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Overview of Invited Talks and Sessions

(Lecture halls H18, H19, and H20; Poster P2)

Invited Talks

DY 2.1	Mon	9:30–10:00	H18	**Roughness growth modes in thin film growth** — •Martin Oettel
DY 9.1	Mon	15:00–15:30	H19	**Granular matter composed of non-convex grains** — •Ralf Stannarius
DY 12.1	Mon	15:30–16:00	H20	**A phononic frequency comb from a single resonantly driven nanomechanical mode** — •Eva Weig
DY 12.4	Mon	16:30–17:00	H20	**From period-doubling bifurcations to time crystals and coherent Ising machines** — •Oded Zilberberg, Toni L. Heugel, Jan Košata, Javier del Pino, R. Chitra, Alexander Eichler
DY 12.6	Mon	17:15–17:45	H20	**2D membranes in motion** — •Herre van der Zant
DY 14.1	Tue	9:30–10:00	H18	**Non-Markovian Brownian systems: from single-particle thermodynamics to collective behavior** — •Sabine Klapp
DY 17.1	Tue	10:30–11:00	H19	**Caustics in turbulent aerosols** — •Bernhard Mehlig
DY 29.1	Wed	12:00–12:30	H18	**Derivation of a continuum description of sheared jammed soft suspensions from particle dynamics** — •Eric Bertin, Nicolas Cuny, Romain Mari
DY 32.1	Wed	15:00–15:30	H19	**Large scale patterns in turbulent Rayleigh-Bénard convection** — •Stephan Weiss
DY 33.1	Wed	15:00–15:30	H20	**Detecting dynamical quantum phase transitions by string observables** — •Anatoli Polkovnikov, Amit Dutta, Souvik Bandyopadhyay
DY 37.1	Thu	9:30–10:00	H20	**Controlled and robust phase separation in cells** — •David Zwicker
DY 48.1	Fri	9:30–10:00	H19	**Photonic Reservoir Computing: Analytic insights and possibilities for optimization** — Lina Jaurigue, Felix Köster, •Kathy Lüdge

Invited Talks of the joint Symposium SKM Dissertation Prize 2022 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:15–10:45	H2	**Charge localisation in halide perovskites from bulk to nano for efficient optoelectronic applications** — •Sascha Feldmann
SYSD 1.2	Mon	10:45–11:15	H2	**Nonequilibrium Transport and Dynamics in Conventional and Topological Superconducting Junctions** — •Raffael L. Klees
SYSD 1.3	Mon	11:15–11:45	H2	**Probing magnetostatic and magnetotransport properties of the antiferromagnetic iron oxide hematite** — •Andrew Ross
SYSD 1.4	Mon	11:45–12:15	H2	**Quantum dot optomechanics with surface acoustic waves** — •Matthias Weiss

Invited Talks of the joint Symposium United Kingdom as Guest of Honor (SYUK)

See SYUK for the full program of the symposium.

SYUK 1.1	Wed	9:30–10:00	H2	**Structure and Dynamics of Interfacial Water** — •Angelos Michaelides
SYUK 1.2	Wed	10:00–10:30	H2	**A molecular view of the water interface** — •Mischa Bonn
SYUK 1.3	Wed	10:30–11:00	H2	**Motile cilia waves: creating and responding to flow** — •Pietro Cicuta

SYUK 1.4	Wed	11:00–11:30	H2	**Cilia and flagella: Building blocks of life and a physicist's playground** — •Oliver Bäumchen
SYUK 1.5	Wed	11:45–12:15	H2	**Computational modelling of the physics of rare earth - transition metal permanent magnets from $SmCo_5$ to $Nd_2Fe_{14}B$** — •Julie Staunton
SYUK 2.1	Wed	15:00–15:30	H2	**Hysteresis Design of Magnetic Materials for Efficient Energy Conversion** — •Oliver Gutfleisch
SYUK 2.2	Wed	15:30–16:00	H2	**Non-equilibrium dynamics of many-body quantum systems versus quantum technologies** — •Irene D'Amico
SYUK 2.3	Wed	16:00–16:30	H2	**Quantum computing with trapped ions** — •Ferdinand Schmidt-Kaler
SYUK 2.4	Wed	16:45–17:15	H2	**Breaking the millikelvin barrier in cooling nanoelectronic devices** — •Richard Haley
SYUK 2.5	Wed	17:15–17:45	H2	**Superconducting Quantum Interference Devices for applications at mK temperatures** — •Sebastian Kempf

Invited Talks of the joint Symposium Interplay of Substrate Adaptivity and Wetting Dynamics from Soft Matter to Biology (SYSM)

See SYSM for the full program of the symposium.

SYSM 1.1	Wed	15:00–15:30	H1	**Statics and Dynamics of Soft Wetting** — •Bruno Andreotti
SYSM 1.2	Wed	15:30–16:00	H1	**Droplets on elastic substrates and membranes - Numerical simulation of soft wetting** — •Sebastian Aland
SYSM 1.3	Wed	16:00–16:30	H1	**Wetting of Polymer Brushes in Air** — Lars Veldscholte, Guido Ritsema van Eck, Liz Mensink, Jacco Snoeijer, •Sissi de Beer
SYSM 1.4	Wed	16:45–17:15	H1	**Elastocapillary phenomena in cells** — •Roland L. Knorr
SYSM 1.5	Wed	17:15–17:45	H1	**Active contact line depinning by micro-organisms spreading on hydrogels** — Marc Hennes, Julien Tailleur, Gaëlle Charron, •Adrian Daerr

Invited Talks of the joint Symposium Collective Social Dynamics from Animals to Humans (SYSO)

See SYSO for the full program of the symposium.

SYSO 1.1	Thu	9:30–10:00	H1	**Capturing group interactions: The next frontier of modeling social and biological systems** — •Frank Schweitzer
SYSO 1.2	Thu	10:00–10:30	H1	**Modelling Individual Mobility Behavior** — •Laura Maria Alessandretti
SYSO 1.3	Thu	10:30–11:00	H1	**Validating argument-based opinion dynamics with survey experiments** — •Sven Banisch
SYSO 1.4	Thu	11:15–11:45	H1	**Self-organization, Criticality and Collective Information Processing in Animal Groups** — •Pawel Romanczuk
SYSO 1.5	Thu	11:45–12:15	H1	**Collective dynamics and physiological interactions in bird colonies** — •Hanja Brandl

Invited Talks of the joint Symposium Complexity and Topology in Quantum Matter (SYQM)

See SYQM for the full program of the symposium.

SYQM 1.1	Fri	9:30–10:00	H1	**The role of crystalline symmetries in topological materials: the topological materials database** — •Maia Vergniory
SYQM 1.2	Fri	10:00–10:30	H1	**Microwave Bulk and Edge Transport in HgTe-Based 2D Topological Insulators** — •Erwann Bocquillon, Matthieu C. Dartiailh, Alexandre Gourmelon, Hiroshi Kamata, Kalle Bendias, Simon Hartinger, Jean-Marc Berroir, Gwendal Fève, Bernard Plaçais, Lukas Lunczer, Raimund Schlereth, Hartmut Buhmann, Laurens Molenkamp
SYQM 1.3	Fri	10:30–11:00	H1	**Spectral Sensitivity of Non-Hermitian Topological Systems** — •Jan Carl Budich
SYQM 1.4	Fri	11:15–11:45	H1	**Topological photonics and topological lasers with coupled vertical resonators** — •Sebastian Klembt
SYQM 1.5	Fri	11:45–12:15	H1	**Spectroscopic Studies of the Topological Magnon Band Structure in a Skyrmion Lattice** — •Markus Garst

Sessions

DY 1.1–1.3	Sun	16:00–18:30	H4	**Tutorial: Stochastic Processes from Financial Risk to Genetics (joint session SOE/TUT/BP/DY)**
DY 2.1–2.1	Mon	9:30–10:00	H18	**Invited Talk Martin Oettel**
DY 3.1–3.9	Mon	10:00–12:30	H18	**Statistical Physics far from Thermal Equilibrium**
DY 4.1–4.8	Mon	10:00–12:15	H19	**Wetting, Droplets and Microfluidics (joint session DY/CPP)**
DY 5.1–5.10	Mon	10:00–12:45	H20	**Many-Body Quantum Dynamics 1 (joint session DY/TT)**
DY 6.1–6.7	Mon	10:30–12:45	H16	**Active Matter 1 (joint session BP/CPP/DY)**
DY 7.1–7.7	Mon	15:00–17:15	H16	**Statistical Physics of Biological Systems 1 (joint session BP/DY)**
DY 8.1–8.10	Mon	15:00–17:45	H18	**Data Analytics for Complex Systems (joint session DY/SOE)**
DY 9.1–9.1	Mon	15:00–15:30	H19	**Invited Talk Ralf Stannarius**
DY 10.1–10.10	Mon	15:00–17:45	H39	**Modeling and Simulation of Soft Matter (joint session CPP/DY)**
DY 11.1–11.9	Mon	15:30–18:00	H19	**Granular Matter and Contact Dynamics**
DY 12.1–12.6	Mon	15:30–17:45	H20	**Focus Session: Nonlinear Dynamics of Nanomechanic Oscillators**
DY 13.1–13.2	Mon	17:45–18:15	H18	**Big Data and Artificial Intelligence (joint session SOE/DY)**
DY 14.1–14.1	Tue	9:30–10:00	H18	**Invited Talk Sabine Klapp**
DY 15.1–15.4	Tue	9:30–10:30	H19	**Delay and Feedback Dynamics**
DY 16.1–16.11	Tue	10:00–13:00	H18	**Active Matter 2 (joint session DY/BP/CPP)**
DY 17.1–17.1	Tue	10:30–11:00	H19	**Invited Talk Bernhard Mehlig**
DY 18.1–18.6	Tue	11:15–12:45	H19	**Nonlinear Dynamics 1: Synchronization and Chaos (joint session DY/SOE)**
DY 19.1–19.6	Tue	11:30–13:00	H20	**Many-Body Quantum Dynamics 2 (joint session DY/TT)**
DY 20.1–20.5	Tue	11:30–13:00	H38	**Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)**
DY 21.1–21.1	Wed	9:30–10:15	H11	**Invited Talk Dirk Brockmann (joint session SOE/DY)**
DY 22.1–22.10	Wed	9:30–12:30	H16	**Active Matter 3 (joint session BP/CPP/DY)**
DY 23.1–23.9	Wed	9:30–12:00	H18	**Complex Fluids and Soft Matter 1 (joint session DY/CPP)**
DY 24.1–24.6	Wed	9:30–11:15	H19	**Stochastic Thermodynamics and Information Processing**
DY 25.1–25.7	Wed	9:30–11:15	H39	**General Session to the Symposium: Interplay of Substrate Adaptivity and Wetting Dynamics from Soft Matter to Biology (joint session CPP/DY)**
DY 26.1–26.6	Wed	10:00–11:30	H20	**Critical Phenomena and Phase Transitions**
DY 27.1–27.6	Wed	10:15–12:45	H11	**Networks: From Topology to Dynamics (joint session SOE/BP/DY)**
DY 28.1–28.7	Wed	11:15–13:00	H19	**Extreme Events, Glasses and Miscellaneous**
DY 29.1–29.1	Wed	12:00–12:30	H18	**Invited Talk Eric Bertin**
DY 30.1–30.2	Wed	12:45–13:15	H11	**Energy Networks (joint session SOE/DY)**
DY 31.1–31.9	Wed	15:00–17:30	H18	**Active Matter 4 (joint session DY/BP/CPP)**
DY 32.1–32.1	Wed	15:00–15:30	H19	**Invited Talk Stephan Weiss**
DY 33.1–33.1	Wed	15:00–15:30	H20	**Invited Talk Anatoli Polkovnikov**
DY 34.1–34.6	Wed	15:30–17:15	H19	**Fluid Physics: Turbulence and Convection**
DY 35.1–35.9	Wed	15:30–18:00	H20	**Quantum Chaos and Coherent Dynamics**
DY 36.1–36.11	Thu	9:30–12:30	H22	**Quantum Coherence and Quantum Information Systems (joint session TT/DY)**
DY 37.1–37.1	Thu	9:30–10:00	H20	**Invited Talk David Zwicker**
DY 38.1–38.6	Thu	10:00–11:30	H18	**Complex Fluids and Soft Matter 2 (joint session DY/CPP)**
DY 39.1–39.8	Thu	10:00–12:15	H19	**Pattern Formation and Reaction-Diffusion Systems**
DY 40.1–40.7	Thu	10:00–12:00	H20	**Brownian Motion and Anomalous Diffusion**
DY 41.1–41.12	Thu	15:00–18:15	H22	**Nonequilibrium Quantum Many-Body Systems (joint session TT/DY)**
DY 42.1–42.6	Thu	15:00–16:30	H16	**Statistical Physics of Biological Systems 2 (joint session BP/DY)**
DY 43.1–43.8	Thu	15:00–18:00	P2	**Poster Session: Quantum Chaos and Many-Body Dynamics**
DY 44.1–44.20	Thu	15:00–18:00	P2	**Poster Session: Statistical Physics and Critical Phenomena**
DY 45.1–45.13	Thu	15:00–18:00	P2	**Poster Session: Nonlinear Dynamics, Pattern Formation, Data Analytics and Machine Learning**
DY 46.1–46.22	Thu	15:00–18:00	P2	**Poster Session: Complex Fluids, Soft Matter, Active Matter, Glasses and Granular Materials**
DY 47	Thu	18:30–19:15	H19	**Members' Assembly**
DY 48.1–48.1	Fri	9:30–10:00	H19	**Invited Talk Kathy Lüdge (joint session DY/SOE)**
DY 49.1–49.10	Fri	9:30–12:15	H20	**Statistical Physics: General**
DY 50.1–50.11	Fri	10:00–12:45	H18	**Active Matter 5 (joint session DY/BP/CPP)**

