thermal environment, random elastic collisions between the background particles and a tracer establish the picture of Brownian motion fulfilling the Einstein relation between diffusivity and mobility. In nature, environments often comprise collections of autonomously moving objects, termed active matter, which exhibit fascinating phenomena. We investigate experimentally the impact of an active environment on a passive tracer by using active granular particles, i.e. vibrationally excited inertial self-propelled units termed vibrobots. They display multiple correlated tapping collisions with the tracer, by bouncing and sliding on its surface. As a consequence, the tracer displays a persistent memory and is described by a generalized active Einstein relation that constrains fluctuations, dissipation, and effective activity due to the tracer memory. Since the resulting persistence can be tuned by the environmental density and motility, our findings can be useful for engineering properties of various active systems in biomedical applications and swarm robotics.

DY 43.10 Thu 12:30 BH-N 334

Stationary particle currents in sedimenting active matter wetting a wall — •Matthieu Mangeat, Shauri Chakraborty, Adam Wysocki, and Heiko Rieger — Saarland University, Saarbrücken, Germany

Recently it was predicted, on the basis of a lattice gas model, that scalar active matter would rise against gravity up a confining wall in spite of repulsive particle-wall interactions [PRL 124, 048001 (2020)]. We confirm this prediction with sedimenting active Brownian particles (ABPs) in a box and elucidate the mechanism leading to the formation of a meniscus rising above the bulk of the sedimentation region. The height of the meniscus increases algebraically with the activity, and the formation of the meniscus is determined by a stationary circular particle current centered at the base of the meniscus. The origin of these vortices can be traced back to the confinement of the ABPs in a box: already the stationary state of non-interacting ABPs without gravitation displays highly symmetric circular currents. Gravitation distorts this vortex configuration downward, leaving two major vortices at the two side walls, with a strong downward flow along the walls. Repulsive interactions between the ABPs change this situation only as soon as motility induced phase separation (MIPS) sets in and forms a dense, sedimented liquid region at the bottom, which pushes the center of the vortex upwards towards the liquid-gas interface. Self-propelled particles therefore represent an impressive realization of scalar active matter that forms stationary particle currents being able to perform visible work against gravity, which we predict to be observable experimentally.

DY 43.11 Thu 12:45 BH-N 334

Velocity-density scaling for active particles in an external field — •Colin-Marius Koch and Michael Wilczek — Theoretical Physics I, University of Bayreuth, Germany

Active particles in external fields can show diverse aggregation phenomena. The emerging collective phenomena and their statistics can thereby depend on microscopic details of active constituents' interactions. Here, we investigate how different steric interactions and self-propulsion mechanisms affect the aggregation of active particles in an external field. While density and velocity profiles individually differ between the studied cases, they consistently scale inversely with each other, when the instantaneous velocity projected onto the particle orientation is considered. The observed velocity-density scaling is robust for relatively dilute systems in which no strong aggregation, i.e. motility-induced phase separation, is present. We conclude that different microscopic details can result in the same statistics of collective behaviour in systems that are dilute enough.

DY 44: Focus Session: Wetting on Adaptive Substrates II (joint session CPP/DY/O)

The focus session aims to discuss recent developments in the wetting dynamics of adaptive, deformable, and switchable surfaces.

Time: Thursday 11:30–13:00 Location: H 0107

Invited Talk DY 44.1 Thu 11:30 H 0107

A multi-scale approach to characterize wetting within a porous medium — •Maja Rücker[1], Ryan T. Armstrong[2], Chenhao Sun[3], Peyman Mostaghimi[2], Steffen Berg[4,5], Paul Luckham[5], Apostolos Georgiadis[4,5], and James E. McClure[6] — [1]Eindhoven University of Technology, Eindhoven, NL — [2]University of New South Wales, Sydney, Australia — [3]China University of Petroleum, Beijing, China — [4]Shell Global Solutions International B.V., Amsterdam, NL — [5]Imperial College London, London, UK — [6]Virginia Tech, Arlington, VA, USA

Considering a porous medium with two fluids in it, the fluid flow and distribution will depend on the wetting characteristic of the system. Recent developments in imaging techniques, such as micro-computed tomography and atomic force microscopy, alongside advances in computational modelling allowed for new concepts linking macroscopic wetting responses to the fundamental microscopic wetting definitions to emerge. We present an approach to upscale wetting parameters building upon energetic and geometric considerations and accounting for the various mechanisms related to wetting, manifesting at those different length scales. Starting from fluid-solid interactions, through the motion of three-phase contact lines to the evolution of fluid configurations in the porous medium, we show experimental observation on a coherent set of fluid/fluid/solid systems and discuss those in relation to the proposed upscaling concept. We will highlight the remaining questions for the characterization of wetting in the context of multiphase flow in porous media and point out future research directions.

DY 44.2 Thu 12:00 H 0107

Soft Wetting Transition — •Christopher Henkel[1], Vincent Bertin[2], Jacco H. Snoeijer[2], and Uwe Thiele[1,3] — [1]Institut für Theoretische Physik, Universität Münster, Germany — [2]Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, The Netherlands — [3]Center for Nonlinear Science (CeNoS), Universität Münster, Germany

We investigate the forced receding dynamics of a three-phase contact line on a viscoelastic substrate. Thereby, we use the Landau-Levich (or dip-coating) geometry, where a solid viscoelastic plate is dragged out of a liquid bath. We employ a mesoscopic hydrodynamic model in long-wave approximation, i.e. valid at small contact angle and plate inclination. The elastic response of the substrate follows the Winkler foundation with a Kelvin-Voigt relaxation. In particular, we investigate how the shape and stability of the meniscus change with the plate velocity and the viscoelastic substrate properties. Finally we compare numeric results with asymptotic analytic calculations.

DY 44.3 Thu 12:15 H 0107

Demixing around liquid droplets — •Khalil Remini and Ralf Seemann — Experimental Physics, Saarland University, Saarbrücken, Germany

Equilibrium polystyrene droplets are explored sitting on soft solid substrates. The soft solid substrates consist of commercial polydimethylsiloxane (PDMS) elastomer kits with elastic module varying across several orders of magnitude (3-1200 kPa). Inspecting the there-phase contact line of the droplets on a nanoscopic length scale by atomic force microscopy, i.e. on a length scale well below the elasto-capillary length, where capillary forces are higher than the elastic force of the substrate, we find that the ridge formed by the elastic substrate around the droplet is similar to that of a liquid. Material contrasts confirm a liquid ring surrounding the droplets at the three-phase contact line, as a result from stress induced demixing of non-crosslinked PDMS molecules from the PDMS elastomer matrix. This liquid ring extends for softer PDMS elastomers having a larger content of non-crosslinked molecules, but it is present also for the stiffer elastomers. So, the Neumann construction at the three-phase contact line is valid for all tested PDMS elastomers when measuring locally with sufficient resolution.

DY 44.4 Thu 12:30 H 0107

Chemical reactions confined in liquid films: dynamics and stability — •Tilman Richter[1], Paolo Malgaretti[1], Thomas M. Koller[2], and Jens Harting[1] — [1]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien (IEK-11), Cauerstr. 1, 91058 Erlangen, Germany — [2]Institute of Advanced Optical Technologies - Thermophysical Properties (AOT-TP), Department of Chemical and Biological Engineering (CBI) and Erlangen Graduate School in Advanced Optical Technologies (SAOT), Friedrich-Alexander-Universit Erlangen-Nuernberg (FAU), Paul-Gordan-Straße 8, 91052 Erlangen, Germany

In catalytic reactions occurring within small liquid droplets or thin liquid films, the yield significantly differs from that in bulk reactions. This variance is primarily due to the fluid interface's substantial surface-to-volume ratio. The fluid interface initiates several phenomena, such as increased surface diffusion, Marangoni flows, and more effective surface interactions, which can boost yield substantially. We develop a theoretical model that demonstrates that the uneven distribution of reactants and products, caused by chemical reactions, can induce Marangoni flows. These flows then alter the spatial distribution of the catalyst. This complex interaction offers novel methods for either inhibiting or promoting the rupture of thin films, as well as for modifying the shape of small droplets.

DY 44.5 Thu 12:45 H 0107

Dynamic vesicles on adaptive surfaces — •Lucia Wesenberg, Ben Rasmus Sprötge, Kai-Uwe Hollborn, and Marcus Müller — Institut für theoretische Physik, Georg-August-Universität Göttingen

Vesicles on substrates play a fundamental role in numerous biological transport processes, such as the neurotransmitter release at the synapse, transport vesicles in cells, or the nutrient intake of trees by large vesicles. For all of these processes the adaptive adhesion of the vesicles to a biological substrate is crucial. Furthermore, it is interesting to compare how these adaptive processes differ from wetting of liquid droplets as their shapes seem similar, however, one is governed by bending rigidity and the other by tension.

Here, we study the equilibrium shapes of vesicles as well as their dynamic adaptation to a changing substrate. Our simulations show the significant impact of buoyancy on the vesicle shape, especially in the contact zone. We are able to construct an adsorption diagram summarizing the metastable region of upward buoyant adsorbed vesicles. Further, we study permeable vesicles, adapting dynamically to substrates with a constant adhesion potential with periodically modulated strength or a steplike potential with a given velocity. A step in the potential allows the steering of vesicles, while periodic switching enables controlled vesicle substrate contact. Thus, both cases prove to be an effective control mechanism for biological transport of vesicles.

DY 45: Wetting, Fluidics and Liquids at Interfaces and Surfaces (joint session CPP/DY)

Time: Thursday 15:00–17:30 Location: H 0107

DY 45.1 Thu 15:00 H 0107

Dynamic wetting of concentrated granular suspensions — •Reza Azizmalayeri, Peyman Rostami, and Günter K. Auernhammer — Leibniz-Institut für Polymerforschung, Dresden, Germany

Concentrated granular suspensions are employed in a variety of applications in which the contact line dynamics and internal structure of the suspension interact. The process can be characterized using individual particle analysis and average suspension descriptions. There is a markedly high shear rate at the droplet's contact line. This localized shear rate profoundly affects the suspension's non-Newtonian rheological behaviour. Recent researches have affirmed the applicability of hydrodynamic solutions like Cox-Voinov relation to granular suspensions. Despite these efforts, the impact of particles on the overall flow field and microstructure of densely packed granular systems along the contact line remains unexplored. In this study, a configuration consisting of a pinned droplet on a moving substrate is utilized. Using astigmatism particle tracking velocimetry (APTV), we precisely track the 3D motion of tracer particles within the suspension. Near the advancing contact line, we observe distinct behaviours based on the interaction between particles. A concentrated suspension of low interacting particles violates the Cox-Voinov relationship with particle friction becoming a significant factor. Meanwhile, when strong particle interactions are present the suspension exhibits a yield stress behaviour. The receding contact line exhibits a dynamic curvature that undergoes a transient phase before reaching a stationary state. The results of this study are supported by rheology measurements.

DY 45.2 Thu 15:15 H 0107

How rheology influences the wetting behavior of droplets — •Günter K. Auernhammer[1], Peyman Rostami[1], Reza Azizmalayeri[1], Valentine Comoy[1], and Mathis Fricke[2] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Department of Mathematics, TU Darmstadt, Germany

We study the spreading of viscous and viscoelastic drops on solid substrates with different wettability. In the early stages of spreading, we find that the viscoelastic drop spreads with faster and a different power law than the Newtonian drop (i.e. aqueous glycerine solution) for the same zero shear rate viscosity. We argue that the effect of viscoelasticity is only observable for experimental time scales in the order of the internal relaxation time of the polymer solution or longer times. Near the contact line, the effective viscosity is lower for the viscoelastic drop than for the Newtonian drop. Together with its shear rate dependency, this difference in effective viscosity can explain the different spreading dynamics. We support our experimental findings with a simple perturbation model that qualitatively agrees with our findings. [https://arxiv.org/abs/2308.14515]

DY 45.3 Thu 15:30 H 0107

Surface Sensitive Fractioning of Microparticles and Microplastics — •Marek Bekir — Institut für Physik und Astronomie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm

Separation of particles of equal size but different surface energies is nowadays a challenging task. With local-light driven diffusioosmosis (local-LDDO) [1] in combination with microfluidic technology [2] we provide a potential tool for separation of such microparticles and microplastics. The local-LDDO is a phenomenon of a photosensitive azobenzene containing surfactant, where under illumination a dynamic exchange of isomers provides a repulsive flow strong enough to elevate particles up to several micrometers from the liquid-glass interface of the microfluidic chamber. In combination of a superimposed lamellar fluid flow the elevation leads to a stronger passive motion along the streamline. We demonstrate that the lift off depends on the size but also on the surface morphology, surface material and surface coating, too, i.e. differently surface modified particles therefore a different motion velocity.[3]

[1] Feldmann, D.; Arya, P.; Molotilin, TY.; Lomadze, N.; Kopyshev, A.; Vinogradova, OI.; Santer, S. Langmuir 2020, 36, 6994-7004.

[2] Sajeesh, P.; Kumar Sen, A. Microfluid Nanofluid 2014, 17, 1-52.

[3] Bekir, M.; Sperling, M.; Vasquez Muñoz, D., Braksch, C.; Böker, A.; Lomadze, N.; Popescu, M. N., Santer, S. Advanced Materials 2023, 35, 2300358.

DY 45.4 Thu 15:45 H 0107

Curvature-dependent adsorption of surfactants in water nanodroplets: Insights from molecular dynamics — •Fabio Staniscia and Matej Kanduč — Department of Theoretical Physics, Jožef Stefan Institute, Ljubljana SI-1000, Slovenia

Adsorption of surfactants at curved air-water interfaces plays a major role in phenomena involving nanodroplets, such as emulsification, wetting, heterogeneous catalysis, and aerosol chemistry. Once the nanodroplet becomes small enough, its large curvature can influence the adsorption of surfactants, which has not been thoroughly investigated. At this scope we investigate the adsorption of short-chain surfactants inside water nanodroplets using molecular dynamics simulations. We show that the curvature of the droplet interface enhances adsorption and affects other interfacial properties, such as the preferred surfactant orientation. We relate this behavior to curvature-dependent surface tension of water, described by the Tolman length correction. We show that the influence of curvature on adsorption grows exponentially with the size of the hydrophobic tail of the surfactant. Finally, we use our theoretical model to predict the behavior of larger surfactants and of larger droplets.

DY 45.5 Thu 16:00 H 0107

Interfacial versus confinement effects in the frequency dependent dielectric response of nanoconfined water — •Maximilian Becker and Roland R. Netz — Freie Universität Berlin, Berlin, Germany

We investigate the frequency-dependent dielectric response of water confined between two graphene sheets with force-field and density-functional-theory based molecular dynamics simulations. We highlight the critical role of the volume over which the dielectric response is averaged when measuring the dielectric susceptibility and introduce a system-size-independent decomposition, allowing us to discern interfacial and confinement contributions to the overall dielectric spectrum. Using this, we discuss the molecular origin of the main absorption features of nanoconfined water from the GHz to the THz regime: While intermolecular orientational correlations govern the interfacial and confinement effects on the 30 GHz Debye peak and the static dielectric constant, the 20 THz librational peak undergoes intensity changes which can be attributed to a change in single-molecule motion. When going from bulk to confinement, DFT-MD simulations reveal the emergence of a broad spectroscopic band arising between 1 and 30 THz, a region which is known to probe the dynamics of hydrogen bonds in water. These results are interpreted in the context of the hydrogen bond network at the water-graphene interface and in two-dimensional water layers which sheds light on the intricate behavior of water molecules within confined environments and contributes to a deeper understanding of their dielectric properties.

30 min. break

DY 45.6 Thu 16:45 H 0107

Improved displacement efficiency in Ganglia size distribution by invasion of complex fluids — Karthik Nuthalapati[1] and •Ralf Seemann[2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Universität des Saarlandes, Saarbrücken, Germany

It is well-known that the viscoelastic nature of polymer solutions affects the displacement process when used as displacing fluids, for example, in enhanced oil recovery. Nevertheless, the microscopic displacement efficiency within porous media remains elusive. In this study, we experimentally investigated the impact of polymer viscosity and elasticity on the displacement efficiency of silicone oils with different viscosities. As displacing fluids, we explored four types of complex fluids, including a highly viscous Newtonian fluid, a shear-thinning solution with negligible elasticity, an elastic polymer with constant viscosity, and a viscoelastic polymer solution made from a polyelectrolyte within the Ganglia size distribution. As a result, viscoelastic polymers demonstrated improved displacement efficiency in Ganglia size distribution through the invasion of complex fluids.

DY 45.7 Thu 17:00 H 0107

The Structure of Water Under Confinement in Periodic Mesoporous Organosilicas Investigated by X-Ray Scatter-

ing — •Niels Christian Giesselmann[1], Philip Lenz[2,3], Sophia-Marie Meinert[2], Tamás Simon[2], Wonhyuk Jo[1,4], Nele Naomi Striker[1], Michael Fröba[2,3], and Felix Lehmkühler[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]University of Hamburg, Institute of Inorganic and Applied Chemistry, Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [4]European XFEL, Schenefeld, Germany

The effect of pore wall chemistry and pore diameter on the structure of confined water was studied by X-ray scattering on water confined in periodic mesoporous organosilicas (PMOs). A shift in the first structure factor peak at $q \approx 1.8$ Å^{-1} reveals a variation in the density of the confined water in dependence of hydrophilicity and pore size. Smaller and more hydrophilic pores induce a lower density in the water. In contrast to bulk water, the pair distribution functions (PDFs) of confined water show a splitting of the second-neighbour peak into either two, in the case of smaller and more hydrophilic pores, or three separate peaks, in larger and more hydrophobic pores. From the running coordination number we conclude that smaller and more hydrophilic confinement leads to a stronger developed tetrahedral network in confined water, while confinement in larger and hydrophobic pores give tetrahedral arrangements that are bulk-like or even less pronounced than in bulk water.

DY 45.8 Thu 17:15 H 0107

Unveiling the Role of Surface Hydrophobicity and Defects in Heterogeneous Cavitation by Atomistic Simulations — •Philip Loche[1,2], Matej Kanduč[3], Emanuel Schneck[4], and Roland R. Netz[2] — [1]EPFL, Lausanne, Switzerland — [2]FU Berlin — [3]Jožef Stefan Institute, Ljubljana, Slovenia — [4]TU Darmstadt, Darmstadt, Germany

The reduction of pressure in liquids can lead to vaporization and the formation of bubbles, a phenomenon known as cavitation. Cavitation is commonly observed in hydraulic machinery, ship propellers, and even within biological systems. Liquids can sustain enormous negative pressures until reaching their stability limits, at which point cavitation occurs. While classical nucleation theory well explains the energetics of these events, little is known about the dynamics of interfacial bubble formation.

We quantify the kinetics of heterogeneous cavitation using classical nucleation theory and atomistic simulations of self-assembled monolayers at various contact angles under a constant rate protocol. Our focus is on the impact of surface hydrophobicity and defects. We find that increased hydrophobicity leads to a predominance of heterogeneous cavitation at surfaces. Simulations reveal an exponential relationship between the contact angle and the kinetic prefactor, with heightened hydrophobicity significantly reducing this parameter. The balance pressure, where homogeneous and heterogeneous cavitation rates converge, indicates a critical contact angle for switching between these two effects under realistic pressures and volumes.

DY 46: Complex Fluids, Colloids, Micelles and Vesicles (joint session CPP/DY)

Time: Thursday 15:00–17:45 Location: H 0110

Invited Talk DY 46.1 Thu 15:00 H 0110

Colloids and the depletion interaction: multi-phase coexistence of colloidal mixtures — •Remco Tuinier — Laboratory of Physical Chemistry, Department of Chemical Engineering and Chemistry & Institute for Complex Molecular Systems, Eindhoven University of Technology, The Netherlands

Colloids are the building blocks of many natural (e.g., clay, milk, blood) and technological (e.g., paint, storage media, cosmetics, shaving foam) systems. The big question underlying related innovations is how can colloidal systems be formulated and designed towards the desired properties? To do this, the forces between the colloidal particles need to be controlled. Adding depletants (non-adsorbing polymers or small colloids) is key to controlling the attractive interactions [1]. This talk provides a detailed exploration of the phase behaviour of complex colloidal mixtures. While hard spheres can undergo a fluid-solid phase transition, anisotropic hard particles such as rods, cuboids, discs or boards exhibit a richer phase behaviour. The addition of depletants to anisotropic colloids gives rise to orientation-dependent attractions resulting in non-trivial phase behaviour. It is demonstrated that such mixtures exhibit a strikingly rich multi-phase coexistence behaviour [2].

[1] H.N.W. Lekkerkerker, R. Tuinier, M. Vis, Colloids and the Depletion Interaction, 2nd edition, Springer, 2024.

[2] J. Opdam, V.F.D. Peters, H.H. Wensink, R. Tuinier, J. Phys. Chem. Lett. 14 (2023) 199-206.

DY 46.2 Thu 15:30 H 0110

Light-induced manipulation of colloidal particles in a photosensitive polymer-dye system — •Anna López de Guereñu and Svetlana Santer — Room 2.025 University of Potsdam Physics and Astronomy Karl-Liebknecht-Str. 24-25 14476 Potsdam Germany

In this study, we explore the optical and physical properties of a photosensitive surfactant system consisting of mesoporous silica particles in an aqueous solution with a fluorescent dye and an azobenzene-containing surfactant. The latter undergoes reversible photo-isomerization from trans- to cis-configuration upon UV/blue light exposure on a picosecond timescale, offering precise control over particle aggregation. The formation of the dye/surfactant complex adds complexity to the system.

Light-driven diffusioosmosis (LDDO) facilitates remote colloid control, with mesoporous colloids acting as a source or sink for the surfactant, influencing mutual interactions between particles.

The surfactant's isomerization state determines its adsorption affinities, influencing particle interactions. The trans-isomer accumulates in pores and forms a complex with the dye, while the cis-isomer remains outside the pores. Upon irradiation, the cis-surfactant generates a diffusioosmotic flow, causing a repulsion of particles. Wavelength and intensity modulate this process, allowing to control these structures. The dye provides an additional dimension to the system, adding to its complexity due to its influence on the surfactant isomerization and the LDDO process.

DY 46.3 Thu 15:45 H 0110

Mesoporous silica colloids: surfactant cleaning, wetting and surface diffusion — •Antonio Stocco — Institut Charles Sadron, University of Strasbourg, CNRS, France

We have investigated the use of mesoporous silica colloids to remove cationic surfactants from water. Porous silica colloids diffuse at the surface of water and in the volume, interacting with cationic surfactants that can adsorb inside the pores of these particles. We observed that surfactant adsorption on mesoporous silica depends dramatically not only on the particle pore size but also on specific counterion effects. We measured striking differences both on a macroscopic property of the interface, i.e. surface tension, and also at a single particle level by evaluating the translational diffusion of partially wetted particles at the fluid interface.

DY 46.4 Thu 16:00 H 0110

Kinetics of phase separation inside complex random porous media — •Rounak Bhattacharyya[1,2] and Bhaskar Sen Gupta[1] — [1]Department of Physics, Vellore Institute of Technology, Vellore, Tamil Nadu, India 632014 — [2]Institute for Theoretical Physics and BioQuant, Heidelberg University, 69120 Heidelberg, Germany

The kinetics of phase separation of segregating fluid mixtures imbibed in porous media is an active field of research due to its great scientific interest and industrial applications. The subject is well understood in the case of ordered pores (e.g., cylindrical pore). But most of the real experimental porous systems are random in nature and are poorly understood. Experimental limitations come from the difficulties in probing the real space geometry using scattering experiments. Also, the theoretical and numerical studies are challenging because of the complex topology of the materials. At this meeting, we will present the findings of our study on the phase separation dynamics of segregating binary fluid mixtures inside random porous materials using large-scale molecular dynamics simulations. Different random porous structures are considered to understand the effect of pore morphology on the coarsening process. We find the existence of two different growth regimes and the crossover is related to the average diameter of random pores. The Porod law and Superuniversality hypothesis are

also examined. Finally, the non-equilibrium aging dynamics and the corresponding scaling laws will be discussed for such systems.

30 min. break

DY 46.5 Thu 16:45 H 0110

Screening Behavior of Nano-Ions in Aqueous Solutions — •Thomas Tilger and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Due to their special properties, which make them suitable for many applications, the interest in nano ions grew during the last years. They turned out to be promising new materials for e.g. wastewater treatment, separation of nuclear waste and to stabilize foams. Especially for the last application, it is crucial to understand how the interaction between nano ions and the interaction betweeen interfaces in the presence of nano ions can be described.

To directly measure the interaction between well-defined interfaces, colloidal probe atomic force microscopy (CP-AFM) has proven to be a powerful tool. As a model system for nano ions, we chose superchaotropic Keggin ions in aqueous solutions at different concentrations and investigated their influence on the interaction between colloidal silica beads.

It turned out that - despite their large size of approximately one nanometer - the interaction between the silica beads can still be described by the DLVO-theory of electrolyte solutions, consisting of a van der Waals attraction and an electrostatic double layer repulsion. However, the obtained screening lengths exhibit a significant deviation from the ones expected according to the nominal ionic strength of the solutions. The strength of this deviation increases with the concentration of the solutions and might be a hint for an ion aggregation.

DY 46.6 Thu 17:00 H 0110

Protein cluster formation in protein-polymer mixtures — •Anusha Hiremath, Fajun Zhang, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

Understanding protein cluster formation is crucial for unraveling the mechanisms behind diseases like Alzheimer's and Parkinson's, which are linked to specific protein aggregation. Protein clusters, serving as precursors in protein crystallization [1], are also essential to comprehend the nature of protein aggregation. In this study, static and dynamic light scattering (SLS and DLS) are employed to investigate Bovine Serum Albumin cluster formation driven by depletion interactions [2] in the presence of Polyethylene Glycol (PEG) with varying sizes and concentrations. Using a two-exponential fit model, we illustrate the decreasing diffusion coefficient trend with increasing PEG concentration and size, marking the transition from a dilute to a semi-dilute regime [2]. This decrease in diffusion coefficients suggests an increased attractive potential between proteins, indicating the formation of small clusters. The apparent molecular weight from SLS indicates the formation of protein clusters above a threshold PEG concentration, which decreases with increasing PEG size. Furthermore, we find that larger PEGs accelerate cluster formation. This work demonstrates that the depletion attraction by adding PEG can balance the electrostatic repulsion, leading to the cluster formation in protein solutions. [1] Zhang, F., J Phys Condens Matter, 29, 443002(2017). [2] Zosel, F. et al., PNAS, 117, 13482(2020).

DY 46.7 Thu 17:15 H 0110

Phase Behaviour and Structures Induced by Adding Cosurfactant to Nonionic Micelles - Rodlike Assembly of Small Micelles — Robert F. Schmidt[1], Sylvain Prévost[2], Miriam Simon[3], Yeshayahu Talmon[3], and •Michael Gradzielski[1] — [1]Stranski-Laboratorium für Physikalische Chemie, Inst f. Chemie, TU Berlin, Str. des 17. Juni 124, D-10623 Berlin, Germany — [2]ILL, 71 Rue de Martyrs, Grenoble, France — [3]Dep. of Chemical Engineering, Technion, Haifa 3200003, Israel

Addition of cosurfactant is a way to control systematically structure and properties of surfactant formulations. Normally this leads to continuously changing the packing parameter and transforming spherical to wormlike micelles and at higher concentration to bilayers via a first order phase transition. Here we show a completely different self-assembly behaviour seen for a classical nonionic surfactant (Tween 20) and 2-ethylhexylglycerol (EHG) as cosurfactant. Structural characterisation by light and neutron scattering (SANS) and cryo-TEM, shows that elongated assemblies are formed, which are composed of individual micelles that are locally ordered in a cylindrical fashion. A first-order phase transition takes place but only a smaller fraction of amphiphile is initially forming a bilayer structure and complete transformation to bilayers occurs within the single-phase region for EHG concentrations higher than the ones of the phase transition. This very uncommon structural evolution can be rationalised by the particular structure of the amphiphilic molecules involved and this finding extends our common assumptions about surfactant assembly.

DY 46.8 Thu 17:30 H 0110

Cryo Atom Probe Studies of 5CB, 8CB and Their Mixture — •Kuan Meng, Patrick Stender, Sebastian Eich, and Guido Schmitz — Stuttgart University, Institute for Materials Science, Heisenbergstr. 3, 70569, Stuttgart, Germany

The development of Cryo-FIB enabled studies of various delicate samples of high interest, such as SEI, ferritin and porous borosilicate. Generally, frozen organic materials exhibit complex mass spectra and a high dependence on measurement parameters. Following our earlier measurements on frozen liquids [1], we are studying the evaporation and fragmentation of different liquid crystals. In detail, 5CB (4-Cyano-4'-pentylbiphenyl) and 8CB (4-Cyano-4'-octylbiphenyl) were chosen for investigation due to their relatively simple chemical structure and hydrophobically-induced stability.

Both types of samples, pure 5CB and 8CB, evaporate predominantly as intact molecules, which suits our previous observation in the n-tetradecane study [1]. As a consequence, these two type of molecules can be distinguished even in the mixture, due to their effective mass difference. The dependence of mass spectra on the evaporation conditions and the miscibility of both species will be presented in the talk.

[1] Meng, K., Schwarz, T., Weikum, E., Stender, P., & Schmitz, G. (2022). Frozen n-Tetradecane Investigated by Cryo-Atom Probe Tomography. Microscopy and Microanalysis, 28(4), 1289-1299.

DY 47: Quantum Chaos and Coherent Dynamics (joint session DY/TT)

Time: Thursday 15:00–17:45 Location: A 151

DY 47.1 Thu 15:00 A 151

Probing the anisotropic scattering model in ultrapure Delafossites — •Linus Holeschovsky, Carsten Putzke, and Philip Moll — Max-Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Anisotropic scattering models have been used to describe the strange metal phase of overdoped cuprates. They stem from the idea of two distinct, k-dependent live-times of quasi-particles. This description is one among many trying to explain the strange metal phase and remains highly debated. On the other hand, the ultrapure delafossite PdCoO2 and PtCoO2 show two distinct quantum coherence lengths that can be explained by two different scattering times. These delafossite are particularly interesting due to their extremely long mean free path and moderate electronic correlation. This gives access to underlying physical properties, which can be theoretically explained within well-established theoretical models.

In this study, angle-dependent magnetic oscillation is used to investigate the anisotropic scattering time in microstructured PdCoO2 and PtCoO2. Specifically, a two-axis rotator is used to probe the coherence peak of interlayer transport in different crystallographic directions, which is particularly sensitive to scattering times. The anisotropy and temperature dependence of the scattering time can therefore be mapped on the Fermi surface. In this talk, we emphasize how the relative simplicity and textbook-like behavior of the delafossite materials make them prime candidates to probe physical models otherwise difficult to verify but were proposed in more complex materials.

DY 47.2 Thu 15:15 A 151

Semiclassical structure of resonance states in chaotic scattering — Roland Ketzmerick, •Florian Lorenz, and Jan Robert Schmidt — TU Dresden, Institute of Theoretical Physics, Dresden, Germany

We introduce a classical multifractal measure that describes resonance states with decay rate γ in the semiclassical limit. This measure (i) maximizes an entropy-like quantity and (ii) is conditionally invariant with the same decay rate γ. It is derived from a local random vector model and replaces previous approximate approaches. This supports the recently proposed factorization conjecture, that resonance states are a product of a classical measure and universal fluctuations [1]. These results are numerically demonstrated for optical microcavities.

[1] R. Ketzmerick, K. Clauß, F. Fritzsch, and A. Bäcker, Chaotic resonance modes in dielectric cavities: Product of conditionally invariant measure and universal fluctuations, Phys. Rev. Lett. **129**, 193901 (2022).

DY 47.3 Thu 15:30 A 151

Quasiclassical description of out-of-time-ordered correlators — •Thomas Michel[1], Juan Diego Urbina[2], and Peter Schlagheck[1] — [1]CESAM Research Unit, University of Liège, 4000 Liège, Belgium — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Out-of-time-ordered correlators (OTOCs) are quantum objects that can be used as a probe for quantum chaos. They characterise information scrambling, more specifically, how a local operator commute with another local operator that is time-evolved. We present a quasiclassical formalism of OTOCs using the semiclassical van Vleck-Gutzwiller propagator in combination with the diagonal approximation. For short time, we recover the same result as with the Wigner-Moyal formalism, yielding an initial exponential growth of the correlator. For long times and fully chaotic dynamics, this quasiclassical formalism yields a finite saturation value of the OTOC. However, as we verified in Bose-Hubbard systems, this quasiclassical saturation value is found to be small compared to the actual quantum OTOC saturation threshold. This finding shows the importance of effects beyond quasiclassical physics related to trajectory pairs with small-angle crossings, as was pointed out in Ref. [1].

[1] 1.Rammensee, J., Urbina, J.-D. & Richter, K. Many-Body Quantum Interference and the Saturation of Out-of-Time-Order Correlators. Phys. Rev. Lett. 121, 124101 (2018).

DY 47.4 Thu 15:45 A 151

A semiclassical approach to mode entanglement in Bose-Hubbard systems — •Sebastian Hörhold, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Entanglement is the fundamental mechanism behind phenomena as equilibration and decoherence [1] in many-body systems. Degrees of freedom of bosonic theories, describing for example cold atoms in optical lattices, are represented by complex matter fields at each lattice point and one speaks then of mode entanglement. In a semiclassical approach [2] based on interfering mean-field paths in Fock space, describing mode entanglement becomes rather cumbersome [3] as the path integral is constructed by using product states.

The aim of our work is to incorporate entanglement at the level of the path integral, similar to what has been done for matrix product states in spin systems [4]. We address then whether the effective classical description, closely related to the time-dependent variational approach [5], captures the emergence of entanglement.

[1] M. Rigol, V. Dunjko and M. Olshanii, Nature 452, 854-858
[2] K. Richter, J. D. Urbina and S. Tomsovic, J. Phys. A: Math. Theor. 55 453001
[3] S. Tomsovic et al., Phys. Rev. A 97, 061606(R)
[4] A. G. Green et al., arXiv:1607.01778v1
[5] J. Haegeman et al., arXiv:1103.0936v2

DY 47.5 Thu 16:00 A 151

Chaotic escape dynamics in the vicinity of hyperbolic fixed points — •Alexander Hempel, Jonas Stöber, and Arnd Bäcker — TU Dresden, Institute of Theoretical Physics, Dresden, Germany

For an ensemble of orbits started in the vicinity of a hyperbolic fixed point in the area-preserving standard map, we find a slow, non-exponential decay of the survival probability. We show that this is governed by the stable and unstable manifolds which form a partial barrier enclosing a resonance zone. The re-entrance of orbits into the resonance zone and the statistics of transit times leads to a simple model, which explains the initial decay of the survival probability. Furthermore we briefly discuss quantum mechanical consequences.

15 min. break

DY 47.6 Thu 16:30 A 151

Higher-order exceptional points in waveguide-coupled microcavities — •Julius Kullig[1], Daniel Grom[1], Sebastian Klembt[2], and Jan Wiersig[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany — [2]Physikalisches Institut and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, University of Würzburg, Würzburg, Germany

Open quantum and wave systems exhibit fascinating and exotic behavior described by non-Hermitian physics. A key feature of such systems are exceptional points (EPs) in the parameter space. At these EPs the eigenvalues of the Hamiltonian become degenerate and simultaneously the corresponding eigenstates coalesce. Consequently, the system has interesting chiral eigenstates and is highly sensitive to external perturbations. A hot topic of current research is the creation of high-order EPs, where more than two eigenstates coalesce. In this talk, we present an intuitive and robust implementation of high-order EPs in photonic structures consisting of waveguide-coupled microring cavities. Combining the unidirectional coupling from the waveguide with mirror-induced asymmetric backscattering, we can increase the order of the EPs even further. Furthermore, we demonstrate that our setup allows for an easy realization of non-generic perturbation schemes.

DY 47.7 Thu 16:45 A 151

Non-Hermitian mesoscopic optics in coupled microcavities — •Tom Rodemund[1], Síle Nic Chormaic[2], and Martina Hentschel[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Okinawa Institute of Science and Technology Graduate University, Okinawa, Japan

Coupled cavities are of interest as they expose qualitatively new effects, such as non-Hermitian properties, that are not accessible using an individual cavity. Here, we study two coupled two-dimensional microdisk cavities of circular and deformed (limaçon) shape, which are in the focus of interest due to their high emission directionality [1].

We investigate their coupling-induced properties as a function of intercavity distance and identify characteristic coupling regimes, with clear signatures of the presence of another cavity even deep in the weak couling regime. For deformed coupled microcavities, the asymmetry of the intercavity coupling implies non-Hermitian properties prominently evident in the chirality of the coupled cavity modes. We use an analytical model to explain our findings and reveal the direct connection between coupling asymmetry and the resulting sense of rotation of the coupled modes. This could prove useful for future applications such as far-field emission control of coupled cavities.

[1] Kreismann et al., *Phys. Rev. Res.* **1** 033171 (2019)

DY 47.8 Thu 17:00 A 151

Tuning phase space and far-field emission in anisotropic bilayer-graphene cavities — •Lukas Seemann[1], Angelika Knothe[2], and Martina Hentschel[1] — [1]Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Universität Regensburg, 93040 Regensburg, Germany

Ray-wave correspondence is a well-known tool in optics. Its generalization to Fermi electron optics in 2D materials allows for the description of ballistic charge carrier transport, e.g. in gate-defined cavities [1]. Here we focus on bilayer graphene (BLG) with a trigonal warped Fermi line. Its anisotropic disperion relation with three preferred propagation directions implies an electron dynamics in BLG cavities that differs significantly from the optical case [2]. In this work we investigate the interplay of momentum and real space asymmetries by combining the anisotropic dispersion relation with a deformed cavity. We investigate the resulting charge carrier dynamics in o'nigiri shaped cavities where the latter provides the same C3 symmetry as the BLG Fermi line. We study its signatures in phase space and explain how it translates into the far-field. Its properties can be fine-tuned by choosing appropriate material parameters for the BLG system, by the cavity geometry, and the tilt angle between BLG lattice and cavity axis which opens a broad venue for applications.

[1] J.-K. Schrepfer, S. Chen, M.-H. Liu, K. Richter, and M. Hentschel, Phys. Rev. B 104, 155436 (2021)
[2] Lukas Seemann, Angelika Knothe, and Martina Hentschel Phys. Rev. B 107, 205404 (2023)

DY 47.9 Thu 17:15 A 151

Non-abelian invariants in periodically-driven quantum rotors — •Volker Karle, Areg Ghazaryan, and Mikhail Lemeshko — Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg

This presentation explores the role of topological invariants in the non-equilibrium dynamics of periodically-driven quantum rotors, inspired by experiments on closed-shell diatomic molecules driven by periodic, far-off-resonant laser pulses. This approach uncovers a complex phase space with both localized and delocalized Floquet states. We demonstrate that the localized states are topological in nature, originating from Dirac cones protected by reflection and time-reversal symmetry. These states can be modified through laser strength adjustments, making them observable in current experiments through molecular alignment and observation of rotational level populations. Notably, in scenarios involving higher-order quantum resonances leading to multiple Floquet bands, the topological charges become non-Abelian. This results in the remarkable finding that the exchange of Dirac cones across different bands is non-commutative, enabling non-Abelian braiding, paving the way for the study of controllable multi-band topological physics in gas-phase experiments with small molecules, as well as for classifying dynamical molecular states by their topological invariants.

DY 47.10 Thu 17:30 A 151

Unveiling out of time correlators in stochastic operator variance — •Aritra Kundu — Univeresity of Luxembourg

This study introduces the stochastic operator variance (SOV) as a tool for investigating quantum systems influenced by noise. We present a protocol that utilizes noise to probe out-of-time-order correlators and extract the Lyapunov exponent in a noisy quantum chaotic system. We demonstrate SOV in both quantum and classical realms by introducing a stochastic version of the Lipkin-Meshkov-Glick (LMG) model. We further examine analytical and numerical demonstrations of a stochastic LMG Hamiltonian undergoing energy dephasing. In the classical limit, we provide analytical results for the Lyapunov exponents. This research contributes to understanding the interplay between noise and quantum dynamics for benchmarking near-term noisy quantum devices.

DY 48: Granular Matter and Contact Dynamics

Time: Thursday 15:00–17:00 Location: BH-N 128

DY 48.1 Thu 15:00 BH-N 128

Columnar Structures of Spheres: Fundamentals and Applications — •Jens Winkelmann[1] and Ho-Kei Chan[2] — [1]Trinity College Dublin, Dublin, Ireland — [2]Harbin Institute of Technology, Shenzhen, China

Columnar structures, many of which are helical, refer to dense cylindrical packings of particles. They are ubiquitous; for example, they exist in the contexts of botany, foams, and nanoscience. There have been in-depth investigations of columnar structures of both hard spheres (e.g., ball bearings) and soft spheres (e.g., wet foams), through computer simulations, analytic derivations, or simple experiments. In this talk, I will present you an overview of the fundamentals and applications of such structures, based on our recently published book on this subject. I will review some of the theoretical and experimental methods employed to assemble such structures, and then discuss some of the latest findings related to the structural transitions and hysteretic behaviour of such systems.

DY 48.2 Thu 15:15 BH-N 128

Rheology of entangled assemblies of granular chains — Mehdi Habibi[1] and •Reza Shaebani[2] — [1]Wageningen University, The Netherlands — [2]Saarland University, Germany

We study the nonlinear rheology of random assemblies of granular chains under oscillatory shear. It is known that a narrow shear zone forms near the moving boundaries in a granular packing upon increasing the strain amplitude. We show that the presence of topological constraints between chains sharpens the transition and broadens the sher zone. Both the shear-zone width and the transition sharpness follow scaling laws as a function of chain length. Above the transition point, we observe shear stiffening behavior as a result of semiloop formation by chains. We also clarify the role of interparticle friction on the rheological response of the assembly.