DY 51.1–51.5	Fri	10:00–11:15	H19	**Machine Learning in Dynamics and Statistical Physics (joint session DY/SOE)**
DY 52.1–52.5	Fri	11:30–12:45	H19	**Nonlinear Dynamics 2: Stochastic and Complex Systems, Networks (joint session DY/SOE)**

Members' Assembly of the Dynamics and Statistical Physics Division

Thursday 18:30–19:15 H19

DY 1: Tutorial: Stochastic Processes from Financial Risk to Genetics (joint session SOE/TUT/BP/DY)

Macroscopic and microscopic models from Economy to Biology must account for stochasticity on various levels. While classical physics strives for deterministic descriptions through differential equations from fundamental level to thermodynamics, many physics-based models on higher level explicitely include stochasticity from various sources. Discrete and continuous stochastic processes then become the mathematical foundation of these models. This tutorial highlights classical as well as current methods and approaches of probabilistic models and stochastic processes in physics, biology as well as socio-economic systems, thereby bridging the risk to extinction in genetics with its economic counterpart. (Session organized by Jens Christian Claussen.)

Time: Sunday 16:00–18:30 Location: H4

Tutorial DY 1.1 Sun 16:00 H4

Diffusion approximations for particles in turbulence — •Bernhard Mehlig — University of Gothenburg, Gothenburg, Sweden

The subject of this tutorial is the dynamics of particles in turbulence, such as micron-sized water droplets in the turbulent air of a cumulus cloud. The particles respond in intricate ways to the turbulent fluctuations. Non-interacting particles may cluster together to form spatial patterns – even though the turbulent fluid is incompressible [1]. In this tutorial I explain how to understand spatial clustering using diffusion approximations, highlighting an analogy with Kramers' escape problem [2]. I introduce/review the necessary elements of diffusion theory. My goal is to give a pedagogical introduction to diffusion approximations in non-equilibrium statistical physics, using particles in turbulence as an example.

[1] K. Gustavsson and B. Mehlig, Statistical models for spatial patterns of heavy particles in turbulence, Adv. Phys. 65 (2016) 57 (read Sections 1, 3.1, and 6.1).

[2] H. A. Kramers, Brownian motion in a field of force and the diffusion model of chemical reactions, Physica 7 (1940) 284 (read up to eq. (17)).

Tutorial DY 1.2 Sun 16:50 H4

Probabilities in physics, paradoxes and populations — •Tobias Galla — Instituto de Física Interdisciplinary Sistemas Complejos, IFISC (CSIC-UIB), Campus Universitat Illes Balears, E-07122 Palma de Mallorca, Spain

It is notoriously hard for humans to develop a good intuition for probabilities and stochastic processes. Our brains are not able to do this naturally, and there are numerous mistakes which are easy to make. These mistakes are in fact made regularly in the press (sometimes perhaps deliberately). More worrisome, decision makers such as judges, doctors or politicians are also prone to mishandling probabilities. In this tutorial I will outline a few of these traps, and how to avoid them. I will also discuss the nature of probabilistic models of physical processes – is there genuine randomness in the world around us? I will then present a number of instances in which physics approaches combined with stochastic modelling can make a difference. As one example, I will outline experimental and theoretical results which highlight the importance of stochastic processes in population dynamics. Other examples will include stochastic processes in genetics, the evolution of cancer and in game theory.

Tutorial DY 1.3 Sun 17:40 H4

Risk Revealed: Cautionary Tales, Understanding and Communication — •Paul Embrechts — Department of Mathematics, ETH Zürich

The title of the tutorial refers to a forthcoming book, to be published by Cambridge University Press, co-authored with Valérie Chavez-Demoulin (Lausanne) and Marius Hofert (Waterloo). Extreme Value Theory (EVT) offers a mathematical tool for the modeling of so-called What-If events, or stress scenarios. I will present several examples of risk-based decision-making and show how EVT can be used as part of the solution. The current pandemic has clearly shown that the communication of scientific evidence has a difficult stand in the ubiquitous environment of social media. I will discuss some examples of this struggle.

DY 2: Invited Talk Martin Oettel

Time: Monday 9:30–10:00 Location: H18

Invited Talk DY 2.1 Mon 9:30 H18

Roughness growth modes in thin film growth — •Martin Oettel — Uni Tübingen, Institut für Angewandte Physik

Thin film growth is one of the fundamental nonequilibrium processes in statistical physics and it is also very relevant for applications. In the past years, experimental attention has shifted from the growth of metallic films (with fairly isotropic particles) to growth of organic films with possibly very anisotropic particles. In view of applications, the film morphology (notably the film roughness) is a central object of interest. To study that, we employ simple lattice models for isotropic and anisotropic particles to elucidate principal film growth modes with a focus on the intermediate thickness regime. For isotropic particles we find 4 principal growth modes with fairly sharp transitions between them [1]. E.g., a dynamic layering transition separates layer-by-layer and island growth and can be viewed as a nonequilibrium counterpart of wetting/layering transitions. Anisotropy in the interactions between the lattice particles does not change the roughness growth modes but adds further orientational transitions [2]. Further, we have studied monolayer growth for lattice particles which are also anisotropic in their hard-core shape. There, the deposition process corresponds to trajectories in the space of macroscopic order parameters (density, orientation) which connect rather small equilibrium domains and which describe generalized nucleation and arrest processes.

[1] E. Empting et al., Phys. Rev. E 103, 023302 (2021). [2] E. Empting, N. Bader, and M. Oettel, Phys. Rev. E 105, 045306 (2022).

DY 3: Statistical Physics far from Thermal Equilibrium

Time: Monday 10:00–12:30 Location: H18

DY 3.1 Mon 10:00 H18

Relaxation to a parity-time symmetric generalized Gibbs ensemble after a quantum quench in a driven-dissipative Kitaev chain — •Elias Starchl and Lukas Sieberer — Institute for Theoretical Physics, University of Innsbruck, Austria

After a quench, isolated thermalizing quantum many-body systems relax locally to an equilibrium state that is universally determined by conservation laws and the principle of maximum entropy. In contrast, open quantum systems, subjected to Markovian drive and dissipation, typically evolve toward nonequilibrium steady states that are highly model-dependent. However, focusing on a driven-dissipative Kitaev chain, we show that relaxation after a quantum quench can be described by a maximum entropy ensemble, if the Liouvillian governing the dynamics has parity-time (PT) symmetry. We dub this ensemble, which is determined by the biorthogonal eigenmodes of the adjoint Liouvillian, the PT-symmetric generalized Gibbs ensemble (PTGGE). Resembling isolated systems, thermalization becomes manifest in the growth and saturation of entanglement, and the relaxation of local observables. In contrast, the directional pumping of fermion parity represents a phenomenon that is unique to relaxation dynamics in driven-dissipative systems. We expect that our results apply rather generally to integrable, driven-dissipative bosonic and fermionic quantum many-body systems with PT symmetry.

DY 3.2 Mon 10:15 H18

Finite-time dynamical phase transition in non-equilibrium relaxation — •Jan Meibohm[1,2] and Massimiliano Esposito[1] — [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

We uncover a finite-time dynamical phase transition in the thermal relaxation of a mean-field magnetic model. The phase transition manifests itself as a cusp singularity in the probability distribution of the magnetization that forms at a critical time. The transition is due to a sudden switch in the dynamics, characterized by a dynamical order parameter. We derive a dynamical Landau theory for the transition that applies to a range of systems with scalar, parity-invariant order parameters. Close to criticalilty, our theory reveals an exact mapping between the dynamical and equilibrium phase transitions of the magnetic model, and implies critical exponents of mean-field type. We argue that interactions between nearby saddle points, neglected at the mean-field level, may lead to critical, spatiotemporal fluctuations of the order parameter, and thus give rise to novel, dynamical critical phenomena.

DY 3.3 Mon 10:30 H18

Mori-Zwanzig formalism for general relativity: a new approach to the averaging problem* — •Michael te Vrugt[1], Sabine Hossenfelder[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [2]Frankfurt Institute for Advanced Studies, D-60438 Frankfurt am Main, Germany

Cosmology provides a coarse-grained description of the universe that is valid on very large length scales. However, the Einstein field equations are not valid for coarse-grained quantities since, due to their nonlinearity, they do not commute with an averaging procedure. Thus, it is unclear in which way small-scale inhomogeneities affect large-scale cosmology (backreaction). In this work [1], we address this problem by extending the Mori-Zwanzig projection operator formalism, a highly successful coarse-graining method from statistical mechanics, towards general relativity. This allows to derive a dynamic equation for the Hubble parameter in which backreaction is taken into account through memory and noise terms. Our results are linked to cosmological observations.