DY 48.3 Thu 15:30 BH-N 128

Rheological properties of fluidized granular matter — •Marlo Kunzner[1], Olfa D'Angelo[2], Till Kranz[3], and Matthias Sperl[1,3] — [1]Institut für Materialphysik im Weltraum, DLR Köln, Deutschland — [2]Institute of Multiscale Simulation, FAU Erlange, Deutschland — [3]Institut für Theoretische Physik, Uni Köln, Deutschland

Aerated granular media are important in several industrial processes; yet, their flow-behavior is poorly understood. On one hand, the well-known Geldart classification [1] divides granulates by their fluidization characteristics; on the other hand, the rheology of air-fluidized granular media has been recently investigated experimentally and theoretically [2], considering the fluidized bed as a homogeneous medium. We propose to link these two approaches by measuring flow curves for polydisperse particles of different diameter regimes ranging from 70*m to 420*m. We find different rheological regimes depending on fluidization velocity and shear-rate, including Newtonian at low shear rate and Bagnoldian shear-thickening at high shear rate. We support the rheometry by light scattering to gain insights on the microscopic behavior of the aerated granular media in the future. [1] Geldart, D "Types of Gas Fluiditation", 1973 [2] O. D*Angelo, A. Shetty, M. Sperl, and W. T. Kranz, *The manifold rheology of fluidized granular media,* 2023.

DY 48.4 Thu 15:45 BH-N 128

How to make Sense of Fluidized Bed Rheology using Shear Banding and Three Time Scales — •W. Till Kranz[1,2], Olfa D'Angelo[2,3], Olivier Coquand[2,4], Abhishek Shetty[5], and Matthias Sperl[2,1] — [1]University of Cologne, Germany — [2]DLR,

Germany — [3]University of Erlangen, Germany — [4]University of Perpignan, France — [5]Anton Paar, USA

The rheology of granular fluids is surprisingly rich if agitation by shear is combined with fluidization and comprises ordinary Newtonian rheology as well as shear thinning and shear thickening regimes. We will report on careful measurements of air-fluidized glass beads in a Taylor-Couette shear cell [1]. We will sketch a procedure to extract quantitative rheological information spanning all the rheological regimes and summarized in only a handful of physically meaningful parameters. Taking into account shear banding this approach embraces and extends the well known empirical μ-$\mathcal{I}$-rheology [2] of non-fluidized granular flows. Using simple arguments involving three relevant time scales, we will show how the seemingly complex rheology stems from intuitive and transparent physical principles [3].

[1] O. D'Angelo, A. Shetty, M. Sperl and W. T. Kranz, arXiv:2309.00413
[2] GDR Midi, EPJ E **14**, 341 (2004)
[3] O. Coquand, W. T. Kranz and M. Sperl, arXiv:2008.05931

DY 48.5 Thu 16:00 BH-N 128

Heating and cooling in a granular gas of spheres in microgravity — •Mahdieh Mohammadi[1,3], Torsten Trittel[1,3], Raul Cruz Hidalgo[2], Dmitry Puzyrev[3], Adrian Niemann[4], Ralf Stannarius[1,3,4], and Kirsten Harth[1,3] — [1]Department of Engineering, Brandenburg University of Applied Sciences, Magdeburger Str. 50, 14770 Brandenburg an der Havel,Germany — [2]Departamento de Física y Matemática Aplicada, Facultad de Ciencias , Universidad de Navarra, Pamplona, Spain — [3]MTRM, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany — [4]Institute of Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

We investigate the dynamic characteristics pertaining to the cooling and heating processes of particles in a microgravity environment. A comprehensive analysis, facilitated by simulations conducted across various regimes with a consistent restitution coefficient and varying friction coefficients, has been undertaken. The determination of characteristic times for the cooling and heating phases is established through an assessment of the system's dynamical parameters. Distinct trends are observed in the attitudes of mean translational and rotational energies within the ensemble of particles during both the cooling and heating phases.

DY 48.6 Thu 16:15 BH-N 128

Clustering of Magnetized Iron Granulate – Less is More Susceptible — •Ali Lakkis[1], Matthias Biersack[1], Oksana Bilous[2], Sofia Kantorovich[2], and Reinhard Richter[1] — [1]University of Bayreuth, Experimental Physics 5, Universitätsstrasse 30, 97440 Bayreuth, Germany — [2]University of Vienna, Faculty of Physics, Kolingasse 14-16, 1090 Vienna, Austria

We are exploring in experiments the aggregation process in a shaken granular mixture of glass and magnetized steel beads, filled in a horizontal vessel. After the shaking amplitude is suddenly decreased, the magnetized beads form a transient network that coarsens in time into compact clusters [1]. Recently it has been quantified how a homogeneous magnetic field B oriented in vertical direction impedes the emergence and growth of the networks [2]. Here we investigate how an increased volume fraction ϕ of the granulate accelerates the coarsening. Moreover, we explore the coarsening dynamics in the (ϕ, B)-control parameter space, and observe that low filling fractions are more susceptible to an increase of B than high ones [3].

[1] A. Kögel, R. Maretzki, E. S. Pyanzina, P. A. Sánchez, S. S. Kantorovich, R. Richter *Soft Matter*, 14 (2018) 1001.
[2] M. Biersack, A. Lakkis, R. Richter, O. Bilous, P. A. Sánchez, S. S. Kantorovich *Phys. Rev. E*, 108 (2023) 054905.
[3] A. Lakkis, M. Biersack, O. Bilous, S. S. Kantorovich, R. Richter, *J. Magn. Magn. Mater*, submitted (2023).

DY 48.7 Thu 16:30 BH-N 128

Magnetic Tubes - Instability of a Drug Deliverer — •Ingo Rehberg — Bayreuth University, Germany

Tubular assemblies of magnetic particles act as microrobots for cargo transport [1]. The magnetization of such tubes comes in two families: Circular magnetization is preferred for short tubes, and axial magnetization for longer ones [2, 3]. Introducing the strength of the outer dipole ring as an order parameter [4] in a numerical simulation unveils the nature of that transition from circular to axial states [5].

[1] Xiaoyu Wang et al., PNAS 120, e2304685120 (2023).
[2] Igor Stanković et al., Nanoscale 11, 2521 (2019).
[3] Adrien Wafflard et al., New J. Phys. 25, 063024 (2023).
[4] Simeon Völkel et al., JMMM 559, 169520 (2022).
[5] Ingo Rehberg, From Tetrahedra to Buckyballs - Examine 486 Dipole Clusters with a Single Python Animation. https://doi.org/10.5281/zenodo.10201571 (2023).

DY 48.8 Thu 16:45 BH-N 128

Exploring the impact of concentration and applied magnetic field on the diffusion coefficient of ferrogranulate: insights from computer simulations — •Oksana Bilous[1], Pedro Sánchez[1], Ali Lakkis[2], Reinhard Richter[2], and Sofia Kantorovich[1] — [1]Computational and Soft Matter Physics, University of Vienna, Vienna, Austria — [2]Experimental Physik, University of Bayreuth, Bayreuth, Germany

We study how an applied magnetic field affects the self-diffusion of magnetic particles in a ferrogranulate layer*a composite of glass and steel millimetre-sized particles on a shaken substrate. Initially, the system is maintained in a non-aggregated state through high shaking amplitude, followed by a step-like quench that induces particle aggregation and a slowdown. When an external magnetic field is applied perpendicular to the layer, aggregation is inhibited, prompting an investigation into its impact on particle diffusion. Molecular dynamics simulations model the ferrogranulate as a mixture of Stockmayer and repulsive spheres, with shaking amplitude mimicked by a thermostat. We find that at low applied field values, the system exhibits a bistable gas-liquid regime at high concentrations, while for stronger fields, the system shows no signs of a phase transition, significantly influencing the system dynamics.

DY 49: Focus Session: Computing with Dynamical Systems: New Perspectives on Reservoirs and Applications II – Applications and Quantum RC

Reservoir Computing uses the dynamic response of driven dynamical systems to predict and analyze temporal signals. The best-known example is the Echo State Networks proposed by H. Jaeger in 2001, where the reservoir consists of a recurrent neural network. However, in recent years, other realizations have been proposed, in particular those in which the reservoir system can be implemented in hardware in a fast and energy-efficient manner (e.g., using optical components). Other recent developments concern the specific incorporation of prior (physical) knowledge about the source of the input signal (physics aware/informed Reservoir Computing) as well as various application examples in different disciplines. Therefore, the goal of this focus session is to highlight the rapidly advancing current developments in the field of Reservoir Computing in order to enable a direct scientific exchange between new methodological approaches and innovative applications.

Organized by Ulrich Parlitz (Göttingen), Kathy Lüdge (Ilmenau), and Christoph Räth (München)

Time: Thursday 15:00–18:00 Location: BH-N 243

Invited Talk DY 49.1 Thu 15:00 BH-N 243

Using reservoir computing to create surrogate models — •Lina Jaurigue — Technische Universität Ilmenau

Reservoir computing is a machine learning approach that utilizes the dynamics of a network or physical system to perform complex tasks while only training the output layer via linear regression. Due to the memory properties of the reservoir, reservoir computing is well suited to perform chaotic timeseries prediction tasks. When a reservoir is trained to perform one-step-ahead prediction of a chaotic trajectory, it can also be used to create a surrogate model for the system that the training trajectory originated from. This is done by feeding the output of the reservoir back in as input in the prediction phase. The resulting system is an autonomous dynamical system with solutions that depend on properties of the reservoir and the weights. We investigate how the properties of the reservoir, the input weights and the trained output weights influence solutions of the resulting autonomous dynamical system.

DY 49.2 Thu 15:30 BH-N 243

Image classification using collective modes of a two-dimensional array of photonic-crystal nanolasers — •Giulio Tirabassi[1], Kaiwen Ji[2], Cristina Masoller[1], and Alejandro Yacomotti[2] — [1]Departament de Fisica, Universitat Politecnica de Catalunya, Rambla Sant Nebridi 22, 08222 Terrassa, Barcelona, Spain — [2]Centre de Nanosciences et de Nanotechnologies, CNRS, Universite Paris-Sud, Université Paris-Saclay, 10 Boulevard Thomas Gobert, 91120 Palaiseau, France

Optical computing is revolutionizing the fields of Artificial Intelligence (AI) and High-Performance Computing (HPC) systems. Due to their ultra-low power consumption, nanolasers are ideal light sources for AI and HPC systems. In particular, two-dimensional photonic-crystal nanolaser arrays can be designed and fabricated with evanescent coupling, whose strength can be precisely controlled by adjusting the radius of the holes that separate adjacent nanocavities. In this work, we exploit the collective modes of nanolaser arrays of different sizes for binary classification of images and data. Using a dataset of hand-written digits (a standard dataset for assessing the performance of image recognition systems), we show numerically that an overall success rate of 98% can be achieved in digit classification. Finally, going beyond simulations, we show with laboratory experiments that the performance of the nanolaser arrays can be comparable to that of common non-linear classification algorithms.

DY 49.3 Thu 15:45 BH-N 243

Memristive devices for chaotic time series prediction — •Kristina Nikiruy[1], Seongae Park[1], Tzvetan Ivanov[1,2], Alon Ascoli[3], Fernando Corinto[4], Ronald Tetzlaff[3], and Martin Ziegler[1,2] — [1]Micro- and Nanoelectronic Systems, Department of Electrical Engineering and Information Technology, TU Ilmenau, Germany — [2]Institute of Micro- and Nanotechnologies MacroNano*, TU Ilmenau, Germany — [3]Faculty of Electrical and Computer Engineering, Institute of Circuits and Systems, TU Dresden, Germany — [4]Department of Electronics and Telecommunications (DET), Politecnico di Torino, Turin, Italy

Neuromorphic hardware, in which memristive devices are key elements, enables an energy-efficient and compact realization of the signal processing concept. Here we show that the application of nonlinear vector autoregression (NVAR), also known as next generation reservoir computing (NGRC), to a single-layer network with memristive weights can be used to predict signals, depending on the nature of the nonlinear functions and the number of weights. The network has been experimentally implemented with HfO2-based memristive devices and allows an accurate prediction of chaotic time series of Mackey-Glass and Duffing oscillators. The effect of the nonlinear combinations of the input data points, the network structure, and the number and nonlinear resistive switching properties of the memristive weights on the output response are studied. In this regard, it is shown how a suitable network structure can be tailored for chaotic time series prediction.

DY 49.4 Thu 16:00 BH-N 243

Computing Functionality in Gold Nanoparticle Networks — •Jonas Mensing[1], Andreas Heuer[1], and Wilfred G. van der Wiel[2] — [1]Institute of Physical Chemistry, University of Münster, Germany — [2]Center for brain-inspired Nano Systems, University of Twente, Enschede

Nanoparticles tunnel-coupled by insulating organic molecules exhibit strong nonlinear switching behavior at low temperatures. When assembling these switches in a recurrent network and manipulating the charge transport dynamics inside through surrounding electrodes, this network can be configured to execute brain-inspired computing applications. Via extensive kinetic Monte Carlo-based simulations we have analyze both stationary and time-dependent charge transport dynamics to assess the network*s computing and memory capabilities. We provide novel metrics to quantify general nonlinear properties of the network such as negative differential resistance and nonlinear separability of different input values, which are essential for future machine learning applications.

DY 49.5 Thu 16:15 BH-N 243

Reservoir computing of thermal convection: Random versus small-world networks — •Shailendra Kumar Rathor, Martin Ziegler, and Jörg Schumacher — Technische Universität Ilmenau, Germany

We study a classical two-dimensional thermal convection flow at a low Rayleigh number which is represented by an energy-conserving Lorenz-type model with eight degrees of freedom. This model accounts for the shear motion and tilted plumes in the flow. We employ a recurrent machine learning approach in the form of a reservoir computing model and test different reservoir architectures. In detail, small-world network architectures with different rewiring probabilities are compared with conventional random network topology. It is found that similar prediction capabilities are obtained on the basis of the mean squared error or the prediction horizon.

DY 49.6 Thu 16:30 BH-N 243

Forecasting Food Security with Reservoir Computing — •Joschka Herteux[1,2], Christoph Räth[1], Amine Baha[3], Giulia Martini[2], and Duccio Piovani[2] — [1]Deutsches Zentrum für Luft- und Raumfahrt e. V. (DLR) — [2]World Food Programme, Research, Assessment and Monitoring Division (RAM) — [3]World Food Programme Innovation Accelerator

Early warning systems are an essential tool for effective humanitar-

ian action. Advance warnings on impending disasters facilitate timely and targeted response which help save lives, livelihoods, and scarce financial resources. We present a quantitative methodology based on Reservoir Computing (RC) to forecast levels of food consumption for 60 consecutive days, at the sub-national level, in four countries: Mali, Nigeria, Syria, and Yemen. The methodology is built on publicly available data from the World Food Programme's integrated global hunger monitoring system (https://hungermap.wfp.org/). We compare the performance of the RC model to various algorithms including ARIMA, XGBoost, LSTMs and CNNs spanning from classical statistical to deep learning approaches. Our findings highlight Reservoir Computing as a particularly well-suited model for this task given both its notable resistance to over-fitting on limited data samples and its efficient training capabilities. This work constitutes a successful application of RC on high-dimensional, heterogenous, real data and has been submitted to Nature Communications.

15 min. break

Invited Talk DY 49.7 Thu 17:00 BH-N 243

Opportunities in Quantum Reservoir Computing — •Roberta Zambrini — IFISC (UIB-CSIC)

Non-conventional computing inspired by the brain, (classical) neuromorphic computing, is a successful approach in a broad spectrum of applications, also burgeoning due to big data availability. Recent proposals go beyond classical substrates for quantum machine learning, as in Quantum Reservoir Computing. The classical version of this approach has been developed in the last 20 years and moving from classical to quantum physical reservoirs, has the potential to remarkably boost the processing performance in temporal tasks by exploiting quantum coherence, not requiring error correction. Furthermore this is naturally suited for fully quantum information processing (with quantum inputs). However, it also opens a series of new challenging questions, related to fundamental as well as implementation aspects. Examples are the identification of the best quantum regimes of operation, the role of statistics, or of quantum coherences and entanglement. After introducing the Quantum Reservoir Computing and showing how memory and non-linearity arise in a quantum formalism, we will discuss some of these issues, providing an overview of the field.

DY 49.8 Thu 17:30 BH-N 243

Exploring quantumness in quantum reservoir computing — •Niclas Götting[1,2], Frederik Lohof[1,2], and Christopher Gies[1,2] — [1]Institute for Theoretical Physics, University of Bremen, Bremen, Germany — [2]Bremen Center for Computational Material Science, University of Bremen, Bremen, Germany

With the advent of sophisticated semiconductor fabrication techniques for quantum photonic systems like coupled-cavity arrays, Quantum Reservoir Computing becomes a promising candidate to elevate Reservoir Computing (RC) to the next level. Not only does the phase space dimension of the quantum system scale exponentially with its size, the property of quantum entanglement also introduces a new resource to RC.

We investigate how these properties are linked to the Quantum Reservoir Computer (QRC) performance in simple benchmarks [1]. As the noisy intermediate-scale quantum (NISQ) devices of our current time are subject to various types of perturbations, we also analyze how dephasing of the quantum state affects the benchmark performance.

[1] N. Götting et al. Exploring Quantumness in Quantum Reservoir Computing. Phys. Rev. A 2023, 108 (5), 052427.

DY 49.9 Thu 17:45 BH-N 243

Enhancing the performance of quantum reservoir computing and solving the time-complexity problem by artificial memory restriction — •Saud Cindrak, Kathy Lüdge, and Lina Jaurigue — Institute of Physics, Technische Universität Ilmenau, Weimarer Str. 25, 98693 Ilmenau, Germany

We propose a novel scheme to optimize the performance and reduce the computational cost of quantum reservoir computing. In quantum reservoir computing, a quantum system serves as a reservoir and measurements are performed to obtain the expected values of observables. However, due to the state's collapse after measurement, computations must be repeated multiple times to construct expected values. This becomes challenging for timeseries tasks, where each new input requires the reinitialization of all prior inputs into the system, leading to quadratic time complexity. Another hurdle in reservoir computing lies in tuning nonlinearities. We address these challenges by artificially restricting the reservoir's memory, achieved by reducing the number of reinitialization time steps to a level below the fading memory capacity. With the proposed algorithm, we decrease the time complexity to linear and introduce an experimentally tunable parameter to change the nonlinear response. We demonstrate our approach on both an Ising reservoir and a quantum circuit reservoir and observe an increase in the information processing capacity and a reduction of the prediction errors for the Lorenz timeseries prediction task. [S. Cindrak, B. Donvil, K.Lüdge, L. Jaurigue, ArXiv:2306.12876 (2023). https://doi.org/10.48550/arXiv.2306.12876]

DY 50: Wetting, Droplets, and Microfluidics (joint session DY/CPP)

Time: Thursday 15:00–17:45 Location: BH-N 334

DY 50.1 Thu 15:00 BH-N 334

Structure Formation in Supraparticles Composed of Spherical and Elongated Colloidal Particles — Yashraj M. Wani[1], Melis Yetkin[2], •Kritika Kritika[1,3,4], Michael Howard[5], Hans-Jürgen Butt[2], Michael Kappl[2], and Arash Nikoubashman[1,3,4] — [1]Johannes Gutenberg Universität Mainz — [2]Max-Planck-Institut für Polymerforschung — [3]Leibniz-Institut für Polymerforschung — [4]Technische Universität Dresden — [5]Department of Chemical Engineering Auburn University

In the present work, we use experiments and computer simulations to investigate the formation of supraparticles (SPs) through the evaporation-driven assembly of spherical and elongated colloidal particles (CPs). We systematically explore how different aspect ratios (λ=4,6,11) of the CPs and the drying conditions influence the final morphologies of SPs. In the evaporation-limited regime, where the rate of CP advection is much larger than the rate of CP diffusion, we find a short-ranged orientational ordering of the CPs on the SP surface and isotropic packing in the core. In contrast, simulations in the diffusion-limited regime show a long-ranged orientational ordering of the rods on the SP surface and local nematic ordering in the core. Additionally, we explore SPs fabricated from rod-sphere mixtures, where a thin shell of rods was observed for the slowly dried SPs. In all cases, we also observe that the porosity of the SPs increases with increasing aspect ratio of the elongated CPs.

DY 50.2 Thu 15:15 BH-N 334

Investigation of nonlinear electrophoresis in microfluidics with alternating voltages — •Robert Epkenhans[1], Ralf Eichhorn[2], Dario Anselmetti[1], and Martina Viefhues[1] — [1]Bielefeld University — [2]Nordita Stockholm

Electrophoresis (EP) is a common phenomenon in microfluidics used for controlled migration of biomolecules like DNA or for size selective migration in gels. In the linear, low-field regime the EP-mobility is dependent only on the particle-zeta and the ambient electrolyte. Yet, recent studies reveled a polynomial velocity increasement for colloid particles exposed to high electric fields above roughly 100 kV/m with the underlying physical mechanisms still under debate.

In our studies, we quantified the nonlinear response in the mobility of charged particles in a microfluidic PDMS-chip as a function of the applied electric field strength. Therefore, we used 1) a superimposition of low DC-fields (0-13 kV/m) and high sinusoidal alternating fields up to 260 kV/m, 2) asymmetric potentials yielding a vanishing time-averaged mean, but non-vanishing higher-order mean value. We present several data sets for the particle velocities with a variation of ionic concentration and types and the respective higher-order electrophoretic mobilities. Our results suggest that nonlinear-EP forces are rather relevant in insultorbased microfluidics instead of dielectrophoresis. This opens new possibilities for particle separation devices, e.g. DNA-molecules, since the up to date data indicates size- and shape-dependent electrophoresis in the nonlinear regime. Concerning these matters, we provide suggestions for future studies on nonlinear electrophoresis.

DY 50.3 Thu 15:30 BH-N 334

Dynamic density functional theory for drying colloidal suspensions: Hydrodynamic interactions in spherical confinement — •Mayukh Kundu[1], Yashraj M. Wani[2], Kritika Kritika[2,3,4], Arash Nikoubashman[2,3,4], and Michael P. Howard[1] — [1]Department of Chemical Engineering, Auburn University, Auburn, USA — [2]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [3]Leibniz-Institut für Polymerforschung Dresden, Germany — [4]Institut für Theoretische Physik, TU Dresden, Germany

We investigate the role hydrodynamic interactions (HI) play in the evolution of structures in one-component drying colloidal suspensions confined within spherical droplets. We develop a continuum model for the distribution of hard-sphere particles in the droplet based on dynamic density functional theory (DDFT). To compute the particle flux during drying, we employ an accurate free-energy functional based on fundamental measure theory (FMT) in conjunction with pairwise far-field HI described by the Rotne-Prager-Yamakawa (RPY) mobility tensor. To validate the DDFT model, we compare the DDFT predictions with particle-based Brownian dynamics (BD) and multiparticle collision dynamics (MPCD) simulations in selected cases. We also compare our model to DDFT and particle-based models, including only free-draining HI, in order to systematically characterize the effects of HI between particles. Our work illustrates the importance of including HI in models of nonequilibrium self-assembly processes such as drying and demonstrates a systematic way of constructing such models.

DY 50.4 Thu 15:45 BH-N 334

Numerical study of evaporation-driven particle deposition on a substrate — •Qingguang Xie[1] and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IEK-11), Forschungszentrum Jülich GmbH, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany

Deposition of functional materials on a substrate is a vital process in printing and coating technologies, playing important roles in numerous applications such as photovoltaics, lithium batteries, and electrolysers. The structure of the deposition is crucial for device performance; however, our understanding of the deposition process is still lacking. We conducted numerical studies on the particle deposition process. Initially, we developed a diffusion-dominated evaporation model using a multicomponent lattice Boltzmann method. We validated the applicability of our model by demonstrating agreement in the time evolution of the interface position of an evaporating planar film and a freely floating droplet with analytical predictions. Subsequently, we investigated the deposition of particles on a substrate by drying a colloidal suspension droplet. We explored, both numerically and theoretically, the effect of friction between the particles and the substrate on the deposition pattern. With an increase in friction force, we observed a transition from a dot-like to a ring-like deposit. More recently, we studied the effect of van der Waals force between particles and substrate wettability on the deposition pattern when drying a thin film. We proposed a strategy to achieve highly uniform deposition.

DY 50.5 Thu 16:00 BH-N 334

Coalescence of biphasic droplets embedded in free-standing smectic A films — •Christoph Klopp[1], Torsten Trittel[2], and Ralf Stannarius[1] — [1]Otto von Guericke Universität Magdeburg, Institut für Physik, ANP — [2]TH Brandenburg, Fachbereich Technik

Coalescence of droplets is ubiquitous in nature and modern technology. Various experimental and theoretical studies explored droplet dynamics in three dimensions (3D) and on two-dimensional (2D) solid or liquid substrates, e.g. [1-3]. We investigate micrometer-sized flat droplets consisting of an isotropic core surrounded by a nematic rim (biphasic droplets) in freely suspended smectic A liquid-crystal films. In contrast to purely isotropic droplets which are characterized by a sharp edge and no long-range interactions, the nematic rim introduces a continuous film thickness change resulting in long-range mutual attraction of droplets. We show the appearance of a unique structural wall separating the isotropic cores of the droplets during the merging process.

[1] J. D. Paulsen et al., Nat. Commun., 5, 3182 (2014) [2] D. G. A. L. Aarts et al., Phys. Rev. Lett., 95, 164503 (2005) [3] N. S. Shuravin et al., Phys. Rev. E, 99, 062702 (2019)

15 min. break

DY 50.6 Thu 16:30 BH-N 334

Mutual information as a measure of mixing efficiency in viscous fluids — •Yihong Shi — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Because of the kinematic reversibility of the Stokes equation, fluid mixing at the microscale requires an interplay between advection and diffusion. Here we introduce mutual information between particle positions before and after mixing as a measure of mixing efficiency. We demonstrate its application in a Couette flow in an annulus and show that the mixing efficiency depends in a non-trivial way on the time sequence of rotation. We also determine mutual information from Brownian dynamics simulations using data compression algorithms and demonstrate that advanced neural network based compression algorithms can be applied to estimate mutual information to a high accuracy. Our results show that mutual information provides a universal and assumption-free measure of mixing efficiency in microscale flows.

DY 50.7 Thu 16:45 BH-N 334

Leveraging geometry and catalyst distribution to optimize the yield of catalytic microreactors — •Goncalo Antunes[1], Paolo Malgaretti[1], and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg für Erneurbare Energien, Forschungszentrum Jülich, Erlangen, Germany — [2]Department Chemie- und Bioinginieurwesen und Department Physik, Friedrichs-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany

We develop a semi-analytical model for transport in heterogeneous catalytic microreactors, where both reactant and product are in the gas phase. Making use of the lubrication and Fick-Jacobs approximations, we reduce the three-dimensional governing equations to an effective one-dimensional set of equations. Our model captures the effect of compressibility, of corrugations in the shape of the reactor, as well as of a non-homogeneous catalytic coating of the reactor walls. We then show how to optimize the output of product by tuning the geometrical and chemical properties of the reactor, such as its length, for which we find an optimum value. We further explore the compressible regime, in which an optimum corrugation height emerges. This height depend on the distribution of catalytic material. Finally, we apply our theory to a model porous material, and find an optimum pore size that maximizes the output of product.

DY 50.8 Thu 17:00 BH-N 334

Rolle of water accumulation in dynamic friction on hydrophobic surfaces — •Igor Stanković[1], Pierre-Emmanuel Mazeran[2], and Olivier Noel[3] — [1]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia — [2]Sorbonne Universites, Universite de Technologie de Compiegne, Laboratoire Roberval, FRE UTC-CNRS 2012, CS 60319, 60203, Compiegne, France — [3]IMMM, UMR CNRS 6283, Le Mans Universite, Avenue O. Messiaen, 72085 Cedex 09, Le Mans, France

The nature of dynamic friction on water molecule-contaminated surfaces is still poorly understood. The capillary phenomena in tribological contact with graphite, a commonly used material, were investigated using circular mode atomic force microscopy and molecular dynamics simulations. Here, we demonstrate that an intuitive paradigm, which asserts that water molecules are squeezed out of hydrophobic contacts, needs to be refined. Consequently, we introduce a mechanism considering a droplet produced within the sliding nanocontact by the accumulation of water adsorbed on the substrate. Our results show that a full slip regime of the droplet sliding on the hydrophobic substrate explains the experimental tribological behaviour.

References 1. O.Noel, P.-E. Mazeran, I.Stanković, ACS Nano 16, 10768-10774 (2022).

DY 50.9 Thu 17:15 BH-N 334

Active-matter-fueled interfacial microflows — •Kuntal Patel[1,2] and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [2]Max-Planck-Institut für Sonnensystemforschung, Göttingen, Germany

Several chemical and biomedical applications require systematic processing of micron-sized fluid samples. To realize this, so-called microfluidic lab-on-a-chip devices with micron-sized channels are widely used. Often, one needs to manipulate interfaces separating immiscible fluids in such channels. The interface separating the two fluid components costs energy, which is quantified by surface tension. Thus, any

deformation of a planar fluid interface increases energy.

In our work, we assign one more property to the interface in the form of dipolar forces acting perpendicular to the interface. We name it the *activity* of the interface, and it is achieved by covering the interface with active particles. The notion of activity is inspired by swimming microorganisms. Using lattice-Boltzmann simulations, we discover that the presence of activity affects the stability of the interface. We notice that dipolar forces pointing towards the interface counter the stabilizing effect of surface tension, so that the interface deforms. In contrast, force components pointing away stabilize the planar interface. We demonstrate that one can leverage such activity-induced instability to generate microfluidic droplets and manipulate liquid sheets. In addition, we can also control droplet formation by varying the magnitude of dipolar forces in real time, which can be accomplished using light-sensitive active particles in practice.

DY 50.10 Thu 17:30 BH-N 334

Extracting oil from an oil and water mixture by using their different wetting properties via the Acoustowetting phenomenon — •Ofer Manor — Technion - Israel Institute of Technology, Haifa, Israel

The free surface of an oil in water emulsion usually catalyzes the formation of a thermodynamically favorable oil film far before the emulsion destabilizes in the bulk of the mixture: We stabilize 170 nm nanoemulsions by surfactants—SDS or Tween 20. The emulsions remain stable for 12 months in closed vessels. However, micron thick oil films appear within minutes on 10 micro-liter sessile drops of the emulsions. We extract the micron-thick oil film off the free surface of the emulsion drops using a traveling 20 MHz-frequency surface acoustic wave (SAW) in the solid.

In our experiments, we place drops of emulsion atop a lithium niobate substrate that supports a traveling SAW therein. Oil films leaks off the emulsion sessile drops 1-20 minutes from the commencement of the experiment, dynamically wetting the solid under acoustic stress—the Acoustowetting phenomenon. The Acoustowetting phenomenon discriminates between the water and oil phases via their wetting properties: The SAW powers the dynamic wetting of the solid by the oil film, extracting oil mass off the emulsion drops, while keeping the higher surface-energy water phase in place. The thickness of the oil film, leaking off the drops, oscillates between 20 to 1 microns and sustains a crystal-like pattern of lateral micron dimensions and submicron thickness of unknown origin in the presence of the SAW.

DY 51: Members' Assembly

Time: Thursday 18:00–19:00 Location: BH-N 243

All members of the Dynamics and Statistical Physics Division are invited to participate.

DY 52: Focus Session: Wetting on Adaptive Substrates III (joint session CPP/DY/O)

The focus session aims to discuss recent developments in the wetting dynamics of adaptive, deformable, and switchable surfaces.

Time: Friday 9:30–12:45 Location: H 0110

Invited Talk DY 52.1 Fri 9:30 H 0110

Condensation on soft substrates — •Ambre Bouillant[1,3], Bruno Andreotti[2], and Jacco H. Snoeijer[3] — [1]Laboratoire MSC, CNRS UMR 7057, Université Paris Cité, FR — [2]Laboratoire LPENS, CNRS UMR 8023, Université PSL, FR — [3]Physics of Fluids, Twente Unversity, NL

Vapor molecules can nucleate on cool substrates, provided the surrounding humidity is high enough. Dew formation has been investigated on both rigid (and rough!) solids as well as on liquids. However, how substrate elasticity affects the condensation process remains elusive. In this talk, I will present how water condenses on soft, elastic gels that are smooth at the nanometer scale. We prepare PDMS gels whose softness varies between that of a rigid substrate and an un-crosslinked polymeric liquid.

Although elasticity should be marginal at the nanometric scale at which drops form, we report that the nuclei density is highly sensitive to the substrate softness. Throughout this talk, I will delve into the intricate dynamics of condensation and try to explain some of the intriguing characteristics we have observed. Among these are the influence of softness on nucleation; the sub-diffusive growth of droplets; and the absence of secondary nucleation events (unlike what is classically observed in heterogeneous nucleation). Later, when neighboring drops get closer, they attract each other due to interactions mediated by substrate deformations. Drops then gather into clusters that seem reluctant to coalesce. This ultimately results in the formation of a persistent, ordered, honeycomb-patterned liquid film.

DY 52.2 Fri 10:00 H 0110

Modelling droplets on substrates with travelling-wave deformations — •Josua Grawitter and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin, Germany

Motivated by strategies for targeted microfluidic transport of droplets, we investigate how sessile droplets can be steered toward a preferred direction using travelling-wave deformations of the substrate. To perform our numerical study, we develop a formalism to apply the boundary-element method to dynamic wetting. It solves the governing Stokes equations for the fluid flow field inside the droplet that is pushed forward by the deforming substrate.

We find two distinct modes of droplet motion. For small wave speed the droplet surfs with a constant velocity on the wave, while beyond a critical wave speed a periodic wobbling motion occurs, the period of which diverges at the transition. In the related case of a flat substrate with travelling waves in wettability, such an observation is well rationalized by the *nonuniform oscillator* model and the transition described by a SNIPER bifurcation. Here, however, the mean droplet velocity in the wobbling state is proportional to the wave speed at large speed values since the droplet always has to move up and down. To rationalize this behavior, the nonuniform oscillator model has to be extended. Since the critical wave speed of the bifurcation depends on the droplet radius, this dependence can be used to sort droplets by size.

DY 52.3 Fri 10:15 H 0110

High Voltages Generated by Moving Water Drops — •Stefan Weber[1,2], Pravash Bista[2], Aaron Ratschow[3], and Hans-Jürgen Butt[2] — [1]Institute for Photovoltaics, University of Stuttgart — [2]MPI for Polymer Research, Mainz — [3]Institute for Nano- and Microfluidics, TU Darmstadt

Water drops on insulating, hydrophobic substrates can generate electric potentials of kilovolts upon sliding for a few centimeters. We show that the drop saturation voltage corresponds to an amplified value of the solid-liquid surface potential at the substrate. The amplification is given by the substrate geometry, the drop and substrate dielectric properties and the Debye length within the liquid. Next to enabling an easy and low-cost way to measure surface- and Zeta potentials, the high drop voltages have implications for energy harvesting, droplet microfluidics and electrostatic discharge protection.

DY 52.4 Fri 10:30 H 0110

Electro(de)wetting with Photoswitches: Control of wetting by electric fields and light — •Billura Shakhayeva and Björn Braunschweig — University of Münster, Institute of Physical Chemistry, 48149 Münster, Germany

Electro-dewetting (EDeW) was introduced as a new method in order to change the wetting properties of surfaces. The underlying mechanism is, however, not fully understood and additional experiments

are needed. For that, we have replaced the DTAB surfactants used in the original work [1] by arylazopyrazole triethylammonium bromide (AAP-TB) which is a cationic surfactant that can change the surface tension at the air-water interface to a large extend through E/Z photoisomerization [2]. This offers to fine tune the contact angle during EDeW by E/Z photoisomerization of AAP-TB and we find a further increase in contact angle by ∼6° when the samples were irradiated by UV light that triggers photoisomerization from the E to the less surface-active Z isomer. Li et al.[1] suggested that surfactants are deposited on the silicon oxide surface through the EDeW process. In order to study the possible deposition of surfactants and the role of a possible prewetting layer outside of the drop and at some distance from the 3-phase contact line we have done sum-frequency generation (SFG) spectroscopy and find that surfactants are deposited even several mm adjacent to the drop and that their structure as well as the structure of the accompanying water layer changes drastically close to the 3-phase contact line. [1] Li et al. Nature, 572, 507-510 (2019) [2] Schnurbus et al. J. Phys. Chem. B 124, 6913 (2020).

DY 52.5 Fri 10:45 H 0110

Light-Triggered Manipulations of Droplets All in One: Reversible Wetting, Transport, Splitting, and Merging — •Maren Umlandt, Nino Lomadze, and Svetlana Santer — University of Potsdam, Potsdam, Germany

We report on light-triggered droplet manipulation such as reversible wetting, splitting, merging, and transport [1]. The unique feature is that the changes in the wetting properties of anisotropic liquids adsorbed on photo-switchable films can be triggered by application of optical stimuli, which lead to changes in the morphology of the surfaces. The adaptive films consist of an azobenzene-containing surfactant attached to oppositely charged polymer chains. Under exposure to irradiation with light, the azobenzene photo-isomerizes between trans- and cis-states, resulting in changes in surface energy and orientation of surfactant tails in film [2]. The increase in the surface temperature due to absorption of light by the azobenzene groups [3] enables diverse processes of droplet manipulation. Using a moving light spot, we demonstrate the locomotion of the droplet over macroscopic distances. Our findings could lead to the application of a programmable workbench for manipulating and operating an ensemble of droplets.

We thanks for funding DFG and RFBR.

[1] Umlandt, M. et al. ACS Applied Materials & Interfaces 2022 14 (36), 41412-41420 [2] Arya, P. et al. J. Chem. Phys. 2020, 152, 024904 [3] Zakharov, A. V.et al. Phys. Rev. E 2017, 96, 052705

15 min. break

Invited Talk DY 52.6 Fri 11:15 H 0110

Of Singularities and Controversies: The Soft Wetting Enigma — •Stefan Karpitschka — University of Konstanz

The surface mechanics of soft solids are ubiquitously important in nature and technology. Static and dynamic wetting of soft polymer gels by simple liquids has emerged as an archetypical model system: The singular capillary traction at the edge of a droplet creates a microscale wetting ridge which slows down dramatically the macroscopic dynamics. Capillary, elastic, viscous and osmotic effects all contribute simultaneously in a highly non-linear regime, which has sparked controversial discussions of the underlying theoretical description. In this talk I will present recent measurements on ultra-thin to ultra-soft materials, along with new theoretical and numerical results, scrutinizing sources of non-linear behavior in both statics and dynamics.

DY 52.7 Fri 11:45 H 0110

Dynamics of Moving Droplets on Lubricated Polymer Brushes — •Rodrique Badr[1], Lukas Hauer[2,3], Doris Vollmer[3], and Friederike Schmid[1] — [1]Johannes Gutenberg University, Mainz — [2]Humboldt-Universität zu Berlin, Berlin — [3]Max Planck Institute for Polymer Research, Mainz

The interaction of liquid droplets with lubricated substrates is rich with interesting physics combining thermodynamics, polymer science, and fluid dynamics, and has the potential for various industrial applications. In this work we focus on the dynamics of droplets moving on lubricated polymer brushes. In previous work, we showed the existence of a cloaking transition where the lubricant covers the surface of the droplet at equilibrium. Here, we investigate the influence of this cloak on the dynamics, in addition to its properties during the dynamical steady state. In addition, we investigate the characteristic of the wetting ridge, as well as the flow of the droplet, and quantify the friction forces felt by the droplet during its motion.

DY 52.8 Fri 12:00 H 0110

Modeling the growth of biofilms on soft substrates — •Anthony Pietz[1], Karin John[2], and Thiele Uwe[3] — [1]Institute for theoretical physics, University of Münster — [2]Institute for theoretical physics, University of Münster — [3]Research Associate at the CNRS Laboratoire Interdisciplinaire de Physique LIPhy Grenoble - France

We investigate the influence of substrate softness on biofilm growth amending the thin-film model developed by Trinschek et al for rigid solid substrates [1] by the inclusion of a simple description of an elastic substrate [2]. Wettability (described in the mesoscopic model by a wetting energy) is a key factor in the transition between arrested and continuous spreading on rigid substrates [1]. Our focus are changes in the spreading process with changing character of the substrate studied by time simulations of 2d drops/biofilms at fixed surface tension and initial drop volume. We find that with increasing softness from rigid via elastic to liquid-like substrate the spreading velocity of the biofilm decreases at fixed biofilm growth rate and wettability. Further, we discus how these changes depend on wettability and growth rate. In particular, we show that the transition between arrested and continuous spreading is for increasing softness shifted towards larger wettability and larger growth rate.

[1] S. Trinschek, K. John, S. Lecuyer, and U. Thiele, Phys. Rev. Lett. 119, 078003 (2017).

[2] C. Henkel, J. H. Snoeijer, and U. Thiele, Soft Matter 17, 10359 (2021).

DY 52.9 Fri 12:15 H 0110

Chemically Active Wetting — •Susanne Liese[1], Xueping Zhao[2], Christoph Weber[1], and Frank Jülicher[3] — [1]Faculty of Mathematics, Natural Sciences, and Materials Engineering: Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Department of Mathematical Sciences, University of Nottingham Ningbo China — [3]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Wetting of liquid droplets on passive surfaces is ubiquitous in our daily lives, and the governing physical laws are well-understood. When surfaces become active, however, the governing laws of wetting remain elusive. Here we derive the non-equilibrium thermodynamic theory for active wetting, where the surface is active due to a binding process that is maintained away from equilibrium. We show that active binding fundamentally changes the wetting behavior, leading to steady, non-equilibrium states with droplet shapes reminiscent of a pancake or a mushroom. The origin of such anomalous shapes can be explained by mapping to electrostatics, where pairs of binding sinks and sources correspond to electrostatic dipoles along the triple line. This is an example of a more general analogy, where localized chemical activity gives rise to a multipole field of the chemical potential. The underlying physics is relevant for cells, where droplet-forming proteins can bind to membranes accompanied by the turnover of biological fuels.