[1] M. te Vrugt, S. Hossenfelder, R. Wittkowski, Physical Review Letters 127, 231101 (2021)

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

DY 3.4 Mon 10:45 H18

Synthetic horizons in 1D tight-binding model and thermalisation of the many-body groundstate — •Lotte Mertens[1,2], Ali G. Moghaddam[2,3], Dmitry Chernyavsky[2], Corentin Morice[1], Jeroen van den Brink[2,4], and Jasper van Wezel[1] — [1]Institute for Theoretical Physics and Delta Institute for Theoretical Physics, University of Amsterdam, 1090 GL Amsterdam, The Netherlands — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [3]Department of Physics, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan 45137-66731, Iran — [4]Institute for Theoretical Physics and Wurzburg-Dresden Cluster of Excellence ct.qmat, Technische Universitat Dresden, 01069 Dresden, Germany

Open problems in general relativity have motivated the search for analogue gravitational systems in condensed matter implementations. In one such system, a 1D tight-binding model with position-dependent hopping, the possibility of realizing an analogue gravitational horizon has recently been demonstrated. Here, we introduce the concept of emergent temperature, inspired by Unruh radiation, and show that it arises naturally in tight-binding lattice models featuring a horizon. Despite finding many similarities between the emergent lattice temperature and the gravitational Unruh temperature, we show that the nature of the thermal spectrum in the lattice theory is radically different from that in the continuum limit. Additionally, we provide a detailed analysis of outgoing radiation showing the conditions under which the horizon behaves purely as a thermal source.

DY 3.5 Mon 11:00 H18

Renormalized Fluctuation Expansion for Non-Equilibrium Disordered Networks — •Michael Dick[1,2,3], Alex van Meegen[1,4], and Moritz Helias[1,5] — [1]Institute of Neuroscience and Medicine (INM-6) and Institute for Advanced Simulation (IAS-6) and JARA-BRAIN Institute I, Jülich Research Centre, 52425 Jülich, Germany — [2]Department of Computer Science 3 - Software Engineering, RWTH Aachen University, Aachen, Germany — [3]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Jülich Research Centre, 52425 Jülich, Germany — [4]Institute of Zoology, University of Cologne, 50674 Cologne, Germany — [5]Department of Physics, Faculty 1, RWTH Aachen University, Aachen, Germany

It is frequently hypothesized that cortical networks display hallmarks of critical dynamics. Such critical dynamics are beyond the validity of a mean-field approximation because it inherently neglects fluctuations. Thus, a renormalized theory is necessary. We consider an archetypal neural network model which displays a magnetic as well as a chaotic transition. Based on the analogue of a quantum effective action, we derive self-consistency equations for the first two renormalized Greens functions. Their self-consistent solution reveals critical slowing down near the transition to the ferromagnetic state and an optimal level of disorder which favors collective behavior. The quantitative theory explains the shape of the single-unit autocorrelation function, featuring multiple temporal scales, and the population autocorrelation function.

15 min. break

DY 3.6 Mon 11:30 H18

Modeling flash sintering conditions with Boltzmann equations — •Magdulin Dwedari, Lothar Brendel, and Dietrich Wolf — University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg

In a flash sintering experiment, a suitable combination of electric field and furnace heating is applied to the sample, which makes it possible to sinter it in a matter of seconds and at significantly lower temperatures compared to conventional sintering. An established hypothesis that explains the key signatures of a flash sintering event, such as a surge in conductivity, is that the electric field causes a rapid generation of Frenkel defects in the sample. With molecular dynamic simulations it has been confirmed that a phonon proliferation at the Brioullin-Zone edge can cause a Frenkel defect concentration 10^{15} times higher than the thermal concentration.
To study the effects of an electric field on the phonon distribution, we model the electron system governed by an electric field and the phonon system coupled to an external heat bath with two coupled Boltzmann equations. The key difference to previous work exciting the electron

system via a laser pulse is that our excitation term models the effects of the electric field and is therefore continuous and imposes a cylindrical symmetry.

DY 3.7 Mon 11:45 H18

Barrier crossing in a viscoelastic bath — •Félix Ginot[1], Juliana Caspers[2], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physiks Universität Konstanz, 78457 Konstanz, Germany — [2]Georg-August Universität Göttingen, 37073 Göttingen, Germany

The activated, i.e., fluctuation-assisted hopping of a Brownian particle across an energy barrier ΔU is a fundamental process with important applications across science, such as in chemical reactions, protein folding, or drug absorption. Such processes can be rationalized using Kramers theory, which predicts the hopping rate $\nu \propto \exp(-\Delta U/k_{\mathrm{B}}T)$ with $k_{\mathrm{B}}T$ the thermal energy, in agreement with experimental observations. Many systems, however, cannot be described in terms of a single degree of freedom, notably when memory effects need to be taken into account. In this work we experimentally investigate barrier crossing of a Brownian particle in a double-well potential suspended in a viscoelastic solvent which exhibits non-Markovian behavior, i.e., memory. For potential barriers up to several $k_{\mathrm{B}}T$ we find the hopping dynamics to be characterized not by a single but by *two* time scales which can differ by more than two orders of magnitude. While the long time scale increases exponentially with ΔU (as in Kramers theory), the short one is almost unaffected by the barrier height. The latter results from elastic energy fluctuations of the viscoelastic bath due to excitations arising from the particle's hopping motion. Our results, which are in agreement with a simple model where the fluid is described as a Maxwell medium, have immediate consequences for the above examples, e.g., altering the interpretation and prediction of lifetimes.

DY 3.8 Mon 12:00 H18

Scalar Active Mixtures: The Nonreciprocal Cahn-Hilliard Model — •Suropriya Saha[1], Jaime Agudo-Canalejo[1], and Ramin Golestanian[1,2] — [1]Department of Living Matter Physics, Max Planck Institute for Dynamics and Self-Organization — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford

Pair interactions between active particles need not follow Newton's third law. In this work, we propose a continuum model of pattern formation due to nonreciprocal interaction between multiple species of scalar active matter. The classical Cahn-Hilliard model is minimally modified by supplementing the equilibrium Ginzburg-Landau dynamics with particle-number-conserving currents, which cannot be derived from a free energy, reflecting the microscopic departure from action-reaction symmetry. The strength of the asymmetry in the interaction determines whether the steady state exhibits a macroscopic phase separation or a traveling density wave displaying global polar order. The latter structure, which is equivalent to an active self- propelled smectic phase, coarsens via annihilation of defects, whereas the former structure undergoes Ostwald ripening. The emergence of traveling density waves, which is a clear signature of broken time- reversal symmetry in this active system, is a generic feature of any multicomponent mixture with microscopic nonreciprocal interactions.

DY 3.9 Mon 12:15 H18

Quantum thermodynamics of nonadiabatically driven systems: The effect of electron-phonon interaction — •Jakob Bätge[1], Amikam Levy[3], Wenjie Dou[2], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg, Freiburg,Germany — [2]Department of Physics, School of Science, Westlake University, Hangzhou, China — [3]Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel

The development and optimization of quantum devices have increased the interest in dynamics and thermodynamics of systems on the scale of single atoms and molecules. In this contribution, we investigate the nonequilibrium quantum dynamics of a driven nanosystem with two different approaches. By comparing results from the numerically exact hierarchical equations of motion method [1] and a Markovian quantum master equation [2], we analyze non-Markovian effects in the system dynamics. Furthermore, we discuss nonadiabatic effects in thermodynamic quantities induced by electronic-vibrational coupling.

[1] J. Bätge *et al.*, Phys. Rev. B **103**, 235413 (2021)
[2] R. Dann *et al.*, Phys. Rev. A **98**, 052129 (2018)

DY 4: Wetting, Droplets and Microfluidics (joint session DY/CPP)

Time: Monday 10:00–12:15 Location: H19

DY 4.1 Mon 10:00 H19

Lattice Boltzmann simulations of dense suspensions of soft particles with interface viscosity — •Fabio Guglietta[1], Othmane Aouane[1], Francesca Pelusi[1], Marcello Sega[1], and Jens Harting[1,2] — [1]Helmholtz Institute Erlangen-Nürnberg, Germany — [2]Department of Chemical and Biological Engineering and Department of Physics, FAU Erlangen-Nüremberg, Germany

Interface viscosity (IV) plays a major role in the dynamics of single droplets and viscoelastic capsules by influencing their transient dynamics and steady-state deformation. For example, it has recently become clear that numerical models for red blood cells must include IV to account for their realistic description. Therefore, IV can be expected to play a significant role in determining also the dynamics and rheology of their dense suspensions. However, as no detailed investigation exists on the effects of IV in the dense suspensions of soft capsules, we aim to fill this gap by including it in computational fluid dynamics models. Here, we address this problem for the first time by performing numerical simulations in the framework of the immersed boundary - lattice Boltzmann method. This approach proved to be a valid numerical tool to provide a realistic description of soft particles immersed in Newtonian fluids. We employ a recent numerical model to account for IV by relying on the discretised Boussinesq-Scriven tensor, which provides a continuum description of a 2D viscous fluid. We show that the IV influences (a) the time it takes for particles to deform during the transient phase and (b) the final shape of the particles in the steady-state at different volume fraction values.

DY 4.2 Mon 10:15 H19

Wetting dynamics of droplets: an immersed boundary lattice Boltzmann approach — •Francesca Pelusi[1], Othmane Aouane[1], Fabio Guglietta[1], Marcello Sega[1], and Jens Harting[1,2] — [1]Helmholtz Institute Erlangen-Nürnberg, Germany — [2]Department of Chemical and Biological Engineering and Department of Physics, FAU, Germany

Many applications in computational fluid dynamics require the immersed boundary (IB) method to couple the dynamics of well-defined structures with that of a surrounding fluid. If the latter is simulated with a lattice Boltzmann (LB) method, the resulting IBLB approach is known to be a very versatile tool, for example, in studying dense suspensions of red blood cells. However, little attention has been devoted so far to applying this approach to substrate wetting problems. Here, we report on an IBLB-based investigation of the wetting of droplets interacting with a solid surface. In our model, the droplet surface tension contributes to the force the droplet (structure) communicates to the surrounding fluid. We characterize Newtonian droplets' static and dynamic contact angles and show how surface/IB-nodes interaction tuning allows obtaining the desired wetting properties. Furthermore, the flexibility of the IBLB approach will enable us to model non-Newtonian surface rheology, opening the possibility of simulating the unusual wetting behavior of gallium droplets. Indeed, liquid gallium develops an oxide layer at the liquid surface when in contact with the oxygen, which affects its adhesive properties with significant consequences for its high-tech applications, such as catalysis.

DY 4.3 Mon 10:30 H19

Viscosity-induced Destabilization of a Liquid Sheet in Inertial Microfluidics — •Kuntal Patel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Lab-on-a-chip devices based on inertial microfluidics function between Stokes and turbulent regimes, which enables to achieve high throughput. In the present work, we study the motion of a liquid sheet of thickness t_s and viscosity μ_1 in a two-dimensional microchannel of width w, filled with a viscous fluid (viscosity μ_2, $m = \mu_2/\mu_1 > 1$). At finite Reynolds number Re, a small perturbation at the interfaces separating the sheet from the surrounding fluid can result in a rapid destabilization of interfaces and may lead to a break-up. The present work gives

a proof-of-concept of how viscosity-driven interfacial instability can be exploited for a controlled droplet production in inertial microfluidics. Such microfluidic droplets are utilized in food and pharmaceutical related applications and as chemical reactors in Lab-on-a-chip devices.

In our computational linear stability analysis based on the Orr-Sommerfeld equation, we observe that the growth rate of the fastest growing mode ξ^* increases with Re. Furthermore, the dependence of ξ^* on m and t_s is quantified by the scaling law $\xi^* \propto m t_s^{2.5}$, which is valid for thin sheets in moderate Re flows with relatively weak interfacial tension Γ. In the second part, our lattice Boltzmann simulations starting from a single-mode perturbation of wavelength λ reveal that the interfacial instability causes the liquid sheet to break up and ultimately to form droplets when $\lambda \geq 0.5w$. We also identify different interface breakup mechanisms leading to droplet formation.

DY 4.4 Mon 10:45 H19

Imaging, Analysis and Sorting in Microfluidic Systems: Correlative Multi-Contrast, Multi-Parameter Applications — •Tobias Neckernuss[1], Patricia Schwilling[2], Jonas Pfeil[1,2], Daniel Geiger[1], and Othmar Marti[2] — [1]Sensific GmbH — [2]Institute for Experimental Physics, Ulm Univeristy

Droplet-based microfluidics is a promising approach in biology, pharmacy, medicine, and lab-on-a-chip applications. One remaining problem is the lack of a suitable fast image-based detection method that enables droplet- and content-based analysis and sorting with rates fast enough to be sufficient for high-throughput measurements and to enable surveilled lab scale production. We demonstrate recent advances for high-speed, real-time, image-based analysis and manipulation of microfluidic systems. With rates of up to 3000 particles or droplets per second we show applications of our system in the field of droplet-based microfluidics. Here, we concentrate on droplet-content analysis and have a sneak look at further potential applications in biology and image-based cell analysis. We introduce new contrast types for image-based analysis like brightfield, darkfield, phase contrast, fluorescence and combinations thereof. Combining new cutting edge hardware technology with specifically tailored software and integration of external lab infrastructure enables us reach new dimensions in image based particle analysis and sorting.

15 min. break

DY 4.5 Mon 11:15 H19

the obstacle effect on soft sphere discharging in quasi-2D silo — •Jing Wang[1], Kirsten Harth[1,2], Dmitry Puzyrev[1], and Ralf Stannarius[1] — [1]Institute of Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany — [2]Department of Engineering, Brandenburg University of Applied Sciences, Magdeburger Straße 50, D-14770 Brandenburg an der Havel, Germany

Soft smooth particles in silo discharge show their own characteristics, for example, non-permanent clogging and intermittent flow. We conduct experiment on soft, low-frictional hydrogel spheres compred with hard, frictional spheres in a quasi-2D silo. We introduce a competitive behavior of these spheres during their discharge by placing an obstacle in front of the outlet of the silo. High-speed optical imaging is applied to capture the process of discharge. By the method of particle tracking velocimetry (PTV), the fields of velocity, egress time, packing fraction, and kinetic stress are analysed in the study.

DY 4.6 Mon 11:30 H19

Coalescence of isotropic and nematic droplets in quasi 2D liquid crystal films — •Christoph Klopp, Alexey Eremin, and Ralf Stannarius — Institute for Physics, Otto von Guericke University Magdeburg, Germany

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]. Here, we demonstrate coalescence of isotropic and nematic droplets in quasi-2D liquids, viz. overheated smectic A freely suspended films. We investigated their dynamics experimentally and measured the shape deformation during the entire merging process using high-speed imaging and interferometry. This system is a unique example where the lubrication approximation can be directly applied, and the smectic membrane plays the role of a precursor film. Our studies reveal the scaling laws of the coalescence time depending on the droplet size and the material parameters. We also compared the dynamics of isotropic and nematic droplets and additionally analyzed the results based on an existing model for liquid lens coalescence on liquid and solid surfaces [4].

Acknowledgements: This study was supported by DLR and DFG within the OASIS and OASIS-Co projects WM2054 and STA 425/40.

References: [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) [4] C. Klopp et al., Langmuir, 36, 10615 (2020)

DY 4.7 Mon 11:45 H19

Using feedback-controlled thermoviscous flows to precisely position microparticles — •Elena Erben, Antonio Minopoli, Nicola Maghelli, Benjamin Seelbinder, Iliya D. Stoev, Sergei Klykov, and Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Optical positioning of microscale objects has proven key for advancing fundamental biological research and holds great potential for other disciplines as well. The most widely used among these methods are optical tweezers which enable the precise control and manipulation of multiple particles. However, they require probes of high refractive index contrast and low absorption and exclude the use of photosensitive samples. Here we present a novel optofluidic technique that leverages optical-control capabilities and the gentle nature of hydrodynamic flows, thus lifting the aforementioned constraints. Our approach is based on optically-induced thermoviscous flows generated by the repeated scanning of a moderately heating infrared laser beam [1]. We have combined thermoviscous flows with feedback control to confine micron-sized particles with a precision of up to 24 nm without exposing them directly to laser light [2]. Recently, we extended this approach beyond single-object manipulation to further enable simultaneous control of multiple particles. With this contribution, we furthermore discuss combinations with implicit force sensing [3] and the potential for future application in and beyond the life science sector.

[1] Weinert et al., *Phys. Rev. Lett.*, 2008; [2] Erben et al., *Opt. Express*, 2021; [3] Stoev et al., *eLight*, 2021.

DY 4.8 Mon 12:00 H19

Active thin films — •Tilman Richter[1], Paolo Malgaretti[1], Stefan Zitz[2], and Jens Harting[1] — [1]Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen- Nürnberg (IEK-11), Dynamics of Complex Fluids and Interfaces, Cauerstraße 1, 91058 Erlangen, Germany — [2]Roskilde University, Department of Science and Environment, Roskilde, Denmark

Thin liquid films are important for many microfluidic applications such as printing or coating of e.g. printable electronics or photovoltaic cells where a evenly spread thin film of certain properties is of utmost importance. It is well known that a thin film on a solid substrate can be unstable and droplet formation may arise, especially for very thin films. The dynamics of thin liquid films and their instability has been the subject of intensive experimental, analytical, and numerical studies, the latter often based on the thin film equation. We propose a set of newly developed equations for the influence of chemical active colloids suspended in a thin liquid film based on the lubrication approximation, advection-diffusion and, the Fick-Jackobs approximation. For this novel set of equations we perform a linear stability analysis (LSA) that reveals surprisingly interesting dynamics. We identify the subset of parameters for which the thin film becomes stable, as well as a variety of different dominating wave-modes. This allows us to control not only the stability but also the droplet size distribution after film rupture. In order to assess the asymptotic state of the thin film, the LSA results are compared against numerical simulations using the Lattice Boltzmann method.

DY 5: Many-Body Quantum Dynamics 1 (joint session DY/TT)

Time: Monday 10:00–12:45 Location: H20

DY 5.1 Mon 10:00 H20

Squeezed-field path integral method for fermionic superfluid systems — •Dapeng Li — Luruper Chaussee 149, Gebäude 69 22761 Hamburg

We develop a squeezed field path integral method for fermionic superfluid systems including BCS superconductors and unconventional superfluid systems. In this method, the squeezing parameters of the Bogoliubov transformation for fermions become dynamical variables representing bosonic collective excitations on superfluid systems. Using this method, we analyze the spectral function of the single particle excitations for BCS superconductors. We demonstrate that, as a main consequence of the method, a bosonic branch corresponding to the Higgs mode appears as a sideband branch, in addition to the single particle excitation branches obtained from the BCS mean-field approximation. Moreover, we show that our framework can also be applied to low-energy excitations of systems with unconventional orders.

DY 5.2 Mon 10:15 H20

Suppression of inter-band heating for random driving — •Hongzheng Zhao[1,2], Johannes Knolle[2,3,4], Roderich Moessner[1], and Florian Mintert[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Imperial College London, London, United Kingdom — [3]Technical University of Munich, Munich, Germany — [4]Munich Center for Quantum Science and Technology, Munich, Germany

Heating to high-lying states strongly limits the experimental observation of driving induced non-equilibrium phenomena, particularly when the drive has a broad spectrum. Here we show that, for entire families of structured random drives known as random multipolar drives, particle excitation to higher bands can be well controlled even away from a high-frequency driving regime. This opens a window for observing drive-induced phenomena in a long-lived prethermal regime in the lowest band. Reference: arXiv:2201.08130

DY 5.3 Mon 10:30 H20

Anomalous hydrodynamics and exact quantum scars in frustration-free Hamiltonians — •Jonas Richter and Arijeet Pal — University College London, UK

We study the interplay between quantum scarring and weak Hilbert-space fragmentation in a class of one-dimensional spin-1 frustration-free projector Hamiltonians, known as deformed Motzkin chain. We show that the particular form of the projectors causes the emergence of disjoint Krylov subspaces, with an exact quantum scar being embedded in each subspace, leading to slow growth of entanglement and localized dynamics for specific out-of-equilibrium initial states. Focusing on infinite temperature, we unveil that spin transport is subdiffusive, which we corroborate by simulations of constrained stochastic cellular automaton circuits. Compared to dipole moment conserving systems, the deformed Motzkin chain belongs to a different universality class with distinct dynamical transport exponent and only polynomially many Krylov subspaces. Based on J. Richter and A. Pal, Phys. Rev. Research 4, L012003 (2022).

DY 5.4 Mon 10:45 H20

Influence functional of quantum many-body systems — •Alessio Lerose, Michael Sonner, Julian Thoenniss, and Dmitry Abanin — University of Geneva, Switzerland

Feynman-Vernon influence functional (IF) was originally introduced to describe the effect of a quantum environment on the dynamics of an open quantum system. We apply the IF approach to describe quantum many-body dynamics in isolated spin systems, viewing the system as an environment for its local subsystems. While the IF can be computed exactly only in certain many-body models, it generally satisfies a self-consistency equation, provided the system, or an ensemble of systems, are translationally invariant. We view the IF as a fictitious wavefunction in the temporal domain, and approximate it using matrix-product states (MPS). This approach is efficient provided the temporal entanglement of the IF is sufficiently low. We illustrate the versatility of the IF approach by analyzing several models that exhibit a range of dynamical behaviors, from thermalizing to many-body localized, in both Floquet and Hamiltonian settings. The IF approach offers a new lens on many-body non-equilibrium phenomena, both in ergodic and non-ergodic regimes, connecting the theory of open quantum systems theory to quantum statistical physics.

DY 5.5 Mon 11:00 H20

Transition from localized to uniform scrambling in locally hyperbolic systems — •Mathias Steinhuber, Juan-Diego Urbina, and Klaus Richter — University of Regensburg, Regensburg, Germany

A major signature of Quantum Chaos is the fast scrambling of quantum correlations, quantified by the exponential initial (pre-Ehrenfest time) growth of out-of-time-order correlators (OTOCs) and by their later saturation. As previously shown by [1] and [2], there is a significant difference in the short time dynamics of the OTOCs in integrable systems around hyperbolic fixed points depending on the initial state being localized or uniform (high-temperature). In these cases, the exponential regime is given respectively by twice the instability-exponent 2λ or only once the stability-exponent λ of the hyperbolic fixed point. We show that a local wave-packet can have a clear *dynamical* transition between these two reported exponential-regions within the pre-Ehrenfest-time regime. Thus, the question arises on how to decide, based on the properties of the hyperbolic fixed point which of the two scenarios applies in each particular situation.

1 Hummel, Q., Geiger, B., Urbina, J. D. & Richter, K. Reversible Quantum Information Spreading in Many-Body Systems near Criticality. Phys. Rev. Lett. 123, 160401 (2019).

2 Xu, T., Scaffidi, T. & Cao, X. Does Scrambling Equal Chaos? Phys. Rev. Lett. 124, 140602 (2020).

15 min. break

DY 5.6 Mon 11:30 H20

Optimal route to quantum chaos in the Bose-Hubbard model — Lukas Pausch[1,2], Edoardo Carnio[1,2], Andreas Buchleitner[1,2], and •Alberto Rodríguez[3] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104, Freiburg, Germany — [2]EUCOR Centre for Quantum Science and Quantum Computing, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104, Freiburg, Germany — [3]Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain

The dependence of the chaotic phase of the Bose-Hubbard Hamiltonian [1,2] on particle number N, system size L and particle density is investigated in terms of spectral and eigenstate features. We analyze the development of the chaotic phase as the limit of infinite Hilbert space dimension is approached along different directions, and show that the fastest route to chaos is the path at fixed density $n \lesssim 1$ [3]. The limit $N \to \infty$ at constant L leads to a slower convergence of the chaotic phase towards the random matrix theory benchmarks. In this case, from the distribution of the eigenstate generalized fractal dimensions, the ergodic phase becomes more distinguishable from random matrix theory for larger N, in a similar way as along trajectories at fixed density.