DY 52.10 Fri 12:30 H 0110

Intracellular wetting between biomembranes and liquid-like condensates — •Lukas Hauer[1], Katharina Sprobeck[1], Amir Houshang Bahrami[2,3], and Roland L. Knorr[1,4] — [1]Humboldt Univeristät zu Berlin — [2]Bilkent University, Ankara — [3]MPI-DS, Göttingen — [4]University of Tokyo

Wetting has been recently identified as physiologically important in fundamental cellular processes: phase-separated condensates (e.g., proteins and RNA) form liquid droplets in cells and interact with membranes, e.g., during autophagy in eukaryotic cells or protein storage in plant vacuoles. Upon contact, the droplets can exert wetting forces on the membrane that deforms. This creates a competition of mechanical forces of the membrane elasticity and the droplet capillarity, giving rise to elastocapillary phenomena. In this talk, I will present a minimal model system comprising giant lamellar vesicles (GUVs) filled with aqueous phase-separating polymers(PEG/Dextran). We create liquid-liquid interfaces inside GUVs by osmotic quenches, yielding deformed vesicles with excess membrane area. The excess membrane accumulates at the liquid-liquid interface and assumes differing morphologies, ranging from micro-tubules to sheets, to stomatocytes. We find that the morphology transition depends on the liquid-liquid surface tension. Our results will help to explain resembling in vivo observations during the morphogenesis of protein storage vacuoles in plants.

DY 53: Statistical Physics of Biological Systems III (joint session BP/DY)

Time: Friday 9:30–13:00 Location: H 2032

DY 53.1 Fri 9:30 H 2032

The Sun within: active processes from two-temperature models — •Faezeh Khodabandehlou and Christian Maes — Department of Physics and Astronomy KU Leuven, Leuven, Belgium

We propose an embedding of standard active particle models in terms of two-temperature processes. One temperature refers to an ambient thermal bath, and the other temperature effectively describes "hot spots," i.e, systems with few degrees of freedom showing important population homogenization or even inversion of energy levels as a result of activation. As a result, the effective Carnot efficiency would get much higher than for our standard macroscopic thermal engines, making connection with the recent conundrum of hot mitochondria. Moreover, that setup allows to quantitatively specify the resulting nonequilibrium driving, useful in particular for bringing the notion of heat into play, and making easy contact with thermodynamic features. Finally, we observe that the shape transition in the steady low-temperature behavior of run-and-tumble particles (with the interesting emergence of edge states at high persistence) is stable and occurs for all temperature differences, including close-to-equilibrium.

DY 53.2 Fri 9:45 H 2032

Irreversibility across a nonreciprocal PT-symmetry-breaking phase transition — •Henry Alston[1], Luca Cocconi[2], and Thibault Bertrand[1] — [1]Imperial College London, London, UK — [2]Max Planck Institute for Dynamics and Self-Organization, Gottingen, Germany

Nonreciprocal interactions are commonplace in continuum-level descriptions of both biological and synthetic active matter, yet studies addressing their implications for time-reversibility have so far been limited to microscopic models. We derive a general expression for the average rate of informational entropy production in the most generic mixture of conserved phase fields with nonreciprocal couplings and additive conservative noise. For the particular case of a binary system with Cahn-Hilliard dynamics augmented by nonreciprocal cross-diffusion terms, we observe a non-trivial scaling of the entropy production rate across a parity-time symmetry breaking phase transition. We derive a closed-form analytic expression in the weak-noise regime for the entropy production rate due to the emergence of a macroscopic dynamic phase, showing it can be written in terms of the global polar order parameter, a measure of parity-time symmetry breaking.

Invited Talk DY 53.3 Fri 10:00 H 2032

Bacterial transport in dilute and porous environments — •Christina Kurzthaler — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Unraveling the motion of microorganisms in dilute and porous media is important for our understanding of both the molecular basis of their swim gait and their survival strategies in microbial habitats. First, I will show that by using renewal processes to analyze experimental measurements of wild-type E. Coli, we can provide a quantitative spatiotemporal characterization of their run-and-tumble dynamics in bulk [1]. We further demonstrate quantitatively how the persistence length of an engineered strain can be controlled by a chemical inducer and characterize a transition from perpetual tumbling to smooth swimming. Second, I will address how this run-and-tumble gait evolves towards a hop-and-trap motility pattern of agents moving in a porous environment [2]. Using computer simulations, we discover a geometric criterion for their optimal spreading, which emerges when their persistence lengths are comparable to the longest straight path available in the porous medium. Our criterion provides a fundamental principle for optimal transport in densely-packed biological and environmental settings, which could be tested experimentally by using engineered cells and may provide insights into microbial adaption mechanisms.

[1] arXiv:2212.11222 (2022) [2] Nat. Commun. 12, 7088 (2021)

DY 53.4 Fri 10:30 H 2032

Signature of (anti)cooperativity in the stochastic fluctuations of small systems: application to the bacterial flagellar motor — •María-José Franco-Oñate[1], Andrea Parmeggiani[2], Jérôme Dorignac[2], Frédéric Geniet[2], Jean-Charles Walter[2], Francesco Pedaci[3], Ashley Nord[3], John Palmeri[2], and Nils-Ole Walliser[2] — [1]MPI Physics of Complex Systems, Dresden, Germany — [2]Laboratoire Charles Coulomb (L2C), Montpellier, France — [3]Centre de Biologie Structurale (CBS), Montpellier, France

The cooperative binding of molecular agents onto a substrate is pervasive in living systems. To study whether a system shows cooperativity, one can rely on the fluctuation analysis of quantities such as the number of substrate-bound units.

Using a general-purpose grand canonical Hamiltonian description of a small one-dimensional (1D) lattice gas with nearest-neighbour interactions as a prototypical example of a cooperativity-influenced adsorption processes, we elucidate how the strength of the interaction potential between neighbouring bound particles on the lattice determines the intensity of the fluctuations of the mean occupancy at steady state.

We then employ this relationship to compare the theoretical predictions of our model to data from single molecule experiments on bacterial flagellar motors (BFM). In this way, we find evidence that cooperativity controls the mechano-sensitive dynamical assembly of the torque-generating units, the so-called stators, onto the BFM.

DY 53.5 Fri 10:45 H 2032

A power-law growth model of pancreatic cancer precursor lesions — Ashley L. Kiemen[1], Denis Wirtz[1], and •David Zwicker[2] — [1]Departments of Pathology, Johns Hopkins University School of Medicine, Baltimore, MD, USA — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Pancreatic cancer often originates from microscopic precursor lesions in the pancreatic ducts. Recent evidence showed that even healthy people possess more and larger lesions than previously believed. A better understanding of the growth of these lesions may thus improve our ability to understand how a minuscule fraction transitions to invasive cancer. Using advanced imaging, we quantified >1,000 lesions and found that lesion size is distributed according to a power law with a fitted exponent of -1.7 over more than three orders of magnitude. To explain these data, we analyze several models of lesion growth and fit the predicted size distributions to the observed data. Our analysis suggests that lesions either (i) grow sub-exponentially and frequently seed new lesions or (ii) grow super-exponentially and frequently merge. Independent genomic mapping of lesions supports both alternatives, suggesting both are relevant. Our work demonstrates how combining experimental measurements of human tissues with dynamic modeling can improve understanding of cancer tumorigenesis.

15 min. break

DY 53.6 Fri 11:15 H 2032

Exclusion model of mRNA translation with collision-induced ribosome drop-off — Johannes Keisers[1] and •Joachim Krug[2] — [1]Centre de Biologie Structurale (CBS), Université de Montpellier, 34090 Montpellier, France — [2]Institute for Biological Physics, University of Cologne, 50937 Köln, Germany

The translation of messenger RNA transcripts to proteins can be modeled as a one-dimensional totally asymmetric exclusion process with extended particles. In this contribution we focus on the effects of premature termination of translation through the irreversible detachment of ribosomes. We consider a model where the detachment is induced by the unsuccessful attempt to move to an occupied site [1]. The model is exactly solvable in a simplified geometry consisting of the translation initiation region followed by a single slow site representing a translation bottleneck. In agreement with a recent experimental study, we find a non-monotonic dependence of the protein production rate on the initiation rate, but only if the leading particle in a colliding pair detaches. The homogeneous version of the model is related to an asymmetric reaction-diffusion model with a localized input of particles. We exploit this connection to show that, for long transcripts, the ribosome density decays asymptotically as the inverse square root of the distance to the initiation site.

[1] J. Keisers, J. Krug, J. Phys. A 56 (2023) 385601

DY 53.7 Fri 11:30 H 2032

Boundary geometry drives three-dimensional defect transitions in a polar fluid — •Pamela Guruciaga[1], Takafumi Ichikawa[2], Takashi Hiiragi[2,3], and Anna Erzberger[1,4] —

[1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Kyoto University, Kyoto, Japan — [3]Hubrecht Institute, Utrecht, The Netherlands — [4]Heidelberg University, Heidelberg, Germany

Motivated by observations of an interplay between apico-basal polarity and boundary geometry in mouse embryo morphogenesis, we develop a minimal model to address the role of boundaries—with emphasis on their geometry—in the surface-induced ordering of a 3D polar fluid. We find that, although material parameters are responsible for the creation of defects in the order parameter field, their location and structure are determined by the system geometry. We test our results in the experimental context of the mouse epiblast, where cells gradually align along their apico-basal axis and eventually form a fluid filled cavity (lumen) at their apical sides. Since field defects represent regions where the apical sides of the cells meet, changes in defect position can be relevant to lumen formation in the biological system. We compare our predictions with imaging data of the morphogenetic process for wild-type and genetically perturbed mice, finding a remarkable quantitative agreement without any fitting parameters. Our work provides insights into luminogenesis and embryonic viability, while paving the way for defect control by geometry manipulation in more general settings.

DY 53.8 Fri 11:45 H 2032

Optimal Memoryless Chemotaxis — •Jacob Knight[1], Paula García-Galindo[2], Johannes Pausch[1], and Gunnar Pruessner[1] — [1]Department of Mathematics, Imperial College London, South Kensington, London SW7 2BZ, UK — [2]Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS, UK

A wide array of biological systems can navigate in shallow gradients of chemoattractant with remarkable precision. Whilst previous models approach such systems using coarse-grained chemical density profiles, we construct a model consisting of a chemotactic cell responding to *discrete* cue particles, giving rise to novel phenomenology. For a cell without internal memory, we derive an effective velocity with which the cell approaches the source. This effective velocity is independent of the chemoattractant diffusivity, which can be tuned such that the cell can navigate in arbitrarily shallow chemical gradients. The effective velocity becomes negative beyond some homing radius, which represents an upper bound on the distance within which chemotaxis can be reliably performed.

DY 53.9 Fri 12:00 H 2032

Two-stage adaptive evolution in a rugged yet highly-accessible fitness landscape model with delayed commitment — •Muhittin Mungan[1], Suman G. Das[2], and Joachim Krug[1] — [1]Institute for Biological Physics, University of Cologne, Köln, Germany — [2]Institute of Ecology and Evolution, University of Bern, Bern, Switzerland

We study an empirically-motivated theoretical fitness landscape model of antibiotic-resistance evolution in bacteria [1]. The fitness of a genotype at any concentration depends on two parameters, the resistance level and the drugless growth rate, with a tradeoff between these. For intermediate concentrations fitness landscapes are rough while the fitness peaks are nevertheless highly accessible. Adaptation on such landscapes occurs in two stages. At first there is rapid accumulation of mutations and fast growth of fitness and resistance level along with a decrease in the drugless growth rate. Next there is slow growth of fitness and resistance level, and recovery of the drugless growth rate through the reversion of some of the mutations. We numerically demonstrate a robust pattern of evolution with qualitative features that are largely independent of specific model assumptions. The basins of individual fitness peaks overlap strongly, so that commitment to a peak is delayed substantially. An analytically tractable special case reproduces our findings rather well, shedding light on the nature of adaptive evolution, basins of fitness peaks and delayed commitment.

[1] S.G. Das et al. eLife 9:e55155 (2020)

DY 53.10 Fri 12:15 H 2032

Optimal memory with niche construction — •Edward Lee[1], Jessica Flack[2], and David Krakauer[2] — [1]Complexity Science Hub Vienna, Vienna, Austria — [2]Santa Fe Institute, Santa Fe, USA

Adaptation to changing environments is a universal feature of life and can involve the organism evolving or learning in response as well as actively modifying the environment to control selection pressures. The latter case couples the organism and environment together. Then, how quickly should the organism adapt in response to the changing environment? We formulate this question using a simple model of adaptive costs that considers timescales of memory and environment. We derive a general, sublinear scaling law for optimal memory as a function of environmental persistence, which encapsulates the trade-off between remembering vs. forgetting. The scaling holds for finite memory but a wide range of mediating factors. We then explore strategic game dynamics, uncovering a ratcheting mechanism that promotes reducing environmental volatility when niche constructors can monopolize benefits; conversely, niche destructors can dominate by degrading a shared environment. Finally, we compare the results with metabolic costs to predict that adaptive costs matter more for smaller organisms. Taken together, we predict stabilizing niche construction will evolve when environments are volatile and niches are separable, possibly enriching the behavioral repertoire of social organisms.

DY 53.11 Fri 12:30 H 2032

Interfaces as a probe for interactions in biological systems — •Nirvana Caballero — University of Geneva

Controlling cells, either individually or as a proliferating cell front, remains elusive because the plethora of interactions at widely varying lengthscales present in these systems leads to highly complex dynamical and geometrical properties. Interfaces separating regions of heterogeneous composition, or domains, can encode critical information about these systems' underlying physics. I will show how physical theories describing interfaces can be used to capture the microscopic interactions dominating a system. I will give examples at different scales from cell membranes [1], where the heterogeneous domain composition is key to biological function, to migrating colonies of cells, where interfaces reveal the main interactions present in a colony [2].

[1] NC, K. Kruse, T. Giamarchi. Phase separation on surfaces in the presence of matter exchange. Phys. Rev. E 108, L012801 (2023)

[2] Roughness and dynamics of proliferating cell fronts as a probe of cell-cell interactions. G. Rapin*, NC*, I. Gaponenko, B. Ziegler, A. Rawleight, E. Moriggi, T. Giamarchi, S. A. Brown, and P. Pruch, Sci. Rep. 11, 8869 (2021)

DY 53.12 Fri 12:45 H 2032

Heterogenity in Mucus by statistical analysis from particle tracking — •Thomas John, Sten Leipnitz, Enkeleda Meziu, and Christian Wagner — Campus, University Saarland, Saarbrücken, Germany

In the respiratory tract, cells constantly produce mucus that transports tiny dust particles out of the lungs. It's a protein solution that consists of more than 95% water. It's believed that the proteins form a heterogeneous network, but this cannot be resolved with light microscopy. We are investigating the diffusion behavior of nanoparticles (multi-particle tracking) in mucus and comparing it to glycerol-water mixtures with comparable viscosity. We show that the probability density function of individual particle diffusion coefficients D_i in mucus is significantly broader than expected from a homogeneous solution. The spatial autocorrelation of D_i also declines more slowly in mucus compared to glycerol-water mixtures. Experiments are compared with numerical simulations of Brownian motion. With these statistical analysis methods, we can support the model of a heterogeneous structure of mucus.

DY 54: Active Matter V (joint session BP/DY)

Time: Friday 9:30–13:00 Location: H 1028

DY 54.1 Fri 9:30 H 1028

Noise reduction with droplets of many components — •Tyler Harmon — Leibniz Institute for Polymer Research, Dresden, Germany

Noise control is critical for cell homeostasis and decision making. We previously showed that phase separation could be used to robustly reduce noise in phase separating systems. Others have suggested that noise buffering has the strongest suppression of noise parallel to the coexistence tie lines. They proposed that correlations from features such as coupled transcription could align the noise with the tie lines, significantly reducing the noise. Here we show how the kinetics associated with phase diagrams naturally aligns the noise to the tie lines. This helps optimize the noise reduction in systems with many components.

DY 54.2 Fri 9:45 H 1028

Pulsatile Control of Actomyosin Contraction — •James Clarke and José Alvarado — Department of Physics, The University of Texas at Austin, Austin, Texas, USA

Cells are always under control and tightly control their mechanics. The actomyosin cytoskeleton is one important cellular structure which receives control signals and turns that into contraction. Existing research has investigated the mechanical properties of actomyosin materials. However, these are usually in terms of responses to external stresses, which may be absent in living systems. Here we instead measure response to biochemical control signals. We apply a control-theoretical framework and investigate quasistatic actomyosin contractility in response to external pulsatile signals of UV light that release ATP molecules from light-sensitive NPE-cages. Across all experimental conditions, we report statistically indistinguishable maximum strains achieved by the gel. We find that the coupling from energy input to contractile strain is weakly nonlinear, with a s^{-2} dependence in Laplace space. Our novel characterization is not only an essential first step in a better understanding of how cells control cytoskeletal contractions via internal control signals. It is also an essential first step towards using biomimetic actomyosin active gels for microrobotic applications.

DY 54.3 Fri 10:00 H 1028

Self-assembly of myofibrils in muscle cells — Francine Kolley[1], Ian D. Estabrook[1], Clara Sidor[2], Clement Rodier[2], Frank Schnorrer[2], and •Benjamin M. Friedrich[1] — [1]Physics of Life, TU Dresden, Germany — [2]IBDM, Marseilles, France

Voluntary motions and heartbeat in animals is driven by contractions of myofibrils, millimeter-long acto-myosin bundles with characteristic periodic patterns of micrometer-sized sarcomeres. Yet, the physical mechanisms that drive the self-assembly of these "cytoskeletal crystals" are not understood. Here, we report data demonstrating that myosin molecular motors and actin-crosslinking Z-disc proteins form sarcomeric patterns first, while actin becomes polarity-sorted only hours later [1]. This data informs mathematical models of sarcomere self-assembly that are able to replicate periodic sarcomeric patterns, either through (i) non-local interactions between spatially-extended myosin filaments and Z-disc proteins, which bind to an actin scaffold, or (ii) catch-bond behavior of the prominent Z-protein α-actinin in response to active myosin forces. Both models are robust to small-number fluctuations for a wide parameter range in agent-based simulations, providing plausible mechanisms of early sarcomere self-assembly.
Next, even after the establishment of sarcomeric patterns, new sarcomeres are added to myofibrils, despite these being under mechanical tension. We report a new mechanism of controlled "self-rupture" in which a mother sarcomere divides into two daughter sarcomeres by splitting its myosin stack, and establishing a new Z-disc in between.
[1] https://www.biorxiv.org/content/10.1101/2023.08.01.551279v1

DY 54.4 Fri 10:15 H 1028

Size-coordination trade-off in Trichoplax adhaerens, an animal lacking a central nervous system — Mircea R. Davidescu[1], •Pawel Romanczuk[2,3], Thomas Gregor[4], and Iain D. Couzin[5,6,7] — [1]Dept. of Ecology and Evolutionary Biology, Princeton University, USA — [2]Dept. of Biology, Humboldt Universität zu Berlin, Germany — [3]Excellence cluster "Science of Intelligence", Berlin, Germany — [4]Lewis-Sigler Institute for Integrative Genomics, Joseph Henry Laboratories of Physics, Princeton University, USA — [5]Dept. of Collective Behaviour, Max Planck Institute for Animal Behavior, Konstanz, Germany — [6]Dept. of Biology, Chair of Biodiversity and Collective Behaviour, University of Konstanz, Germany — [7]Centre for the Advanced Study of Collective Behavior, University of Konstanz, Germany

Coordination with increasing size is a fundamental challenge affecting collective systems from biofilms to governments. The earliest multicellular organisms were decentralized, with indeterminate sizes and morphologies, as exemplified by Trichoplax adhaerens, arguably the earliest-diverged and simplest motile animal. We investigated the coordination in T. adhaerens by observing the degree of collective order in locomotion across animals of differing sizes and found that larger individuals exhibit increasingly disordered locomotion. We reproduced this effect using an active elastic cellular sheets model and show that this relationship is best recapitulated across all body sizes when the simulation parameters are tuned to criticality. We discuss possible implications of this on the evolution hierarchical structures such as nervous systems in larger organisms.

DY 54.5 Fri 10:30 H 1028

SwarmRL: Lowering the entry barrier to reinforcement learning for active matter research — •Samuel Tovey, Christoph Lohrmann, and Christian Holm — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

As scientists learn to better design and control devices at a microscopic scale, so too must the tools used to control these devices develop. Multi-agent reinforcement learning (MARL) is a powerful machine learning paradigm for learning control strategies in agents at all scales. Recent work has applied MARL to controlling microscopic agents, whether in learning chemo-taxis behaviour, object manipulation, or swarming.