[1] L. Pausch *et al.*, Phys. Rev. Lett. 126, 150601 (2021)
[2] L. Pausch *et al.*, New J. Phys. 23, 123036 (2021)
[3] L. Pausch *et al.*, arxiv:2205.04209

DY 5.7 Mon 11:45 H20

Observation of phase synchronization and alignment during free induction decay of quantum spins with Heisenberg interactions — •Jürgen Schnack[1], Heinz-Jürgen Schmidt[2], Christian Schröder[3], and Patrick Vorndamme[1] — [1]Universität Bielefeld — [2]Universität Osnabrück — [3]Fachhochschule Bielefeld

Equilibration of observables in closed quantum systems that are described by a unitary time evolution is a meanwhile well-established phenomenon apart from a few equally well-established exceptions. Here we report the surprising theoretical observation that integrable as well as non-integrable spin rings with nearest-neighbor or long-range isotropic Heisenberg interaction not only equilibrate but moreover also synchronize the directions of the expectation values of the individual spins (New J. Phys. 23 (2021) 083038). We highlight that this differs from

spontaneous synchronization in quantum dissipative systems. In our numerical simulations, we investigate the free induction decay (FID) of an ensemble of up to N = 25 quantum spins with s = 1/2 each by solving the time-dependent Schrödinger equation numerically exactly. Our findings are related to, but not fully explained by conservation laws of the system. The phenomenon very robust against for instance random fluctuations of the Heisenberg couplings. Synchronization is not observed with strong enough symmetry-breaking interactions such as the dipolar interaction and is also not observed in closed-system classical spin dynamics.

DY 5.8 Mon 12:00 H20

Long-lived coherence in driven spin systems: from two to infinite spatial dimensions — •Walter Hahn[1,2,3] and Viatcheslav Dobrovitski[2,4] — [1]Fraunhofer IAF, Fraunhofer Institute for Applied Solid State Physics, Freiburg, Germany — [2]QuTech, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands — [3]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, Innsbruck, Austria — [4]Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands

Long-lived coherences, emerging under periodic pulse driving in the disordered ensembles of strongly interacting spins, offer immense advantages for future quantum technologies but the physical origin and the key properties of this phenomenon remain poorly understood. We theoretically investigate this effect in ensembles of different spatial dimensionality, and predict existence of the long-lived coherences in all such systems, from two-dimensional to infinite-dimensional, which are of particular importance for quantum sensing and quantum information processing. We explore the transition from two to infinite dimensions and show that the long-time coherence dynamics in all dimensionalities is qualitatively similar, although the short-time behavior is drastically different exhibiting dimensionality-dependent singularity

DY 5.9 Mon 12:15 H20

A Flow Equation Approach to Many-Body Localisation — •Steven Thomson — Dahlem Centre for Complex Quantum Systems, Freie Universität Berlin

Many-body localisation is a fascinating example of a scenario in which interacting quantum systems isolated from their environments can fail to thermalise, usually due to some form of disorder. Key to our understanding of this enigmatic phase of matter are emergent conserved quantities known as local integrals of motion (LIOMs, or l-bits), which prevent thermalisation from occurring. In this talk, I will present a powerful new numerical method known as the tensor flow equation technique ideally suited for computing LIOMs.

I will demonstrate how this method can be used to compute the integrals of motion in a variety of different systems, including disorder-free potentials and models of spinful fermions. I will show how this method gives an insight into the nature of many-body localisation in these different models, with LIOMs that retain a strong 'fingerprint' of the underlying potential, and will show that in some cases the method can also predict the onset of a delocalised phase. I will end by outlining promising future applications of the method, including to periodically driven and dissipative systems.

DY 5.10 Mon 12:30 H20

Towards a dictionary between JT gravity and periodic orbit theory — •Torsten Weber, Fabian Haneder, Juan-Diego Urbina, and Klaus Richter — University of Regensburg, Germany

Periodic orbit theory is a far reaching development of the semiclassical methods where the most fundamental signatures of the quantum nature of closed systems, like the discreteness of their energy spectrum, emerges from interference between amplitudes constructed from the classical properties of periodic solutions [1]. This conceptual basis, leading to the celebrated Gutzwiller trace formula, has provided impressive achievements from quantum transport to atomic physics and multi-particle scattering. In particular, together with the necessary existence of periodic orbit bunching in ergodic systems, it has lead to an understading of the emergence of universal spectral correlations in chaotic systems, the BGS conjecture [2].

We report our progress in studying how a loss of information (characterized by a coarse graining of classical bunches of orbits) at the level of the trace formula implies the emergence of genus-like expansions with formally the same structure as the solution of JT quantum gravity found in [3]. Our work thus gives convincing hints toward a possible dictionary between quantum-gravitational and periodic orbit objects and concepts.

[1] See e.g. F. Haake, Quantum Signatures of Chaos, Springer, 2000
[3] S. Müller et al., Phys. Rev. E 72, 046207 (2005)
[3] P. Saad, S. Shenker, D. Stanford, arXiv:1903.11115

DY 6: Active Matter 1 (joint session BP/CPP/DY)

Time: Monday 10:30–12:45 Location: H16

Invited Talk DY 6.1 Mon 10:30 H16

Computer simulations of self-motile active droplets and colloid-active gels composites — •Davide Davide Marenduzzo — School of Physics and Astronomy, University of Edinburgh, Edinburgh, UK

In this talk we will show results from computer simulations probing the behaviour of composite materials based on active gels.

In the first part of the talk we will investigate the behavior of active nematic or cholesteric droplets inside an isotropic fluid. In different regions of parameter space, we find regular motility and chaotic behaviour, and discuss the relevance of these results to biophysical systems such as microbial motility.

In the second part of the talk, we will study the dynamics of a dispersion of passive colloidal particles in an active nematic host. We find that activity induces a dynamic clustering of colloids even in the absence of any preferential anchoring of the active nematic director at the particle surface. When such an anchoring is present, active stresses instead compete with elastic forces and re-disperse the aggregates observed in passive colloid-liquid crystal composites.

DY 6.2 Mon 11:00 H16

Chloroplasts in dark-adapted plants show active glassy behavior — •Nico Schramma, Cintia Perugachi Israëls, and Mazi Jalaal — University of Amsterdam, Amsterdam, Netherlands

Photosynthesis in plants is one of the main drivers for the survival of whole ecosystems on earth. To guarantee the efficiency of this process, plants have to actively adapt to ever-changing light conditions. On large time scales plants can grow towards the light. However, this process is too slow to adapt towards transient stimuli. To do this plants can re-arrange the intracellular structure by the active motion of chloroplasts on short timescales. These organelles are confined between the cell membrane and vacuole and can move inside the cytoplasm via actin polymerization forces. Remarkably, the simple - yet elegant - interplay of light-sensing and active forces leads to various modes of collective motion. Here, we show that the chloroplasts under dark conditions are densely packed systems, driven by a-thermal noise and can exhibit active glassy motion. Furthermore, we aim to establish chloroplast motion as a new framework to study the dynamics of light-controlled dense biological systems featuring intriguing dynamic phase transitions.

DY 6.3 Mon 11:15 H16

Activity-induced polar patterns of filaments gliding on a sphere — •Chiao-Peng Hsu, Alfredo Sciortino, Yu Alice de la Trobe, and Andreas Bausch — Center for Protein Assemblies and Lehrstuhl für Zellbiophysik E27, Physics Department, Technische Universität München, Garching, Germany

Active matter systems feature the ability to form collective patterns as observed in a plethora of living systems, from schools of fish to swimming bacteria. While many of these systems move in a wide, three-dimensional environment, several biological systems are confined by a curved topology. The role played by a non-Euclidean geometry on the self-organization of active systems is not yet fully understood, and few experimental systems are available to study it. Here, we introduce an experimental setup in which actin filaments glide on the inner surface of a spherical lipid vesicle, thus embedding them in a curved geometry. We show that filaments self-assemble into polar, elongated structures

and that, when these match the size of the spherical geometry, both confinement and topological constraints become relevant for the emergent patterns, leading to the formation of polar vortices and jammed states. These results experimentally demonstrate that activity-induced complex patterns can be shaped by spherical confinement and topology.

15 min. break

DY 6.4 Mon 11:45 H16

The effect of chiral flows on pattern formation on active cell surfaces — Lucas Wittwer[2], Eloy de Kinkelder[1], and •Sebastian Aland[1,2] — [1]TU Freiberg — [2]HTW Dresden

Mechanochemical processes play a crucial role during morphogenesis, the formation of complex shapes and tissues out of a single cell. On the cellular level, the actomyosin cortex governs shape and shape changes. This thin layer of active material underneath the cell surface exerts an active contractile tension, the strength of which being controlled by the concentration of force-generating molecules. Advective transport of such molecules leads to a complex interplay of hydrodynamics and molecule concentration which gives rise to pattern formation and self-organized shape dynamics. In this talk, we present a novel numerical model to simulate an active viscoelastic surface immersed in viscous fluids. The resulting patterning, flows and cell shape dynamics are shown for different parameter configurations. It is further demonstrated that adding a chiral (i.e. counter-rotating) force at the cell surface can promote a ring of high molecule concentration and facilitate cell division.

DY 6.5 Mon 12:00 H16

Premelting controlled active matter in ice — •Jeremy Vachier[1] and John S. Wettlaufer[1,2] — [1]Nordita, KTH Royal Institute of Technology and Stockholm University, Hannes Alfvéns väg 12, SE-106 91 Stockholm, Sweden — [2]Yale University, New Haven, Connecticut 06520-8109, USA

Self-propelled particles can undergo complex dynamics due to a range of bulk and surface interactions. In the case of a foreign particle inside a subfreezing solid, such as a particle in ice, a premelted film can form around it allowing the particle to migrate under the influence of an external temperature gradient, which is a phenomenon called thermal regelation. It has recently been shown that the migration of particles of a biological origin can accelerate melting in a column of ice and thereby migrate faster. We have previously shown that the effect of regelation plays a major role in the migration of inert particles and impurities inside ice, with important environmental implications. In particular, the question of how the activity affects a particle's position over time is essential for paleoclimate dating methods in ice cores. We re-cast this class of regelation phenomena in the stochastic framework of active Ornstein-Uhlenbeck dynamics and make predictions relevant to this and related problems of interest in geophysical and biological problems.

DY 6.6 Mon 12:15 H16

Emergent collective behavior of active Brownian particles with visual perception — •Rajendra Singh Negi, Roland G. Winker, and Gerhard Gompper — Theoretical Physics of Living Matter, Institute of Biological Information Processing (IBI-5), Forschungszentrum Jülich, 52425 Jülich, Germany

Collective behavior of self-propelled agents emerges from the dynamic response of individuals to various input signals [1,2]. One such input signal is visual perception. We explore the behavior of a model of self-steering active Brownian particles with visual perception in two dimensions [3]. Several non-equilibrium structures like motile worms, worm-aggregate coexistence, aggregates, and a dilute-gas phase are obtained, depending on the system parameters. The strength of the response to the visual signal, vision angle, packing fraction,rotational diffusion, and activity (velocity v_0) determine the location and extent of these phases in the phase diagram. The radius-of-gyration tensor is used to distinguish between the worm and the aggregate phase. Our results help to understand the collective behavior of cognitive self-propelled particles, like animal herds and micro-robotic swarms.

[1]. J. Elgeti, R. G. Winkler, and G. Gompper, Rep. Prog. Phys. **78**, 056601 (2015).

[2]. M. R. Shaebani, A. Wysocki, R. G. Winkler, G. Gompper, and H. Rieger, Nat. Rev. Phys. **2**, 181 (2020).

[3]. L. Barberis and F. Peruani, Phys. Rev. Lett. **117**, 248001 (2016).

DY 6.7 Mon 12:30 H16

Diffusiophoretic propulsion of an isotropic active particle near a finite-sized disk — •Abdallah Daddi-Moussa-Ider[1], Andrej Vilfan[1,2], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Jozef Stefan Institute, 1000 Ljubljana, Slovenia — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We employ a far-field analytical model to quantify the leading-order contribution to the induced phoretic velocity of an isotropic active colloid near a finite-sized disk of circular shape resting on an interface separating two immiscible viscous incompressible Newtonian fluids. To this aim, we formulate the solution of the phoretic problem as a mixed-boundary-value problem which we then transform into a system of dual integral equations on the inner and outer domains. Depending on the ratio of different involved viscosities and solute solubilities, the sign of phoretic mobility and chemical activity, as well as the ratio of particle-interface distance to the radius of the disk, we find the isotropic active particle to be repelled from the interface, be attracted to it, or reach a stable hovering state and remain immobile near the interface. Our results may prove useful in controlling and guiding the motion of self-propelled phoretic active particles near aqueous interfaces.

Reference: A. Daddi-Moussa-Ider, A. Vilfan, and R. Golestanian, *J. Fluid Mech.* **940** A12 (2022)

DY 7: Statistical Physics of Biological Systems 1 (joint session BP/DY)

Time: Monday 15:00–17:15 Location: H16

DY 7.1 Mon 15:00 H16

Dynamics and Fair Risk Sharing in Groups of Intelligent, Egoistic Individuals — Samuel Monter[1], •Veit-Lorenz Heuthe[1], Emanuele Panizon[2], and Clemens Bechinger[1] — [1]FB Physik, Universität Konstanz, Konstanz, Germany — [2]Department of Quantitative Life Science, ICTP, Trieste, Italy

Many animal species organize in social groups of fascinating complexity. The evolutionary biologist W.D. Hamilton hypothesized that the gregariousness of some animals can be explained solely from the egoistic motivation to decrease the risk of predation [1]. As a quantitative measure of this risk, he considered the Voronoi area around each animal. Many collective behavior studies try to capture this motivation by imposing interaction rules or neglect the driving motive altogether when modeling the dynamics of animals. In this study we train a swarm of individuals in a Multi Agent Reinforcement Learning (MARL) framework according to Hamilton's hypothesis, i.e. to decrease their predation risk. Thus, we gain insights into the dynamics of an ensemble of selfishly motivated individuals unbiased by any a priori assumption about interactions. We find that the individuals learn to cluster into groups which exhibit dynamic steady states resembling the behavior of natural swarms. Additionally, the predation risk is shared evenly within the groups, counterintuitive to the selfish motivation of each individual. Our findings suggest that gregariousness could indeed be driven by selfish motives in accordance with Hamilton's hypothesis.

[1] W. D. Hamilton, Journal of theoretical Biology 1971, 31, 295-311.

DY 7.2 Mon 15:15 H16

Boundary-driven epithelial ordering: from the mouse embryo to topological defects — •Pamela Guruciaga[1], Takafumi Ichikawa[2], Takashi Hiiragi[3], and Anna Erzberger[1] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Kyoto University, Kyoto, Japan — [3]Hubrecht Institute, Utrecht, The Netherlands

In physical problems boundaries are typically considered to be simple, static and externally fixed. Biological systems however not only interact with their surroundings, but also alter them in ways that feed back on their own dynamics. We address this complex interaction in the context of epithelial development. Motivated by observations of an interplay between apico-basal polarity and boundary geometry in mouse epiblast morphogenesis, we develop a theory for epithelial ordering based on the Landau-de Gennes approach to surface-induced order in liquid crystals. We introduce a vector order parameter to represent the polarity, and model its interaction with the boundaries by a weak anchoring energy. We calculate the alignment fields arising from different boundary curvatures, and compare our predictions with imaging data of the morphogenetic process. Our work highlights the role of extraembryonic tissue in embryogenesis, while identifying interesting physical phenomena, such as boundary-dependent transitions in the structure of topological defects.

DY 7.3 Mon 15:30 H16

A competitive advantage through fast dead matter elimination in confined cellular aggregates — •Yoav G. Pollack[1,2], Philip Bittihn[1], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), Göttingen, 37077, Germany. — [2]Max Planck Institute for Multidisciplinary Sciences (MPI-NAT), Göttingen, 37077, Germany. — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, OX1 3PU, UK.

Competition of different cell types for limited space is relevant in biological processes such as tissue morphogenesis and tumor growth. Predicting the outcome for non-adversarial competition of such growing active matter is non-trivial, as it depends on how processes like growth, proliferation and the degradation of cellular matter are regulated in confinement; regulation that happens even in the absence of competition to achieve homeostasis. We show that passive by-products of the processes maintaining homeostasis can significantly alter fitness, enabling cell types with lower homeostatic pressure to outcompete those with higher homeostatic pressure. We reveal that interfaces play a critical role for this specific kind of competition: There, growing matter with a higher proportion of active cells can better exploit local growth opportunities that continuously arise as the active processes keep the system out of mechanical equilibrium. Our results show that optimizing the ratio of growing (active) to dead (passive) cells can be as important to survival as growth rates and their sensitivity to mechanical cues.

DY 7.4 Mon 15:45 H16

A biophysical model of DNA methylation ageing — •Aida Hashtroud and Steffen Rulands — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Machine learning models can accurately predict biological age and time of death based on sequencing measurements of DNA methylation marks. The mechanistic basis underlying these methylation clocks is poorly understood. Here, using a combination of tools from statistical physics and sequencing experiments we show that biological age can be predicted as a result of collective processes in the boundaries between genomic regions of different densities of cytosine-guanine pairs (CpGs). Specifically, we define a biophysical model predicting the time evolution of DNA methylation patterns during ageing based on a wave localization mechanism of tilted competition between antagonistic chromatin modifiers. Our work shows that biological age can be predicted from DNA methylation patterns using models with few parameters inspired by statistical physics.

15 min. break

Invited Talk DY 7.5 Mon 16:15 H16

From active bacterial microcolonies to biofilms as model tissues — •Vasily Zaburdaev — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Bacterial intrinsic activity is evident on all stages of their life cycle. We will start by following how individual cells deploy forces to attach and move on surfaces. We suggest how these active movements may be harnessed to generate work and, for example, cells can power the rotation of micro-turbines. When let to move and interact, however, bacteria will find each other and form microcolonies that consist of several thousands of cells. Microcolonies are often the functional units of the bacterial existence in natural settings and in the context of disease. We will provide theoretical framework describing the bacterial microcolonies as active viscoelastic materials and discuss how this theory might be useful in eukaryotic systems such as organoids, tumour spheroids or clustering immune cells. Microcolonies may further develop into even more complex bacterial communities known as biofilms - there, bacteria embed themselves in the self-secreted extracellular matrix creating an analogue of multicellular tissues. We will outline some future research avenues deepening this analogy and illustrate it with an intriguing example of wound healing in bacterial biofilms.

DY 7.6 Mon 16:45 H16

Playing it safe: information constrains collective betting strategies — •Philipp Fleig[1,2] and Vijay Balasubramanian[2] — [1]Max Planck Institute for Medical Research, 69120 Heidelberg, Germany — [2]Department of Physics & Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA

Risk is an inherent part of life and biological functions are partly shaped by the need to reduce risk. Broadly, risk arises from stochastic interactions of an organism with its environment. Every time an organism displays a particular response or behaviour (e.g. expresses a phenotype or exhibits a certain immune response), it is placing a bet with potential impact on its biological fitness. The more precisely the statistics of the environment are known to the organism, the more successfully bets can be placed. However, an organism typically has limited information about the statistics of the environment. This limitation should be accounted for in the adaptation of biological functions to the environment. We develop a theoretical principle where information geometric model complexity guides stochastic biological functions towards less risky betting strategies. In the framework of Bayesian inference, we show that given finite information about the environment, there is an optimally safe adaptation strategy set by the Bayesian prior. Furthermore, in a toy model of stochastic phenotypic switching by bacteria, we demonstrate how the implementation of our principle of "playing it safe" increases the fitness (population growth rate) of the bacterial collective. We suggest that the principle applies broadly to problems of adaptation, learning and evolution.

DY 7.7 Mon 17:00 H16

Quantification of intracellular information flow — •Mirna Kramar[1], Mathieu Coppey[1], Thierry Mora[2], and Aleksandra Walczak[2] — [1]UMR 168, Institut Curie, Paris — [2]Laboratoire de Physique, Ecole Normale Supérieure, Paris

Signalling pathways are cascades of biochemical reactions which transduce signals from the exterior to the interior of the cell. By essence, these pathways convey information about the outside world which cells collect and process to adapt and guide decisions. The cell's ability to govern its functions correctly and precisely while relying on these intricate biochemical networks is surprising given the crowded and noisy cell interior, which indicates that the mechanisms cells use to process information are highly sophisticated. While our understanding of the constituents of the cellular machinery and the processes taking place in the cell is steadily increasing, little is known about the information flow within the cell. Are pathways conveying only on/off signals, or is there more graded information being transduced?

Here, we measure and quantify the information relayed through the MAPK signalling pathway, one of the key signalling pathways in eukaryotic systems. Using a synergy of an optogenetic experimental setup and a data analysis pipeline based on information theory, we quantify the input-output relationships within the MAPK signalling pathway. We show that the capacity of the pathway far exceeds the 1-bit value (on/off), and that collective systems of cell seem to exploit this capacity.

DY 8: Data Analytics for Complex Systems (joint session DY/SOE)

Time: Monday 15:00–17:45 Location: H18

DY 8.1 Mon 15:00 H18

Estimating covariant Lyapunov vectors from data — •Nahal Sharafi, Christoph Martin und Sarah Hallerberg — Hamburg University of Applied Sciences, Hamburg, Germany

Covariant Lyapunov vectors characterize the directions along which perturbations in dynamical systems grow. They have also been studied as predictors of critical transitions and extreme events. For many applications, it is necessary to estimate these vectors from data since model equations are unknown for many interesting phenomena. We propose a novel approach for estimating covariant Lyapunov vectors based on data records without knowing the underlying equations of the system. In contrast to previous approaches, our approach can be applied to high-dimensional datasets. We demonstrate that this purely data-driven approach can accurately estimate covariant Lyapunpov vectors from data records generated by low and high-dimensional dynamical systems. Additionally we test for the robustness against noise in a low-dimensional dynamical system.

DY 8.2 Mon 15:15 H18

Extending the limits of Electrochemical Impedance Spectroscopy with Machine Learning and Digital Twins — •Limei Jin[1,2], Franz P. Bereck[2], Christian H. Bartsch[2], Josef Granwehr[2], Rüdiger-A. Eichel[2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]IEK-9, Forschungszentrum Jülich, Jülich, Germany

Electrochemical impedance spectroscopy (EIS) is widely used to characterize electrochemical energy conversion systems. The traditional analysis with equivalent circuit models (ECM) has recently been augmented by a transform based distribution of relaxation times (DRT) analysis which allows one to reduce the ambiguity in the construction of ECMs and thus overfitting. Yet, DRT, just like most traditional analyses, is firmly based in the linear response regime as well as based on frequency sweeps on a logarithmic scale. The latter makes these approaches time-consuming, the first limits their scope severely. To develop novel experimental spectroscopic excitation schemes that address these limitations, a model space of sufficiently realistic systems is required that substitutes for time-consuming measurements in terms of a digital twin. We present a joint experimental and theoretical approach for the construction of such a target space for the case of battery cell performance and ageing behaviour.