This talk introduces SwarmRL, a powerful open-source library for applying MARL to microscopic environments. We demonstrate how SwarmRL is used in our group to control micro-scale agents in simulation and experiments and how to interpret the learned policies. The talk introduces the library broadly before looking into results from our recent work using SwarmRL, including a better understanding of the role of temperature on learned strategy and the emergence of chemotactic behaviour in unstable regimes. Finally, we discuss our vision for the future of the library and its integration into experiments and simulations.

DY 54.6 Fri 10:45 H 1028

Sensitive shape dependence in agent-based simulations of growth — •Jonas Isensee[1,2], Lukas Hupe[1,2], Ramin Golestanian[1,2,3], and Philip Bittihn[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Faculty of Physics, University of Göttingen, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom

We consider purely sterically interacting particles that grow and divide in two-dimensional confinement. Such models have been used to study cell dynamics in tissues and bacterial aggregates. A common feature in these is the rich emergent orientation dynamics due to anisotropic shapes, directed growth, and confinement. By introducing continuously tuneable tip variations around a common rod shape and characterizing the resulting orientation dynamics in space and time, we identify trends in the collective dynamics caused by certain shape features. In particular, we find a strong effect of small deviations from the traditional rod shape. Our results separate the effects of aspect ratio and particle shape, contribute to the characterization of the effective dynamics at large and intermediate length scales, and thereby also provide strategies for the design of future artificial systems.

15 min. break

Invited Talk DY 54.7 Fri 11:15 H 1028

Large scale collective dynamics of bacteria suspensions — •Eric Clement[1], Benjamin Perez Estay[1], Anke Lindner[1], Carine Douarche[2], Jochen Arlt[3], Vincent Martinez[3], Wilson Poon[3], and Alexander Morosov[3] — [1]PMMH-ESPCI, Sorbonne University, Paris , France — [2]FAST, University Paris-Saclay —

[3]School of Physics & Astronomy, University of Edinburgh

Fluids laden with swimming micro-organisms have become a rich domain of applications and a conceptual playground for the statistical physics of active matter. Such active bacterial fluids display original emergent phases as well as unconventional macroscopic transport properties, hence leading to revisit standard concepts in the physics and hydrodynamics of suspensions.

Here, I will present and discuss some recent advances on the spontaneous emergence of a "critical fluid" state for dense bacteria suspensions, characterized by a vanishing viscosity and and a divergent "active turbulence" scale controlled by the confinement. Close to the transition I will also describe a novel collective state leading to very large scale coherent motion of the bacteria.

DY 54.8 Fri 11:45 H 1028

Analysis techniques for active matter simulations — •Lukas Hecht, Kay-Robert Dormann, Aritra Mukhopadhyay, Kai Spanheimer, Mahdieh Ebrahimi, Suvendu Mandal, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, D-64289 Darmstadt, Germany

Simulations of active matter systems provide a promising route to understand collective phenomena and the non-equilibrium physics of active matter. Prominent models for active matter systems comprise particle-based models such as the active Brownian particle model and continuum models such as the active model B+. To analyze the data obtained from the numerical solution of these models, currently, many researchers develop in-house code. Here, we present the Active Matter Evaluation Package (AMEP), a unified framework to analyze active matter simulations. This Python library is easy to use and provides a powerful and simple interface for handling large data sets. The package features various methods for calculating observables, visualizing results, and analyzing data from molecular-dynamics, Brownian-dynamics, and continuum simulations. These features allow the user, for example, to easily calculate spatial and temporal correlation functions, to perform cluster analyses, to visualize simulation results, and to study phase separation, pattern formation, and critical phenomena in active matter systems.

DY 54.9 Fri 12:00 H 1028

Unveiling Active Fluctuations in Cellular Aggregates through Derivation of Hydrodynamic Transport — •Subhadip Chakraborti[1,2] and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

The biological functionality of cellular aggregates is a collective result of the activities and displacements of individual constituent cells. The theoretical characterization of this activity involves hydrodynamic transport coefficients, such as diffusivity and conductivity. Motivated by the clustering dynamics in bacterial microcolonies, we propose a model for active multicellular aggregates on 1D lattice. Employing macroscopic fluctuation theory, we derive a fluctuating hydrodynamics framework for this model system. Both semi-analytical theory and microscopic simulations reveal that non-equilibrium microscopic parameters exert a significant influence on the hydrodynamic transport coefficients, causing a notable decrease within the clusters. Additionally, we illustrate how the active nature of intercellular interactions disrupts the conventional Einstein relation that establishes a connection between transport coefficients and fluctuations. This study not only provides a comprehensive understanding of the hydrodynamic transport in bacterial microcolonies but also offers valuable tools for experimental investigations in other systems involving active cellular aggregates, such as tumor spheroids and organoids.

DY 54.10 Fri 12:15 H 1028

Expansion-flow driven orientation patterns in systems of growing rods — •Lukas Hupe[1,2], Jonas Isensee[1,2], Ramin Golestanian[1,2,3], and Philip Bittihn[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Faculty of Physics, University of Göttingen, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom

In densely-packed two-dimensional systems of growing rods, such as bacteria, a number of experimental and numerical studies report long-range nematic alignment in the presence of confinement. In some geometries, spatially heterogeneous preferred orientations are observed. So far, these effects have been qualitatively explained using continuum theories of growing active nematics adapted to the specific geometry under investigation.

Here, we first show how the shear rate tensor of the expansion flow alone can be used to qualitatively predict time-averaged orientation patterns from the geometry of the confinement. We apply this method to a series of example geometries and compare with results from agent-based simulations. To quantitatively describe alignment strength, we then develop a simple model which takes into account advection and explore its potential for cross-prediction across different geometries.

Our results provide a unifying theoretical framework and highlight the role of domain geometry in shaping nematic order of growing systems.

DY 54.11 Fri 12:30 H 1028

Walking the Road to Active Nematic Turbulence — •Malcolm Hillebrand[1,2] and Ricard Alert[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzerstr 38, Dresden 01187 — [2]Center for Systems Biology Dresden, Pfotenhauerstr 108, 01307 Dresden, Germany

Active matter, where internal energy consumption drives motion, exhibits a richly complex array of behaviours. In particular, the appearance of turbulent-like flows at very low Reynolds number, termed active turbulence, provides possibilities for chaotic fluid motion at scales as small as the surface of a cell. Here, in a hydrodynamic model of an active nematic, we thoroughly investigate the transition from smooth shear flow all the way to fully developed active turbulence. We utilise tools from dynamical systems theory, including Lyapunov exponents and time series analysis of velocity fields, as well as energy spectra and scaling laws, to describe the series of changes in dynamics that occur as we increase the activity. We find a sequence of increasingly unpredictable rearrangements between steady flow states that eventually give rise to continuously unstable chaos via a regime of apparent multistability. In addition, intermittent flow characteristics of fully active turbulent flows from simulations are compared to data from kinesin-microtubule experiments.

DY 54.12 Fri 12:45 H 1028

Activation fronts, fluctuations and criticality in the initiation of collective motion — •Parisa Rahmani[1], Hadrien-Matthieu Gascuel[2,3], Richard Bon[2], and Fernando Peruani[1,3] — [1]LPTM, UMR 8089, CY Cergy Paris Universite, 95302 Cergy-Pontoise, France — [2]CNRS, Centre de Recherches sur la Cognition Animale, F-31062 Toulouse Cedex 9, France — [3]Universite Cote d'Azur, Laboratoire J. A. Dieudonne, UMR 7351 CNRS, F-06108 Nice Cedex 02, France

Collective motion is generally not a continuous process, and collectives display repeated transitions from static to moving phases. The initiation of collective motion – of an initially static group – is a crucial process to ensure group cohesion and behavioral synchrony that remains largely unexplored. Here, we investigate the statistical properties of the initiation of collective motion. We find that the information propagates as an activation wave, whose speed is modulated by the velocity of the active agents, where both, the magnitude and direction of the agents' velocity play a crucial role. The analysis reveals a series of distinct dynamic regimes, including a selfish regimes that allow the first informed individuals to avoid predation by swapping position with uninformed individuals. Furthermore, we unravel the existence of a generic and intimate connection between the initiation of collective motion and critical phenomena in systems with an absorbing phase, showing that in a range of agents' velocities the initiation process displays criticality. The obtained results provide an insight in the way collectives distribute, process, and respond to the local environmental cues.

DY 55: Power Grids (joint session SOE/DY)

Time: Friday 9:30–10:00 Location: MA 001

Invited Talk DY 55.1 Fri 9:30 MA 001

Resilience of power grids against extreme events — •Mehrnaz Anvari — Fraunhofer Institute for Algorithms and Scientific Computing, Sankt Augustin, Germany

Societies are experiencing rapid and pressing changes in the way they generate and consume energy. As part of the necessary transformation towards carbon dioxide neutral energy networks, power systems are increasingly incorporating renewable energy sources (RES) into the energy mix. However, RES such as wind and solar power are inherently uncertain and intermittent, which can result in rapid transitions from maximum power to no power in just a few seconds. These non-Gaussian characteristics, combined with fluctuations in electricity consumption, can create vulnerabilities in the power system. This will be the main topic of the first part of this talk. In addition, to exploit the surplus of RES in other sectors such as transportation and heating, their coupling with power grid will become stronger. This means that failures in the power grid, driven by uncertain RES or extreme weather events can lead to cascading failures not only in the power grid but also in other sectors, creating a domino effect. Therefore, identifying the critical components in the complex power grid whose failures lead to large cascading failures is essential to improve the grid's resilience. In the second part of this talk, the co-evolution method will be introduced as a way of identifying these critical components.

DY 56: Many-body Quantum Dynamics II (joint session DY/TT)

Time: Friday 9:30–10:30 Location: A 151

DY 56.1 Fri 9:30 A 151

Cavity control of quantum materials — •Daniele Fausti — Friedrich Alexander University of Erlangen-Nuremberg

This seminar will focus on the potential of cavity electrodynamics in shaping material properties, opened by on our recent investigation into cavity-mediated thermal control of the metal-to-insulator transition in 1T-TaS2, which demonstrated the feasibility of reversible cavity manipulation of a phase transition in a correlated solid-state material. By immersing the charge density wave material 1T-TaS2 into cryogenic tunable terahertz cavities, we unveil a remarkable shift between conductive states. This transition, triggered by a substantial alteration in sample temperature, is controlled by mechanical adjustments of the distance between cavity mirrors and their alignment[1]. The discussion will extend to unpublished data on vibrational strong coupling within higher frequency cavities, emphasizing the position-dependent coupling strength that underscores the influence of the mode structure on the observed effects. Our findings rationalized in a scenario reminiscent of the Purcell effects, wherein the spectral profile of the cavity significantly shapes the energy exchange between the quantum material and the external electromagnetic field unfolds promising opportunities for tailoring the thermodynamics and macroscopic transport properties of quantum materials through strategic engineering of their electromagnetic surroundings. The seminar will discuss some perspectives for cavity control of material functionalities in correlated complex quantum materials.

[1] Nature 622, pages 487*492 (2023)

DY 56.2 Fri 9:45 A 151

Phase transition driven by ultrashort laser pulses in the charge-density-wave material $K_{0.3}MoO_3$ — •Rafael T. Winkler[1,2], Larissa Boie[1], Yunpei Deng[2], Matteo Savoini[1], Serhane Zerdane[2], Abhishek Nag[2], Sabina Gurung[1], Davide Soranzio[1], Tim Suter[1], Vladimir Ovuka[1], Janine Zemp-Dössegger[1], Elsa Abreu[1], Simone Biasco[1], Roman Mankowsky[2], Edwin J. Divall[2], Alexander R. Oggenfuss[2], Mathias Sander[2], Christopher Arrell[2], Danylo Babich[2], Henrik T. Lemke[2], Paul Beaud[2], Urs Staub[2], Jure Demsar[3], and Steven L. Johnson[1,2] — [1]Institute for Quantum Electronics, Physics Department, ETH Zurich, Zurich, Switzerland. — [2]SwissFEL, Paul Scherrer Institute, Villigen, Switzerland. — [3]Faculty - Institute of Physics, Johannes Gutenberg-University Mainz

Blue Bronze ($K_{0.3}MoO_3$) is a quasi 1D material exhibiting a charge density wave with a periodic lattice distortion (PLD). In a time resolved x-ray experiment at SwissFEL, we study the dynamics of the PLD by pumping $K_{0.3}MoO_3$ with short laser pulses and probing it using x-ray diffraction. We construct reciprocal space maps (RSM) of superlattice reflections at different delays. The RSM along the surface normal gets broader at the delay equal to half the amplitude mode oscillation period, indicating a transient inversion of the PLD. For longer delays, this broadening is not visible. However, the diffracted x-ray intensity drops below the unpumped value indicating a molten CDW near the surface.

DY 56.3 Fri 10:00 A 151

Equilibrium parametric amplification in Raman-cavity hybrids — •Hector Pablo Ojeda Collado[1,2], Marios H. Michael[3], Jim Skulte[1,2], Angel Rubio[3,4], and Ludwig Mathey[1,2] — [1]Center for Optical Quantum Technologies and Institute for Quantum Physics, University of Hamburg, 22761 Hamburg, Germany — [2]The Hamburg Center for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chausse 149, 22761 Hamburg, Germany — [4]Center for Computational Quantum Physics, The Flatiron Institute, 162 Fifth Avenue, New York, New York 10010, USA

Parametric amplification have led to extraordinary photo-induced phenomena in recent pump-probe experiments. While these phenomena manifest themselves in out-of-equilibrium settings, in this work, we present the striking result of parametric amplification in equilibrium. We demonstrate that quantum and thermal noise of a Raman-active mode amplifies light inside a cavity when the Raman mode frequency is twice the cavity frequency. This noise-driven amplification leads to the creation of an unusual parametric Raman polariton with smoking gun signatures in Raman spectroscopy. We show distinctive properties of this polariton, including localization and static shift of the Raman mode, together with an increase of quantum light fluctuations within the cavity. Our study suggests a resonant mechanism for controlling Raman modes and thus matter properties by cavity fluctuations. We conclude by outlining how to compute the Raman-cavity coupling, and suggest possible experimental realizations.

DY 56.4 Fri 10:15 A 151

Real-time transport of short electron pulses trough an impurity on a 1D quantum wire — •Thomas Kloss[1,2], Yuriel Nunez Fernandez[1,2], and Xavier Waintal[2] — [1]Univ. Grenoble Alpes, CNRS, Institut Néel, 38000 Grenoble, France — [2]Université Grenoble Alpes, CEA, Grenoble INP, IRIG, Pheliqs, F-38000 Grenoble, France

We study the transmission of pulses which are propagating through a weakly coupled impurity site, which is located on an infinitely long 1D tight-binding chain. For short pulses, the number of transmitted charges deviates from the adiabatic regime and shows a periodic dependence on the number of injected charges. In the limit of ultrashort pulses an analytic formula can be derived which matches perfectly the results obtained by numerical simulations using the Tkwant software. In a next step, a Hubbard-like interaction with strength U is added on the impurity site. Onside density and currents are obtained in a perturbative expansion in U using a real-time Green function approach. We apply a tensor-train technique to integrate over the high-dimensional integrals, which has been shown to outperform diagrammatic quantum Monte Carlo by orders of magnitude in speed an accuracy. The results are compared to self-consistent mean-field calculations and to the non-interacting limit.

DY 57: Networks: From Topology to Dynamics II (joint session DY/SOE)

Time: Friday 9:30–12:15 Location: BH-N 128

Invited Talk DY 57.1 Fri 9:30 BH-N 128

A simulation approach for the emerging mechanical properties of multi-network systems — •Kirsten Martens — CNRS & Univ. Grenoble Alpes

Network-forming materials are ubiquitous, from industrial products (tires, food, cosmetics...) to living organisms (e.g. in the cytoskeleton). Network-based materials often possess remarkable properties, such as high reversible deformability, light weight, optical transparency. Understanding the mechanical properties of multi-array gels at the molecular scale is essential to improve the quality of these new macromolecular architectures.

In this talk I will present a coarse grained numerical model for elastomer materials to address the question how these systems deform and fracture. Our double networks are characterised by a first pre-streched network that is close to failure coupled to a second floppy one that only breaks at later stages. We show that depending on the preparation protocol we can control the ductility of the double network depending on the volume fraction of the second network. Further we have direct access to the local bond breaking dynamics. We show that in single networks bond breaking events are strongly correlated in space and lead to brittle failure, whereas in double networks the damage is more delocalised promoting ductile failure. We show that this is the effect of a two stage process that can be controlled by the densities in the initial preparation protocol of the double network.

DY 57.2 Fri 10:00 BH-N 128

Topological data analysis applied to networks modeling porous media transport — •Lou Kondic[1], Matt Illingworth[1], Binan Gu[2], and Linda Cummings[1] — [1]New Jersey Institute of Technology, Newark, NJ, USA — [2]Worcester Polytechnic University, Worcester, MA, USA

We model porous medium as a random pore network and focus on the influence of the medium internal structure on its flow and adsorptive behavior. A particular focus is modeling suspension flow, where the particles adsorb on the pore walls. We first formulate the governing equations of fluid flow on a general network. Then, we model adsorption by imposing an advection equation with a sink term on each pore and study the influence of network parameters on the flow and transport. The presentation will focus on developing a better understanding of the connection between the topology of the medium (pore network) and the flow properties. The challenging aspect of understanding and quantifying evolving pore network topology is addressed by using topological methods that allow for simplified network descriptions, both regarding their static and their dynamic properties. For this purpose, we use tools based on persistent homology. These tools allow us to connect topology, transport, and adsorption as the basic step toward designing porous media of desired properties.

DY 57.3 Fri 10:15 BH-N 128

Stimulating self-optimisation of flow networks for transport — Julien Bouvard[1], •Swarnavo Basu[2], Charlotte Leu[3], Onurcan Bektas[2,3], Joachim Rädler[3], Gabriel Amselem[1], and Karen Alim[2] — [1]Laboratoire d'Hydrodynamique, CNRS, École polytechnique, Institut Polytechnique de Paris, France — [2]School of Natural Sciences, Technical University of Munich, Germany — [3]Soft Condensed Matter Group, Ludwig-Maximilians-Universität München, Germany

Transport of substances via fluid flow in networks is ubiquitous in biology (e.g. blood vasculature) and engineering (e.g. porous media). Many biological networks can self-organise in response to stimuli by homogenising flow to achieve optimal perfusion and transport. In contrast, engineered networks of random media have heterogeneous flow velocity distributions. Self-organising engineered networks that can homogenise flow will have many applications, e.g. cooling batteries, chemical reactors and *in vitro* vasculature for perfusing tissues and implants. We show, experimentally and theoretically, that self-optimisation can be achieved in networks with eroding walls. Perfusing such a network with short pulses of an eroding agent achieves homogenisation of flow velocities across the network, thus, providing us with a framework for engineering self-optimising networks.

DY 57.4 Fri 10:30 BH-N 128

Partial event coincidence analysis for distinguishing direct and indirect coupling in functional network construction — •Reik V. Donner[1,2] and Yong Zou[3] — [1]Magdeburg-Stendal University of Applied Sciences, Magdeburg, Germany — [2]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [3]East China Normal University, Shanghai, China

Correctly identifying interaction patterns from multivariate time series presents an important step in functional network construction. In this context, the widespread use of bivariate statistical association measures often results in a false identification of links because of strong similarity originating from indirect interaction or common drivers. In order to properly distinguish such direct and indirect links for the special case of event-like data, we present a partial version of event coincidence analysis (PECA) aimed at excluding possible transitive effects of indirect couplings. Using coupled chaotic systems and stochastic processes on two generic coupling topologies, we demonstrate that the proposed methodology allows for the correct identification of indirect interactions in case of just a few coupled systems. Finally, we apply PECA to multi-channel EEG recordings to investigate possible differences in coordinated alpha band activity among macroscopic brain regions in resting states with eyes open (EO) and closed (EC) conditions. Our approach leads to a significant reduction in the number of indirect connections and thereby contributes to a better understanding of the alpha band desynchronization phenomenon in the EO state.

DY 57.5 Fri 10:45 BH-N 128

Meta-reinforcement adds a second memory time-scale to random walk dynamics — •Gianmarco Zanardi[1,2], Paolo Bettotti[1], Lorenzo Pavesi[1], and Luca Tubiana[1,2] — [1]Physics Department, University of Trento, via Sommarive, 14 I-38123 Trento (IT) — [2]INFN-TIFPA, Trento Institute for Fundamental Physics and Applications, I-38123 Trento (IT)

Stochastic processes on networks have successfully been employed to model a multitude of phenomena. Non-Markovianity allows to account for history, introducing a memory effect that biases the evolution. Amongst all the variations that have been developed, in the reinforced random walk (RW) the walker is attracted towards its past trajectory: this process manifests emergent memory where edge weights in the network store information on the path of the RW.

We focus on this emergent memory feature and expand the model to introduce another memory level on a longer time-scale. We extend the reinforcement dynamics to feature a bounded non-linear function and a decay mechanism to interpret weights as short-term memory. We pair this with a second dynamics that is stochastic, irreversible and adapts the reinforcement function during the RW: the walk becomes "meta-reinforced". The result is a long-term memory form on top of the short-term one.

We simulate the RW on a recurrent feed-forward network under many parameter combinations to study the ability of the system to learn and recall traversal paths of the walker.

15 min. break

DY 57.6 Fri 11:15 BH-N 128

Exploiting memory effects to detect the boundaries of biochemical subnetworks — •Moshir Harsh[1], Leonhard Vulpius[1], and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen — [2]Department of Mathematics, King's College London, London WC2R 2LS, UK

Partial measurements of biochemical reaction networks are ubiquitous and limit our ability to reconstruct the topology of the reaction network and the strength of the interactions amongst both the observed and the unobserved molecular species. Here, we show how we can utilise noisy time series of such partially observed networks to determine which species of the observed part form its boundary, i.e. have significant interactions with the unobserved part. This opens a route to reliable network reconstruction. The method exploits the memory terms arising from projecting the dynamics of the entire network onto the observed subnetwork. We apply it to the dynamics of the Epidermal Growth Factor Receptor (EGFR) network and show that it works even for substantial noise levels.

DY 57.7 Fri 11:30 BH-N 128

Linear Stability of Adaptive Dynamical Networks — •Frank Hellmann — Potsdam Institute for Climate Impact Research

I present new stability results for heterogeneous adaptive dynamical networks. As a first application I present a universal stability condition for power grids based on the complex couplings formulation [1].

[1] https://arxiv.org/abs/2308.15285

DY 57.8 Fri 11:45 BH-N 128

Network Science and Beyond – Can Network Measures capture Mechanisms of Desynchronization in Complex Networks? — •Christian Nauck — Potsdam Institute for Climate Impact Research, Germany

This study addresses the fundamental question of how network function emerges from topology, particularly in nonlinear oscillator networks. While traditionally network measures have been discovered, recent advances in Machine Learning (ML), notably Graph Neural Networks (GNNs), provide an alternative for predicting network function. Through a comprehensive literature review, we identify 46 network measures, integrating them with conventional ML (NetSciML) to predict dynamic stability in power grids. Our findings reveal that a complete set of measures rivals GNNs in performance on the same ensemble, offering advantages such as reduced data requirements, shorter training times, and enhanced interpretability. However, NetSciML falls short in predicting stability across varied grid sizes, suggesting that GNNs employ a distinct and potentially more mechanistic approach. This underscores GNNs' potential to overcome challenges faced by current network science-based methods, providing novel solutions for desired outcomes.

DY 57.9 Fri 12:00 BH-N 128

Network dynamics in urban mobility: a case study of Berlin during and after COVID-19 — •Marlli Zambrano, Andrzej Jarynowski, and Vitaly Belik — Freie Universität Berlin, Berlin, Germany

In response to the urgent need for better models in the face of public health crises like the COVID-19 pandemic, this study presents a temporal network analysis of urban mobility and contact patterns in Berlin. To this end we leverage GPS mobile phone data (provided by Net Check GmbH) from 2020 and 2022, focusing on the month of November to reduce seasonal or holiday influences. The dataset encompasses 72,301 records with 14,908 nodes (persons) in 2020, and 96,844 records with 11,094 nodes in 2022. Two persons were in contact, if they spent at least 2 minutes on a 8x8 meters geolocation tile. Our approach highlights the temporal evolution of contact network clusters and community dynamics. We investigate the temporal motifs in people's movements between common locations like home and work, and the temporal heterogeneity in activity patterns. Our results indicate a significant temporal shift in mobility patterns during the pandemic, characterized by less path-like average nearest neighbor distances, as opposed to the post-pandemic period. Despite these temporal shifts, the frequency of contact motifs remained surprisingly consistent. This study not only offers a physics-focused lens on the impact of the pandemic on urban temporal networks but also paves the way for developing advanced models for urban dynamics in crisis situations.

DY 58: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Friday 9:30–12:15 Location: BH-N 243

DY 58.1 Fri 9:30 BH-N 243

Percolation in Suspensions of Rod-like Colloids under Shear Flow — •Victor Tänzel, Fabian Coupette, and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Suspensions of electrically conductive fillers are an interesting class of material for applications in energy storage and sensor technology. Their practicality depends on the behavior of the fillers, which is intricate and complex for elongated particles in flow.

We use multi-particle collision dynamics (MPC) to model rod-like particles in shear flow of a hydrodynamic medium. Percolation and conductivity are characterized with regard to the system's properties. MPC also allows us to turn off the hydrodynamic interactions from the solvent, so we can assess their influence.

DY 58.2 Fri 9:45 BH-N 243

orientational order and topological defects in a dilute solutions of rodlike polymers at low reynolds number — •Leonardo Puggioni[1,2], Stefano Musacchio[1], and Guido Boffetta[1] — [1]Dipartimento di Fisica and INFN, Università degli Studi di Torino, via P. Giuria 1, 10125 Torino, Italy — [2]Instituut-Lorentz, Leiden Institute of Physics, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

The relationship between the polymer orientation and the chaotic flow, in a dilute solution of rigid rodlike polymers at low Reynolds number, is investigated, by means of direct numerical simulations. It is found that the rods tend to align with the velocity field in order to minimize the friction with the solvent fluid, while regions of rotational disorder are related to strong vorticity gradients, and therefore to the chaotic flow. The "turbulent-like" behavior of the system is therefore associated to the emergence and interaction of topological defects of the mean director field, similarly to active nematic turbulence. The analysis has been carried out both in two and three spatial dimensions.

DY 58.3 Fri 10:00 BH-N 243

Phase Behaviour of Hard Convex Particles — •Poshika Gandhi and Anja Kuhnhold — Institute of Physics, University of Freiburg, Germany

The shape of a particle has a significant influence on its phase behaviour. A simple uniaxial particle, like a spherocylinder, produces a larger variety of phases as compared to a sphere. From the existence of the biaxial nematic phase to the search for a polar nematic one, simulations of hard particles of different shapes and symmetries continue to invoke interest.

We used Monte Carlo NVT simulations to produce phase diagrams of convex biaxial particles with both chiral and achiral compositions. The effect of particle shape on the phase behaviour and the effect of initial configurations on particles with C_{2v} symmetry was analysed. The results show generalised behaviour across particles of varying shapes and sizes which betters our understanding of the entropic forces in simulations of hard particles.

DY 58.4 Fri 10:15 BH-N 243

Stochastic rotational dynamics of strongly coupled superparamagnetic particles — •Andrey Kuznetsov[1], Sofia Kantorovich[1], Vladimir Zverev[2], and Ekaterina Elfimova[2] — [1]University of Vienna, Vienna, Austria — [2]Ekaterinburg, Russia

We report a theoretical study of the rotational dynamics of interacting superparamagnetic nanoparticles in time-varying magnetic fields. The research is motivated by an increasing interest in biomedical applications of magnetic nanoparticles (such as cancer hyperthermia or magnetic particle imaging). We consider an ensemble of spherical single-domain particles with a uniaxial crystallographic anisotropy. Particles are uniformly distributed in a 3D space, while their easy axes are either co-aligned or distributed at random. We develop a mean-field approach that allows one to describe the dynamics of the system magnetization under oscillating field of arbitrary frequency and magnitude. To test the validity of the theory, its predictions are compared to Langevin dynamics simulations. It is shown, that if the energy of dipolar interactions is comparable to the energy of thermal fluctuations, the theory works well in wide ranges of particle concentrations and anisotropy constants. However, at lower temperatures the agreement breaks down. In particular, for isotropic nanoparticles our theory predicts a Debye-like susceptibility spectrum with a single relaxation time. In simulations we instead observe an emergence of a uniform band of relaxation times, that broadens with the increase of dipolar coupling parameter.

DY 58.5 Fri 10:30 BH-N 243

Nonequilibrium evolution in long-range attractive systems: initial state dependence and averaging in simulations and theory — •Johannes Bleibel[1] and Martin Oettel[2] — [1]Fachbereich Physik, Universität Tübingen, Tübingen, Germany — [2]Institut für angewandte Physik, Universität Tübingen, Tübingen, Germany

We investigate the dynamics of the so–called capillary collapse of colloidal particles trapped a fluid interface with 1D Brownian Dynamics (BD) simulations and Dynamical Density Functional Theory (DDFT). Interfacially trapped, micrometer–sized colloidal particles interact via long–ranged capillary attraction. The interaction is formally analogous to screened Newtonian gravity with the capillary length λ as the tuneable screening length. Within intensive studies of the dynamics in 2D, it turned out that radially averaged DDFT only captures the dynamics at initial times and largely deviates from simulation results later on. This discrepancy has been traced to the role of an initially averaged configuration in DDFT[1].

In order to shed light on the precise role of initial fluctuations in the averaging process and subsequent dynamics both in BD simulations and DDFT, we investigate the dynamics of infinitely long rods trapped at a fluid interface and thus study the dynamics of a long–ranged attractive 1D fluid under a temperature quench. We apply several distinct averaging recipes for initial conditions and noise and discuss possible effects of averaging in an alternative description using Power Functional Theory (PFT).

[1] Bleibel, Domínguez, Oettel, JPCM 28, 244021 (2016)

15 min. break

DY 58.6 Fri 11:00 BH-N 243

Towards a standard model of liquid matter — •Alessio Zaccone — University of Milan, Department of Physics, 20133 Milan, Italy — Institute of Theoretical Physics, University of Göttingen, Germany

Our understanding of liquid matter made a leap in 20th century physics thanks to the successful mathematical and numerical development of pair correlation functions, which gave unprecedented insights into the structure of liquids. The same is however not true for the dynamical, mechanical and thermodynamic properties of liquids. The most striking example is the inability of celebrated theories to explain the specific heat of liquids or the propagation of acoustic waves in liquids as they are observed experimentally or in simulations. This of course includes the emergence of rigidity as a function of frequency of mechanical oscillation or as a function of confinement, and the Maxwell interpolation between viscous (Newton) and elastic (Hooke) limits, which has remained largely an empirical assumption in many theories of liquids and supercooled liquids, from generalized hydrodynamics to mode-coupling theory. In my talk I will show that these open issues can be understood mechanistically, and in comparison with experiments, by combining advances from different conceptual frameworks: i) the Instantaneous Normal Modes theory of liquid dynamics, and iii) the nonaffine response theory of liquids and glasses [1-3]. [1] A. Zaccone, "Theory of Disordered Solids", Springer, 2023, [2] A. Zaccone, Phys. Rev. E 108, 044101 (2023), [3] K. Trachenko and A. Zaccone, PNAS 117 (33) 19653-19655 (2020).

DY 58.7 Fri 11:15 BH-N 243

Dilute gel networks vs. clumpy gels in colloid-polymer mixtures — Matthias Gimperlein and •Michael Schmiedeberg — Inst. für Theor. Phys. 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The formation of gels differs from the behavior observed in other slowly relaxing systems [1,2]. A simple system to explore gelation is a colloid-polymer mixture, where there are complex heterogeneous phases due to the competition of short-ranged repulsions, depletion attractions, and longer-ranged screened Coulomb repulsions.

Here we study the differences of dense clumpy gels and dilute gel networks in terms of dynamics and structure formation. For example, we apply reduction algorithms [3,4] and observe that dilute and dense structures differ in the way structural properties like the typical thickness of the strands emerge. We also analyze the percolation behavior [5] and the formation of pentagonal bipyramids (as in [1]).

Finally we demonstrate that neural networks can be trained to recognize the differences between dilute gel networks and clumpy gels.

[1] H. Tsurusawa and H. Tanaka, Nat. Phys. **19**, 1171 (2023).
[2] M. Schmiedeberg, Nat. Phys. **19**, 1078 (2023).
[3] M. Gimperlein and M. Schmiedeberg, J. Chem. Phys. **154**, 244904 (2021).
[4] J. N. Immink, J. J. Erik Maris, R. F. Capellmann, S. U. Egelhaaf, P. Schurtenberger and J. Stenhammar, Soft Matter **17**, 8354 (2021).
[5] M. Kohl, R.F. Capellmann, M. Laurati, S.U. Egelhaaf, and M. Schmiedeberg, Nat. Comm. **7**, 11817 (2016).

DY 58.8 Fri 11:30 BH-N 243

Thermofluidic Non-equilibrium assembly of Functional Structures — •Desmond Quinn, Diptabrata Paul, and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig

Assembly in equilibrium is dictated by static energy landscapes. Non-equilibrium assembly on the other hand is driven by fluxes that can be controlled by external energy inputs, enabling reconfigurable structures. The non-equilibrium assembly of colloids was explored here, which was mediated by optically driven heat dissipation. The heat dissipated leads to thermofluidic flows and osmotic pressures that drive the colloidal particle towards the heated regions and lead to the formation of ordered structures.

The mechanisms of assembly were disentangled, and the growth dynamics of the structures was modeled. 3D structures were found to assembly in a matter of a few minutes, and the growth dynamics was found to be dependent on the particle fluxes. Analysis of the structure revealed its crystallinity. The emergent photonic properties of such colloidal crystal structures were investigated. A photonic stopband was observed and fit well with theoretical expectations. Furthermore, the photonic property could be modulated by modulating the assembled structure. This shows that non-equilibrium processes could be useful in assembly of reconfigurable functional materials. The manipulation of bacteria was also explored, which is useful to study bacterial interactions.

DY 58.9 Fri 11:45 BH-N 243

Analysing seismic waves and velocities including interference effects in granular matter of volcanoes — •Regine Frank[1,2], Marcel van Laaten[3], Birger Lühr[4], and Ulrich Wegeler[3] — [1]College of Biomedical Sciences, Larkin University, Miami, Florida, USA — [2]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain — [3]Institut für angewandte Geowissenschaften, Friedrich-Schiller-Universitaet Jena — [4]Deutsches GeoforschungsZentrum GFZ, Helmholtz-Zentrum Potsdam

We present self consistent diagrammatic transport theory and numerical solutions for the analysis of seismic waves and velocities including interference effects in granular matter of volcanoes. We introduce weighted essentially non-oscillatory solvers (WENO) which are suitable to treat extreme non-linear properties and rogue waves. We compare our numerical results to recent experiments and several other theoretical models.

[1] A. Lubatsch, R. Frank, Phys. Rev. Research 2, 013324 (2020) [2] C. Sens-Schönfelder, U. Wegler, Geophys. Res. Lett., v. 33, no. 21, L21302 (2006) [3] U. Wegler, B.-G. Lühr, R. Snieder, A. Ratdomopurbo, Geophys. Res. Lett., v. 33, L09303 (2006) [4] C. Friedrich, U. Wegler, Geophys. Res. Lett., v. 32, L14312, (2005)

DY 58.10 Fri 12:00 BH-N 243

Optimal low-resolution representations as a probe of a system's emergent features — •Raffaello Potestio — University of Trento, Trento, Italy

Gathering data from computer simulations of soft and biological matter systems is becoming increasingly easy as our available computational power keeps growing. While hoarding data is thus "easy", making sense of them is a fully different story. Here, I will illustrate how information can be extracted from data by leveraging reduced representations, that is, by looking at the system under examination in terms of a wisely chosen subset of its constituents - be these atoms, spins, pixels, or else. Taking the moves from the theory of bottom-up coarse-graining in soft matter, it is possible to show that the level of resolution at which a system is described can be leveraged as a magnifying glass to investigate its properties, and that a precise notion of optimal resolution level can be given that is tightly connected with its key emergent features.

DY 59: Brownian Motion and Anomalous Diffusion

Time: Friday 9:30–13:00 Location: BH-N 334

DY 59.1 Fri 9:30 BH-N 334

Being heterogeneous is advantageous: Extreme Brownian non-Gaussian searches — •Vittoria Sposini — Faculty of Physics, University of Vienna, Vienna (Austria)

Diffusing diffusivity models, polymers in the grand canonical ensemble and polydisperse, and continuous time random walks, all exhibit stages of non-Gaussian diffusion. Is non-Gaussian targeting more efficient than Gaussian? In this talk I will show that non-Gaussian rare fluctuations in Brownian diffusion dominates extreme searches, introducing drastic corrections to the known Gaussian behavior. Our demonstration entails different physical systems and pinpoints the relevance of diversity within redundancy to boost fast targeting.

Joint work with Sankaran Nampoothiri, Aleksei Chechkin, Enzo Orlandini, Flavio Seno, and Fulvio Baldovin.

DY 59.2 Fri 9:45 BH-N 334

Non-Gaussian displacements in active transport on a carpet of motile cells — •Robert Grossmann[1], Lara S. Bort[1], Ted Moldenhawer[1], Setareh Sharifi Panah[1], Ralf Metzler[1,2], and Carsten Beta[1] — [1]University of Potsdam, Potsdam, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang, Republic of Korea

In this talk, we discuss the dynamics of micron-sized particles on a layer of motile cells [1]. This cell carpet acts as an active bath that propels passive tracer particles via direct mechanical contact. The resulting nonequilibrium transport shows a crossover from superdiffusive to normal-diffusive dynamics. The particle displacement distribution is distinctly non-Gaussian even in the limit of long measurement times—different from typically reported Fickian yet non-Gaussian transport, for which Gaussianity is restored beyond some system-specific correlation time. We obtain the distribution of diffusion coefficients from the experimental data and introduce a model for the displacement distribution that matches the experimentally observed non-Gaussian statistics. We argue why similar transport properties are expected for many composite active matter systems.

[1] Großmann, Bort, Moldenhawer *et al.* (2023) arXiv:2311.05377

DY 59.3 Fri 10:00 BH-N 334

Brownian particle in a Poisson-shot-noise active bath: exact statistics, effective temperature, and inference — •costantino di bello[1], rita majumdar[2,3], rahul marathe[2], ralf metzler[1,4], and edgar roldan[3] — [1]Institute of Physics & Astronomy, University of Potsdam, Germany — [2]Department of Physics, Indian Institute of Technology, New Delhi, India — [3]ICTP - The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy — [4]Asia Pacific Centre for Theoretical Physics, Pohang, Republic of Korea

This work studies the fluctuating, nonequilibrium dynamics of an optically trapped Brownian particle within a dilute solution of active particles. The authors propose a stochastic model in which the particle moves in a harmonic potential and experiences both thermal and Poisson shot-noise kicks with specified amplitude distribution due to moving active particles in the bath. A variety of exact analytical results for the particle position statistics are derived, like mean, variance, skewness and excess kurtosis. Interestingly, the positions' distribution, for any choice of the parameters of the system, is leptokurtic, in accordance with recent experimental studies.

The work also sheds light on when and how to use the notion of effective temperature in such active systems.

DY 59.4 Fri 10:15 BH-N 334

Run-and-trap motility of self-propelled particles — •Agniva Datta, Sönke Beier, Veronika Pfeifer, Carsten Beta, and Robert Grossmann — University of Potsdam, Potsdam, Germany

In many experimental manifestations of active matter, self-propelled particles have been observed to exhibit dynamic transitions between different states of motility that are characterized by various features such as velocity and rotational diffusion coefficients as well as their duration. These multi-state motility behaviors often result in non-Gaussian statistics, anomalous diffusion and ergodicity breaking. We introduce a comprehensive dynamical motility model for self-propelled particles whose active run motility is intermittently interrupted by a trap state as it is observed, for example, for active motion in disordered media. Thereby, we provide a unified framework to study Lévy walks, classical continuous-time random walks and active diffusion models such as active Brownian motion, run-and-tumble or run-and-reverse. We analytically derive expressions for essential quantities, including mean-squared displacements and diffusion coefficients, crucial for understanding the intricacies of these processes. We illustrate the applicability of our model to experimental data using the example of soil bacteria spreading in agar.

DY 59.5 Fri 10:30 BH-N 334

Machine-Learning-Based Classification of Anomalous Diffusion - How well does it generalize? — •Henrik Seckler[1], Janusz Szwabiński[2], and Ralf Metzler[1] — [1]University of Potsdam, Germany — [2]Wrocław University of Science and Technology, Poland

Single-particle traces of the diffusive motion of molecules, cells, or animals are by now routinely measured, similar to stochastic records of stock prices or weather data. Deciphering the stochastic mechanism behind the recorded dynamics is vital in understanding the observed systems. Typically, the task is to decipher the exact type of diffusion and/or to determine the system parameters. The tools used in this endeavor are currently being revolutionized by modern machine-learning techniques. As such methods are often criticized for their lack of interpretability, we focus on means to include uncertainty estimates and feature-based approaches, both improving interpretability and providing concrete insight into the learning process of the machine. We expand the discussion by examining predictions on different out-of-distribution data.