DY 8.3 Mon 15:30 H18

Bayesian approach to anticipate critical transitions in complex systems — •Martin Hessler[1,2] and Oliver Kamps[2] — [1]Westfälische Wilhelms-Universität Münster, 48149 Münster — [2]Center for Nonlinear Science, Westfälische Wilhelms-Universität Münster, 48149 Münster

Complex systems in nature, technology and society can undergo sudden transitions between system states with very different behaviour. In order to avoid undesired consequences of these tipping events, statistical measures as variance, autocorrelation, skewness and kurtosis have been proposed as leading indicators based on time series analysis. Under favourable conditions they can give a hint of an ongoing bifurcation-induced destabilization process. However, they suffer from their loose connection to complex system dynamics, sensitivity to noise and sometimes misleading trends. Therefore, we want to present an alternative approach assuming the dynamical system being described by a Langevin equation. Starting from this stochastic description, we combine MCMC sampling, rolling window methods and Bayesian reasoning to derive the drift slope as an alternative early warning sign. The Bayesian approach enables us to define credibility bands which make it easier to distinguish random fluctuations from real trends that imply a less resilient system. Our investigations suggest that the estimation procedure is rather robust even under strong noise. Besides, the noise level of the system is computed to get insights into the probability of a noise induced transition. We want to present some of the results and discuss possible limitations and tasks of future research.

DY 8.4 Mon 15:45 H18

Stochastic Interpolation of Sparsely Sampled Time Series by a Superstatistical Random Process and its Synthesis in Fourier and Wavelet Space — •Jeremiah Lübke[1], Jan Friedrich[2], and Rainer Grauer[1] — [1]Institute for Theoretical Physics I, Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany — [2]ForWind, Institute of Physics, University of Oldenburg, Küpkersweg 70, 26129 Oldenburg, Germany

A novel method is presented for stochastic interpolation of a sparsely sampled time signal based on a superstatistical random process generated from a Gaussian scale mixture. In comparison to other stochastic interpolation methods such as kriging, this method possesses strong non-Gaussian properties and is thus applicable to a broad range of real-world time series. A precise sampling algorithm is provided in terms of a mixing procedure that consists of generating a field $u(\xi, t)$, where each component $u_\xi(t)$ is synthesized with identical underlying noise but covariance $C_\xi(t, s)$ parameterized by a log-normally distributed parameter ξ. Due to the Gaussianity of each component $u_\xi(t)$, standard sampling algorithms and methods to constrain the process on the sparse measurement points can be exploited. The scale mixture $u(t)$ is then obtained by assigning each point in time t a $\xi(t)$ and therefore a specific value from $u(\xi, t)$, where $\log \xi(t)$ is itself a realization of a Gaussian process with a correlation time large compared to the correlation time of $u(\xi, t)$. Finally, a wavelet-based hierarchical representation of the interpolating paths is introduced, which is shown to provide an adequate method to locally interpolate large datasets.

DY 8.5 Mon 16:00 H18

Global sensitivity analysis of Monte Carlo models using Cramer-von Mises distance — •Sina Dortaj[1,2] and Sebastian Matera[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute for Mathematics, Freie Universität Berlin, Arnimallee 6, 14195 Berlin, Germany

Typically, the parameters entering a physical simulation model carry some kind of uncertainty, e.g. due to the intrinsic approximations in a higher fidelity theory from which they have been obtained. Global sensitivity analysis (GSA) targets quantifying which parameters uncertainties impact the accuracy of the simulation results, e.g. to identify which parameters need to be determined more accurately.

We present a GSA approach on basis of the Cramers-von Mises distance. Unlike prevalent approaches it combines the following properties: i) it is equally suited for deterministic as well as stochastic model outputs, ii) it is free of gradients, and iii) it can be estimated from any suitable numerical quadrature (NQ) without further numerical tricks. Using Quasi-Monte Carlo for NQ and prototypical first-principles kinetic Monte Carlo models (kMC), we examine the performance of the approach. We find that the approach typically converges in a modest number of NQ points. Furthermore, it is robust against even extreme relative noise. All these properties make the method particularly suited for expensive (kinetic) Monte Carlo models, because we can reduce the number of simulations as well as the target variance of each of these.

15 min. break

DY 8.6 Mon 16:30 H18

Reproducible and transparent research software pipelines using semantic research data management and common workflow language — •Alexander Schlemmer[1,2,5], Inga Kottlarz[1,3], Baltasar Rüchardt[1,5], Ulrich Parlitz[1,3,5], and Stefan Luther[1,4,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]IndiScale GmbH, Göttingen — [3]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen — [4]Institute of Pharmacology and Toxicology, University Medical Center Göttingen — [5]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen

Sustainable and well-documented scientific software is essential for effectiveness and reproducibility in data-intensive research. In practice, incompletely documented software hinders in many cases replicability, reproducibility and method comparison. In our terminology, documentation includes method and algorithm descriptions as well as human- and machine-readable representations of parameters, initial conditions and data, versions and dependencies and a well-defined software execution environment. We present an approach combining semantic data management with CaosDB and processing pipelines with Common Workflow Language (CWL), showing use cases from dynamical systems research. The CWL-based environment provides a transparent

description of the process and includes metadata that can be searched within CaosDB. Input-/output-data and parameters can be directly linked to algorithms and software snapshots. The employment of containers simplifies reproducibility and interoperability.

DY 8.7 Mon 16:45 H18

MDSuite: A post-processing engine for particle simulations — •Fabian Zills[1], Samuel Tovey[1], Francisco Torres-Herrador[2], Christoph Lohrmann[1], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany — [2]von Karman Institute for Fluid Dynamics, Rhode-St-Genese, Belgium

Particle-based simulations are experiencing a rapid growth wherein system sizes in the hundreds of thousands or even millions are becoming commonplace. With this growth in system size comes the additional challenge of post-processing the simulation data.

In this talk, we introduce the Python package MDSuite. MDSuite is designed for the post-processing of particle-based simulation in an efficient manner and on modern hardware. Built on top of TensorFlow, MDSuite calculators are fully parallelised, gpu-enabled, and, due to the use of modern data pipe-lining methods, completely memory safe. Furthermore, the use of HDF5 and SQL database structures enables effective tracking of calcualtion parameters as well as a compressed trajectory storage medium. We present MDSuite as a standalone package for the storage, analysis, and comparison of large-scale simulation studies.

DY 8.8 Mon 17:00 H18

Distinguishing noise from high-dimensional chaos — •Inga Kottlarz[1,2] and Ulrich Parlitz[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Dynamics of Complex Systems, Georg-August-Universität Göttingen, Göttingen, Germany

The ordinal pattern-based Complexity-Entropy Plane is a popular tool in nonlinear dynamics for distinguishing noise from chaos. While successful attempts to do so have been documented for low-dimensional maps and continuous-time systems, high-dimensional systems have been somewhat neglected so far. To address the question in which way time series from highdimensional chaotic attractors can be characterized by their location in the Complexity-Entropy Plane we analyze data from the high-dimensional continuous-time Lorenz-96 system, the discrete generalized Hénon map and the Mackey-Glass equation as a delay system and discuss the crucial role of the lag and the pattern length or the ordinal pattern, and the length of the available time series.

DY 8.9 Mon 17:15 H18

The impact of the UEFA European Football Championship on the spread of COVID-19 — •Jonas Dehning[1], Sebastian B. Mohr[1], Sebastian Contreras[1], Philipp Dönges[1], Emil Iftekhar[1], Oliver Schulz[2], Philip Bechtle[3], and Viola Priesemann[1,4] — [1]MPI for Dynamics and Self-Organization, 37077 Göttingen — [2]MPI for Physics, 80805 München — [3]Physikalisches Institut, University of Bonn — [4]Institute for the Dynamics of Complex Systems, University of Göttingen

Large-scale international events like the UEFA Euro 2020 football championship offer a unique opportunity to quantify the impact of match-related social gatherings on COVID-19, as the number of matches played by participating countries resembles a randomized trial. Moreover, soccer-related activities have a marked gender-imbalance that we can exploit for inference. In our work, we build a differentiable Bayesian SEIR-like model. Its parameters are inferred with Hamiltonian Monte-Carlo using the PyMC3 package. Our model simulates COVID-19 spread in each country using a discrete renewal process and gender-resolved case numbers. On average, 3.2% (95% CI: [1.3%, 5.2%]) of new cases in the 12 analyzed countries can be associated with the match-related social gatherings throughout our analysis period. Individually, England, the Czech Republic and Scotland showed a significant effect. Besides these insights on the spread of COVID-19 during large-scale events, our approach is an example of how modern Bayesian tools can be leveraged to gain insights on a complex dynamic process.

DY 8.10 Mon 17:30 H18

Recurrence-based analysis of instantaneous fractal characteristics of geomagnetic variability — •Reik V. Donner[1,2], Tommaso Alberti[3], and Davide Faranda[4] — [1]Hochschule Magdeburg-Stendal, Magdeburg, Germany — [2]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [3]National Institute for Astrophysics, Rome, Italy — [4]LSCE, Université Paris-Saclay, Gif-sur-Yvette, France

We employ two complementary approaches based on the concept of recurrences in phase space to quantify the local (instantaneous) and global fractal dimensions of the temporal variations of a suite of low (SYM-H, ASY-H) and high latitude (AE, AL, AU) geomagnetic indices and discuss similarities and dissimilarities of the obtained patterns for one year of observations during a solar activity maximum. Subsequently, we introduce bivariate extensions of both approaches, and demonstrate their capability of tracing different levels of interdependency between low and high latitude geomagnetic variability during periods of magnetospheric quiescence and along with perturbations associated with geomagnetic storms and magnetospheric substorms, respectively. Our results open new perspectives on the nonlinear dynamics and intermittent mutual entanglement of different parts of the geospace electromagnetic environment, including the equatorial and westward auroral electrojets, in dependence of the overall state of the geospace system affected by temporary variations of the solar wind forcing.

DY 9: Invited Talk Ralf Stannarius

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

Invited Talk DY 9.1 Mon 15:00 H19

Granular matter composed of non-convex grains — •Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

The majority of granular matter studies so far has been devoted to hard, spherical grains. Recently, efforts have been increasingly focused on the investigation of shape-anisotropic and soft particle systems. We report experimental investigations of granular matter composed of non-convex particles. The random packing and orientational short-range order of flat crosses is studied in a two-dimensional geometry, and the influence of the aspect ratio (arm length divided by arm length) is analyzed. With spatial crosses (hexapods), we perform shear experiments and report an unexpected phenomenon in split-bottom containers, a 'reversed Weissenberg effect' of granular matter. Secondary flow leads to convection rolls normal to the shear direction.