DY 59.6 Fri 10:45 BH-N 334

First-passage area distribution and optimal fluctuations of fractional Brownian motion — •Alexander K. Hartmann[1] and Baruch Meerson[2] — [1]University of Oldenburg, Germany — [2]Hebrew University of Jerusalem, Israel

We study the probability distribution $P(A)$ of the area $A = \int_0^T x(t)dt$ swept under fractional Brownian motion (fBm) $x(t)$ until its first passage time T to the origin. The process starts at $t = 0$ from a specified point $x = L$. We show that $P(A)$ obeys the exact scaling relation $P(A) = \frac{D^{\frac{1}{2H}}}{L^{1+\frac{1}{H}}}\,\Phi_H\left(\frac{D^{\frac{1}{2H}}A}{L^{1+\frac{1}{H}}}\right)$, where $0 < H < 1$ is the Hurst exponent characterizing the fBm, D is the coefficient of fractional diffusion, and $\Phi_H(z)$ is a scaling function. The small-A tail of $P(A)$ has been recently predicted [1] as having an essential singularity at $A = 0$. Here [2] we determine the large-A tail of $P(A)$. It is a fat tail, with the average value A diverging for all H. We also verify the predictions for both tails by performing simple-sampling as well as large-deviation Monte Carlo [3] simulations. The verification includes measurements of $P(A)$ up to probability densities as small as 10^{-190}. We also perform direct observations of paths conditioned on the area A. For the steep small-A tail of $P(A)$ the "optimal paths", *i.e.* the most probable trajectories of the fBm, dominate the statistics. Finally, we discuss extensions of theory to a more general first-passage functional of the fBm.

[1] B. Meerson and G. Oshanin, Phys. Rev. E **105**, 064137 (2022).
[2] A.K. Hartmann and B. Meerson, preprint arXiv:2310.14003 (2023).
[3] A.K. Hartmann, Phys. Rev. E **89**, 052103 (2014).

DY 59.7 Fri 11:00 BH-N 334

Density fluctuation analysis of biological matter — •Conrad Möckel[1,2,3], Abin Biswas[1,2,4], Simone Reber[4], Vasily Zaburdaev[2,3], and Jochen Guck[1,2,3] — [1]Max Planck Institute for the Science of Light, 91058 Erlangen, Germany — [2]Max Planck Zentrum für Physik und Medizin, 91058 Erlangen, Germany — [3]Friedrich Alexander Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [4]Max Planck Institute for Infection Biology, 10117 Berlin, Germany

The characterization of the dynamical properties of biological matter plays an important role in unraveling its complexity and associated functions. Here we employ differential dynamic microscopy in combination with bright field microscopy to probe and evaluate the inherent density fluctuations at present in the sample under study. Using theoretical models, this approach allows for quantification of the time and length scale dependent viscoelastic properties of optically transparent

systems as demonstrated for high speed supernatant (HSS) *Xenopus laevis* egg extract. We find that upon microtubule formation, the HSS exhibits subdiffusive characteristics at two distinct time scales which can be connected to dynamical caging and escape events. Our findings illustrate the relevance of this methodology for characterizing dynamical heterogeneities of cytoplasm non-invasively, beyond multiple particle tracking.

15 min. break

DY 59.8 Fri 11:30 BH-N 334

The Role of Cross-Correlations in the Fluctuation-Dissipation-Theorem of the Generalized Langevin Equation — •Niklas Wolf, Viktor Klippenstein, and Nico van der Vegt — TU Darmstadt, 64287 Darmstadt, Germany

In molecular dynamics, the development of dynamically consistent coarse-grained models revolves around modeling friction and random forces to reintroduce fluctuations in the force that are lost when choosing a more coarse description of a problem/system. Modeling these fluctuations with Markovian approaches like the Langevin equation or dissipative particle dynamics assumes time scale separation between the degrees of freedom in the atomistic and coarse model. Usually, this is not given in condensed matter systems but can be accounted for with non-Markovian models like the generalized Langevin equation (GLE), which we focused on in this work.

Recent works[1, 2] have demonstrated that for a GLE with position-independent friction, the usual second fluctuation-dissipation theorem connecting friction and random force should be modified with a cross-correlation term. We investigated these cross-correlations and their effect on dynamic properties in several model systems and found that discarding them does generally not lead to a correct description of the dynamics. To remedy this, we discuss different approaches to include cross-correlations in a GLE equation of motion.

[1] V. Klippenstein, N. F. A. van der Vegt, *J. Chem. Phys.* **154**, 191102 (2021)

[2] H. Vroylandt, *EPL* **140**, 62003 (2022)

DY 59.9 Fri 11:45 BH-N 334

Iterative parameterization of Markovian embedded generalized Langevin equations for molecular dynamics — •Viktor Klippenstein, Niklas Wolf, and Nico F. A. Van Der Vegt — Technical University of Darmstadt, Darmstadt, Germany

In molecular dynamics, coarse-grained (CG) models which aim to describe dynamic properties consistently with the underlying fine-grained (FG) system, typically introduce some dissipative thermostat to account for friction and fluctuations due to removed degrees of freedom. In many cases, the time scales of CG and FG degrees of freedom are not separated which necessitates a non-Markovian (NM) description typically based on a generalized Langevin equation (GLE).

To keep the CG models tractable, we augment the Hamiltonian equation of motion by individually coupling every coarse-grained particle to an isotropic GLE thermostat, where NM friction is fully characterized by a single scalar function termed memory kernel. For computational efficiency, the NM GLE thermostat can be mapped on a Markovian auxiliary variable thermostat (aux-GLE). While our recently introduced method (iterative optimization of memory kernels (IOMK)[1]) allows for efficient optimization of the GLE the parameterization of the aux-GLE is by itself non-trivial, and potentially both error-prone and computationally expensive. To sidestep this problem, we propose a Gauss-Newton type method (IOMK-GN), which allows us to directly optimize the aux-GLE parameters.

[1] Klippenstein V., van der Vegt N. F. A., *J. Chem. Theory Comput.* 2023, 19, 4, 1099-1110

DY 59.10 Fri 12:00 BH-N 334

Concentration-of-measure in time-average statistical mechanics — •Rick Bebon and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Nowadays, state-of-the-art single-molecule or particle-tracking experiments provide direct access to path-dependent observables by probing individual trajectories. Obtained by means of time-averaging a limited number of individual realizations each with a finite duration, inferred estimates are typically afflicted by large systematic uncertainties, making a correct interpretation *a priori* non-trivial. Recent theoretical advances motivate a deeper understanding of fluctuating path-observables, as the latter would allow for decoding important and otherwise hidden information about the underlying microscopic dynamics. Reliably interpreting sample-to-sample fluctuations of time-averaged functionals of noisy trajectories therefore remains a crucial but challenging task, especially in the presence of subsampling. Instigated by these difficulties, we propose a non-asymptotic concentration-of-measure perspective on functionals of overdamped Langevin dynamics that allows a general and correct rationalization of time-averaged observables and their fluctuations for arbitrary times. Subsequently, we demonstrate how bounding the probability that an individual realization deviates from the mean value by more than any fixed amount provides a new outlook on time-averaged observables.

DY 59.11 Fri 12:15 BH-N 334

Langevin Dynamics of Oriented Active Particles on Curved Surfaces — •Balázs Németh and Ronojoy Adhikari — Department of Applied Mathematics and Theoretical Physics, Centre for Mathematical Sciences, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, United Kingdom

The motion of active particles constrained to curved surfaces is an intriguing problem with wide range of applications in biological physics and soft matter, from rotating motors on membranes to Janus particles on interfaces. In this talk, we construct Langevin equations for oriented active particles on fixed surfaces using differential geometric principles. We derive the deterministic equations of motion for the translational and rotational velocities in the body frame of the particle in Hamiltonian form. We find that surface curvature couples the linear and angular momenta of the particle. To these Hamiltonian equations, we add linear friction and white noise to obtain a generalized Ornstein-Uhlenbeck process in phase space. We obtain the corresponding Fokker-Planck equation and the fluctuation-dissipation relation. The equations of Brownian dynamics are derived by adiabatically eliminating the momenta. These can be used to simulate biophysical diffusion processes on surfaces.

DY 59.12 Fri 12:30 BH-N 334

Depinning transition of self-propelled particles — Arthur Straube[1,2] and •Felix Höfling[2,1] — [1]Zuse Institute Berlin — [2]Fachbereich Mathematik und Informatik, Freie Universität Berlin

A depinning transition is observed in a variety of contexts when a certain threshold force must be applied to drive a system out of an immobile state. A well-studied example is the depinning of colloidal particles from a corrugated landscape, whereas its active-matter analogue has remained unexplored. Here, we discuss how active noise due to self-propulsion impacts the nature of the transition [1]: it causes a change of the critical exponent from 1/2 for quickly reorienting particles to 3/2 for slowly reorienting ones. In between these analytically tractable limits, the drift velocity exhibits a superexponential behavior as is corroborated by high-precision data. Giant diffusion phenomena occur in the two different regimes. Our predictions appear amenable to experimental tests, lay foundations for insight into the depinning of collective variables in active matter, and are relevant for any system with a saddle-node bifurcation in the presence of a bounded noise.

[1] A.V. Straube, F. Höfling, under review with Phys. Rev. Lett. (preprint arXiv:2306.09150).

DY 59.13 Fri 12:45 BH-N 334

Coupled long-time dynamics in binary mixtures of colloidal Yukawa-systems — •Daniel Weidig and Joachim Wagner — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

We investigate structure and dynamics of binary mixtures consisting of particles interacting via a screened Coulomb potential. In mixtures of equally charged, but differently sized particles, the partial correlation functions $g_{\mathrm{AA}}(r) = g_{\mathrm{AB}}(r) = g_{\mathrm{BB}}(r)$ and thus partial static structure factors are identical due to identical time-averaged interactions between all present species. Different particle sizes, however, yield different Stokes-Einstein diffusion coefficients with $\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = D_{0,\mathrm{B}}/D_{0,\mathrm{A}}$. Mediated by electrostatic interactions, different mobilities of the species influence the long-time diffusion: In presence of a smaller species, the long-time diffusion of the larger species is accelerated and vice versa as visible both in self- and collective dynamics. A nearly universal dependence of the relative acceleration or deceleration of long-time self-diffusion coefficients in mixtures on the product of size-ratio $\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}}$ of the larger to the smaller species and number-density ratio ϱ_i^*/ϱ_i is observed. Here, ϱ_i^* denotes the number density of species i in a suspension containing only species i and ϱ_i the number density of species i in a mixture. The magnitude of the relative acceleration or deceleration depends in first approximation on the electrostatic interaction at the maximum $r_{\max}$ of the pair correlation functions $g_{ij}(r)$.

DY 60: Quantum Dynamics, Decoherence and Quantum Information (joint session DY/TT)

Time: Friday 10:45–13:00 Location: A 151

DY 60.1 Fri 10:45 A 151

Photon-Resolved Floquet Theory and its Application to Quantum Communication — •Georg Engelhardt[1], Sayan Choudhury[2,3], W. Vincent Liu[2,1], JunYan Luo[4], Victor M. Bastidas[5,6], and Gloria Platero[7] — [1]Southern University of Science and Technology, Shenzhen, China — [2]University of Pittsburgh, Pittsburgh, USA — [3]Harish Chandra Research Institute, UttarPradesh, India — [4]Zhejiang University of Science and Technology, Hangzhou, China — [5]NTT Research, Sunnyvale, USA — [6]Massachusetts Institute of Technology, Cambridge, USA — [7]Instituto de Ciencia de Materiales de Madrid ICMM-CSIC, Madrid, Spain

The semiclassical analysis of Floquet systems can not account for quantum-optical phenomena that rely on the quantized nature of light. Here, we go beyond the semiclassical description by unifying Floquet theory with quantum optics using the framework of Full-Counting Statistics. This formalism, which we dub 'Photon-resolved Floquet theory' (PRFT), is based on two-point tomographic measurements, instead of the two-point projective measurements used in standard Full-Counting Statistics [1,2]. The PRFT predicts the generation of macroscopic light-matter entanglement when atoms interact with multimode electromagnetic fields, thereby leading to complete decoherence in the Floquet-state basis. Employing the PRFT, we propose a quantum communication protocol that may outperform the state-of-art few-photon protocols by two orders of magnitude or better.

[1] G. Engelhardt et al., arXiv:2207.08558 [2] G. Engelhardt et al., arXiv:2311.01509

DY 60.2 Fri 11:00 A 151

Information currents in disordered region — •Nicolas Bauer and Björn Trauzettel — Julius Maximilians Universität Würzburg, Würzburg, Germany

The information lattice is a tool to organize quantum information into different scales and allows the definition of local information and information currents. Hence, it allows to study the flow of information in various systems. We apply the information lattice to a hybrid quench-probe setup, where one part of the system undergoes a quench while another part remains inert. The quench creates a propagating entanglement wave packet, visible in the information lattice, and we study how a disordered region in the probe affects this information current, i.e. scattering and localization of information within the disordered region. In addition, the hybrid setup has an energy selective coupling feature, which allows us to analyze and compare the scattering/localization properties of e.g. fermions at varying energy levels or topological excitations like Majorana zero modes.

DY 60.3 Fri 11:15 A 151

Single-Qubit Error Mitigation by Simulating Non-Markovian Dynamics — •Mirko Rossini, Dominik Maile, Joachim Ankerhold, and Brecht Donvil — Institute for Complex Quantum Systems and IQST, Ulm, Germany

Quantum simulation is a powerful tool to study the properties of quantum systems. The dynamics of open quantum systems are often described by completely positive (CP) maps, for which several quantum simulation schemes exist. Such maps, however, represent only a subset of a larger class of maps: the general dynamical maps which are linear, Hermitian preserving, and trace-preserving but not necessarily positivity preserving. In this talk, I show a simulation scheme for these general dynamical maps, which occur when the underlying system-reservoir model undergoes entangling (and thus non-Markovian) dynamics. Such maps also arise as the inverse of CP maps, which are commonly used in error mitigation. Our simulation scheme is illustrated on an IBM quantum processor, demonstrating its ability to recover the initial state of a Lindblad evolution. This paves the way for a novel form of quantum error mitigation. Our scheme only requires one ancilla qubit as an overhead and a small number of one and two-qubit gates. Consequently, we expect it to be of practical use in near-term quantum devices.

DY 60.4 Fri 11:30 A 151

Generalisation of the Landauer-Buettiker theory onto the case of dissipative contacts — •Andrey Kolovsky — Krasnoyarsk, Russia

We revisit the problem of two-terminal transport of non-interacting Fermi particles in a mesoscopic device by employing the semi-microscopic model for the contacts, where we mimic the self-thermalisation property of the contacts by using the Lindblad relaxation operators. It is argued that the dissipative dynamics of the contacts causes partial decoherence of the quantum states of fermionic carriers in the device which, in its turn, can essentially modify the system conductance as compared to predictions of the standard Landauer-Buettiker theory.

DY 60.5 Fri 11:45 A 151

Iterative construction of conserved quantities in dissipative nearly integrable systems — •Iris Ulčakar[1,2] and Zala Lenarčič[1] — [1]Jožef Stefan Institute, 1000 Ljubljana, Slovenia — [2]University of Ljubljana, Faculty for physics and mathematics, 1000 Ljubljana, Slovenia

Integrable systems offer rare examples of solvable many-body problems in the quantum world. Due to the fine-tuned structure, their realization in nature and experiment is never completely accurate, therefore effects of integrability are observed only transiently. One way to surpass that is to couple nearly integrable systems to baths and driving: these will stabilize integrable effects up to arbitrary time, as encoded in the time dependent, and eventually, the stationary state of form of a generalized Gibbs ensemble. However, the description of such driven dissipative nearly integrable models is challenging and no exact analytical methods have been proposed so far. Here we develop an iterative scheme in which integrability breaking perturbations (baths) determine the most necessary conserved quantities to be added into a truncated generalized Gibbs ensemble description. Our scheme significantly reduces the complexity of the problem, paving the way for thermodynamic results.

DY 60.6 Fri 12:00 A 151

Quantum thermodynamics of impurity models using the principle of minimal dissipation — •Salvatore Gatto, Alessandra Colla, Heinz-Peter Breuer, and Michael Thoss — University of Freiburg

Quantum thermodynamics has witnessed significant attention and advancement in recent years. A central challenge in this field revolves around establishing a consistent and universally accepted definition for work, heat, and entropy production in open quantum systems subjected to thermal reservoirs. Despite numerous proposals, the absence of generally accepted definitions, particularly in scenarios involving strong interactions between the system and reservoirs, remains a contentious issue. A recently developed approach, known as principle of minimal dissipation [1], leads to a unique decomposition of the quantum master equation into coherent and dissipative dynamics, allowing to identify uniquely the contributions describing work and heat.

In this contribution, we apply this approach to investigate the thermodynamic characteristics of impurity models, with a particular focus on memory effects and strong system-bath couplings. The study uses the hierarchical equations of motion approach, which allows a numerically exact simulation of nonequilibrium transport in general open quantum systems involving multiple bosonic and fermionic environments [2].

[1] A. Colla and H. Breuer, Phys. Rev. A 105, 052216 (2022)

[2] J. Bätge, Y. Ke, C. Kaspar, and M. Thoss, Phys. Rev. B 103, 235413 (2021)

DY 60.7 Fri 12:15 A 151

Control phase transitions analysis in the quantum control landscape — •Nicolò Beato, Pranay Patil, and Marin Bukov — Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

In recent years, the presence of control phase transitions emerged while numerically surveying the quantum control landscape associated with population-transfer problems in few-qubit systems [10.1103/PhysRevX.8.031086]. Despite all efforts, an analytical understanding of quantum optimal control landscapes is largely missing.

In this work, we present a set of perturbative methods that allow for the analytical characterization of various control phase transitions. These methods provide an explicit mapping between quantum control

problems and classical many-body systems at thermal equilibrium (exhibiting long-range, multi-body interactions). We demonstrate the effectiveness of these approaches by explicitly considering the single- and two- qubit state-preparation problems, previously extensively studied via numerical optimization algorithms [10.1103/PhysRevA.97.052114]. Through this approach, control phase transitions are connected to dramatic changes in the topological and geometrical properties of the near-optimal part of the control landscape.

The methods developed are largely independent from the quantum systems underlying the control problem and can be easily adapted to more complicated settings. Our work shed new light on the close connection between optimal quantum control and (spin) glassy systems.

DY 60.8 Fri 12:30 A 151

Engineering unsteerable quantum states with active feedback — •Samuel Morales[1], Yuval Gefen[2], Igor Gornyi[3,4], Alex Zazunov[1], and Reinhold Egger[1] — [1]Institut für Theoretische Physik, Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute, 7610001 Rehovot, Israel — [3]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [4]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

We propose active steering protocols for quantum state preparation in quantum circuits where each system qubit is connected to a single detector qubit, employing a simple coupling selected from a small set of steering operators. The decision is made such that the expected cost-function gain in one time step is maximized. We apply these protocols to several many-qubit models. Our results are underlined by three remarkable insights. First, we show that the standard fidelity does not give a useful cost function; instead, successful steering is achieved by including local fidelity terms. Second, although the steering dynamics acts on each system qubit separately, entanglement in the generated target state is introduced, and can be tuned at will, by performing Bell measurements on detector qubit pairs after every time step. This implements a weak-measurement variant of entanglement swapping. Third, numerical simulations suggest that the active steering protocol can reach arbitrarily designated target states, including passively unsteerable states such as the N-qubit W state.

DY 60.9 Fri 12:45 A 151

Extended Hilbert Space for Discontinuous Floquet Drives in the Walsh Basis — •James Walkling and Marin Bukov — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The form of the Floquet counterdiabatic protocol has recently been found and formulated in terms of a variational principle. While good convergence is achieved in a number of systems for harmonic drives, for step drives, the convergence of the numerics is poorly behaved. As a result, we explore a reformulation of Floquet Hilbert space in terms of a more natural basis for step drives: the Walsh basis. Among other nice properties, this basis forms a group for certain finite truncations. We investigate the results of this change of basis on the overall Hamiltonian in the extended space.

DY 61: Closing Talk (joint session BP/CPP/DY)

Time: Friday 13:15–14:00 Location: H 0104

Invited Talk DY 61.1 Fri 13:15 H 0104

Virus traps and other molecular machines of the future — •Hendrik Dietz — Technische Universität München, Garching b. München, Deutschland

Our interest is in learning how to build molecular devices and machines that can execute user-defined tasks. To this end, we investigate how to adapt the physical principles underlying the formation of natural macromolecular assemblies such as viruses or molecular motors for our purposes. Programmable molecular self-assembly with DNA origami is an attractive route toward implementing these principles to create synthetic molecular machinery. We combine computational design and cryo electron microscopy to learn how to construct synthetic molecular objects with increasing accuracy and increasing complexity.

For example, we have learned from viruses how to program DNA blocks to self-assemble into icosahedral shells with specific geometry and apertures, which led to an interesting application: the virus trap, which we hope to develop into a programmable antiviral drug to neutralize viruses. We have also learned how to design DNA origami so that genetic instructions included within them can be read by mammalian cells.

We also have recently learned how to control the movement of nanoscale assemblies. For example, we have built autonomous, power-generating rotary DNA motors driven by AC fields and also turbines that can be driven by ion flux across membranes. With these new machines, opportunities are created to accomplish user-defined, energy-consuming tasks in various contexts.