DY 10: Modeling and Simulation of Soft Matter (joint session CPP/DY)

Time: Monday 15:00–17:45 Location: H39

DY 10.1 Mon 15:00 H39

Machine Learning of consistent thermodynamic models using automatic differentiation — •David Rosenberger[1], Kipton Barros[2], Timothy Germann[2], and Nicholas Lubbers[2] — [1]Freie Universität Berlin, Berlin, Germany — [2]Los Alamos National Laboratory, Los Alamaos, NM, USA

Instead of fitting suitable analytical expressions to thermophysical data, we propose to combine automatic differentiation and artificial neural networks (ANNs) to obtain complex equations of state (EOS) for arbitrary systems. Rather than training directly on the properties of interest, we train an ANN on a model free energy whose partial derivatives match the thermophysical properties measured in experiment. We show that this method is advantageous over direct learning of thermodynamic properties, in terms of both accuracy and the exact preservation of the Maxwell relations. Furthermore, the method can implicitly solve the integration problem of computing the free energy of a system without explicit integration given appropriate data to learn from.

DY 10.2 Mon 15:15 H39

Atomistic Machine Learning for Aqueous Ionic Solutions — •Philip Loche, Kevin K. Huguenin-Dumittan, and Michele Ceriotti — Laboratory of Computational Science and Modeling, IMX, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Accurate modeling of matter at the atomic scale requires to simultaneously account for the quantum nature of the chemical bond - that usually manifests itself on short time and length scales - and long-range interactions, such as electrostatics and dispersion, that occur on a large scale and often result in phenomena with a long characteristic time. Electronic structure calculations provide an accurate description of both quantum and long-range effects, but are computationally demanding, and scale poorly with system size. Machine learning (ML) approaches have emerged as a very effective strategy to build surrogate models that provide comparable accuracy at a fraction of the cost, but the most widespread techniques base their efficiency and transferability on a local description of atomic structure, which makes them ill-equipped to deal with long-range effects.

Here, we are going to to connect local and long range physics in a data driven ML approach by applying the current ML techniques to, condensed-phase systems, involving the characterization of aqueous ionic solutions. We show that only a combination of a long and a short range approach is able to predict short distanced molecular vibrations as well a long ranged ionic screening lengths.

DY 10.3 Mon 15:30 H39

Identification of glass transition temperature for polymer melts using data-driven methods — •Atreyee Banerjee, Hsiao-ping Hsu, Oleksandra Kukharenko, and Kurt Kremer — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

On fast cooling, the dynamics of polymer melts slow down exponentially, leading to solid glassy states without any drastic change in the structural structure. We employ data-driven methods based on purely confomational fluctuations to identify the glass transition temperature for a coarse-grained weakly semi-flexible polymer model. More precisely, we used principal component analysis (PCA) to quantify the conformational fluctuations and identify a sharp change in fluctuation around the glass transition temperature. The first eigen value of PCA shows a clear difference below and above glass transition temperatures. The new method of glass transition temperature predicted from PCA considers local structural fluctuations and does not depend on any fitting parameters like the existing methods.

DY 10.4 Mon 15:45 H39

Systematic parametrization of non-Markovian dissipative thermostats for coarse-grained molecular simulations with accurate dynamics — •Viktor Klippenstein and Nico F. A. Van Der Vegt — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, 64287 Darmstadt, Germany

The Mori-Zwanzig theory, in principle, allows to derive an exact equation of motion for coarse-grained degrees of freedom based on the dynamics of an underlying fine-grained reference system.[1] Still, in practice the simultaneous representation of structural and dynamic properties in particle-based models poses a complicated problem, e.g. due to the non-linearity of the exact coarse-grained equation of motion.

A viable approximate approach is to start from a conservative coarse-grained force-field and to extend the standard Newtonian equation of motion used in molecular simulation with a linear generalized Langevin thermostat. We demonstrate how such a thermostat can be parametrized to correctly represent dynamic properties, both in a purely bottom-up approach[2,3] or by applying iterative optimization.[3] We consider the Asakura-Oosawa model as a simple test case.[3]

[1] V. Klippenstein, M. Tripathy, G. Jung, F. Schmid, and N. F. A. van der Vegt, The Journal of Physical Chemistry B 125, 4931 (2021).
[2] V. Klippenstein and N. F. A. van der Vegt, The Journal of Chemical Physics 154, 191102 (2021).
[3] V. Klippenstein and N. F. A. Van Der Vegt, The Journal of Chemical Physics under review (2022).

DY 10.5 Mon 16:00 H39

Stretching biopolymers with fluctuating bending stiffness — •Panayotis Benetatos — Kyungpook National University, Daegu, South Korea

In many biopolymers, the local bending stiffness fluctuates. For example, DNA-binding proteins attach to and detach from DNA to regulate cellular functions, thus causing a change in the local bending stiffness of the polymer backbone. This could also happen due to internal conformational transitions, such as the DNA denaturation or the helix-coil transition in polypeptides. What all these cases have in common is that the change in the local flexibility is transient and reversible. In order to analyse the conformational and elastic behaviour of such biopolymers, we propose a minimal but encompassing model of a freely jointed chain with reversible hinges (rFJC). We show that the tensile response of a rFJC is remarkably different from that of the usual freely jointed chain (uFJC). At small stretching forces, the rFJC is more compliant than the uFJC and the size (mean square end-to-end distance) of the former is greater than that of the latter. At strong stretching forces, in contrast, the rFJC is much stiffer than the uFJC. In this talk, we also discuss a strongly stretched wormlike chain with fluctuating local bending stiffness. We show that, under certain conditions, we get significant ensemble inequivalence (Gibbs vs Helmholtz).

DY 10.6 Mon 16:15 H39

Modulating internal transition kinetics of responsive macromolecules by collective crowding — •Nils Göth, Upayan Baul, Michael Bley, and Joachim Dzubiella — Applied Theoretical Physics—Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

Packing and crowding are used in biology as mechanisms to (self-) regulate internal molecular or cellular processes based on collective signaling. Here, we study how the transition kinetics of an internal "switch" of responsive macromolecules is modified collectively by their spatial packing. We employ Brownian dynamics simulations of a model of Responsive Colloids, in which an explicit internal degree of freedom–here, the particle size–moving in a bimodal energy landscape self-consistently responds to the density fluctuations of the crowded environment. The bimodal energy landscape is motivated by existing two-state behavior like in protein folding or hydrogels with bimodal volume transitions. We demonstrate that populations and transition times for the two-state switching kinetics can be tuned over one order of magnitude by "self-crowding". An exponential scaling law derived from a combination of Kramers' and liquid state perturbation theory is in very good agreement with the simulations.

[1] Upayan Baul, NG, MB, and JD, J. Chem. Phys. 155, 244902 (2021).

15 min. break

DY 10.7 Mon 16:45 H39

Modelling process-structure-properties of polymer nanocomposites — •Janett Prehl, Constantin Huster, and Karl Heinz Hoffmann — TU Chemnitz, Chemnitz, Germany

Twin polymerization is a complex chemical reaction process leading to a broad range of organic-inorganic nano composite materials.

Within this presentation we will show our latest results [1] on the theoretical analysis of the structure formation process of twin polymerization via a previously introduced lattice-based Monte Carlo method, the reactive bond fluctuation model [2]. We analyze the effects of various model parameters, such as movability, attraction, or reaction probabilities on structural properties, like the specific surface area, the radial distribution function, the local porosity distribution, or the total fraction of percolating elements.

From these examinations, we may identify structural key factors and thus chemical properties of the underlying components that need to be adapted to fulfill desired requirements for possible applications.

[1] Prehl, J. and Huster, C., *polymers* **11** (2019) 878

[2] Hoffmann, K.H. and Prehl, J., *Reac. Kinet. Mech. Cat.* **123** (2018) 367-383; Huster, C., Nagel, K., Spange, S., and Prehl, J., *Chem. Phys. Lett.* **713** (2018) 145-148

DY 10.8 Mon 17:00 H39

A cosolvent surfactant mechanism affects polymer collapse in miscible good solvents — •Swaminath Bharadwaj[1], Divya Nayar[1,2], Cahit Dalgicdir[1], and Nico van der Vegt[1] — [1]Technische Universität Darmstadt, Germany — [2]IIT Delhi, India

The coil-globule transitions of aqueous polymers are of profound significance in understanding the structure and function of responsive soft matter. In particular, the remarkable effect of amphiphilic cosolvents (which preferentially adsorb on the polymer surface) that leads to both swelling and collapse of stimuli responsive polymers is still hotly debated in the literature [1]. The predominant focus has been on the attractive polymer-(co)solvent interactions and the role of solvent-excluded volume interactions has been largely neglected. The solvent-excluded volume contribution to the solvation free energy corresponds to the formation of a repulsive polymer-solvent interface.

Using MD simulations, we herein demonstrate that alcohols reduce the free energy cost of creating a repulsive polymer-solvent interface via a surfactant-like mechanism which surprisingly drives polymer collapse at low alcohol concentrations. This hitherto neglected role of interfacial solvation thermodynamics is common to all coil-globule transitions [2], and rationalizes the experimentally observed effects of higher alcohols and polymer molecular weight on the coil-to-globule transition of thermoresponsive polymers [2]. This mechanism is generic and applicable to other solutions containing amphiphilic cosolvents or cosolutes.

References: [1] S. Bharadwaj et al., Soft Matter, 2022, 18, 2884. [2] S. Bharadwaj et al., Commun. Chem., 2020, 3, 165.

DY 10.9 Mon 17:15 H39

Water transport in soft nanoporous materials: Impact of mechanical response on dynamics, slippage and permeance — •Alexander Schlaich[1,2], Matthieu Vandamme[3], Marie Plazanet[2], and Benoit Coasne[2] — [1]Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, Germany — [2]Univ. Grenoble Alpes, CNRS, LIPhy, 38000 Grenoble, France — [3]Navier, Ecole des Ponts, Univ. Gustave Eiffel, CNRS, Marne-la-Vallee, France

Transport of water in soft porous materials is relevant to applications such as ultrafiltration and reverse osmosis processes, where polymeric membranes are employed in filtration/separation, or energy related processes. While water transport in hard porous materials such as porous silica glasses is well studied, the situation in soft matter is much more puzzling and remains unclear due to the combination of surface heterogeneity, the diffuse boundary location and pore deformations due to mechanical stresses.

In this work we study water in chemically realistic hydrophobic pores at different thermodynamic and mechanical conditions using atomistic molecular dynamics simulations. In detail, we analyze pore swelling, adsorption and confinement effects as well as microscopic diffusion mechanisms and transport effects due to pore size fluctuations. Strikingly, we find that hydrodynamic continuum models remain valid for planar flow of water even in monolayer confinement in soft pores.

DY 10.10 Mon 17:30 H39

Solvation structure of polymer cathodes for Li/S batteries — •Diptesh Gayen[1], Yannik Schuetze[2], Sebastien Groh[1], and Joachim Dzubiella[1] — [1]Institute of Physik, University of Freiburg, Freiburg, Germany — [2]Helmholtz Zentrum Berlin, Berlin

Lithium-sulfur (Li/S) batteries are regarded as one of the most promising next-generation energy storage devices. Meanwhile, some challenges inherent to Li/S batteries remain to be solved, for instance, the polysulfide shuttle effect and the volume expansion of the cathode during discharge. To suppress the above-mentioned drawbacks, polymeric cathodes, e.g., based on poly(4-(thiophen-3-yl) benzenethiol) (PTBT) are considered sulfur host material (S/PTBT). Here, we use molecular dynamics (MD) computer simulations to study the structure and dynamics of a single PTBT chain at 300 K in different concentrations and compositions of dimethoxyethane (DME) and dioxolane (DOL) solvents. The force-field parameters for this polymer were constructed based on the OPLS database, with missing parameters newly developed by us by benchmarking to density-functional theory calculations. We report results on polymer conformational behavior, solvent-specific adsorption, and thermodynamic properties such as the partial molar volume. Our results show that DOL is more absorbed at the PTBT compare to DME. We find no significant effect of the solvent on the structure factor of the polymer. Our simulation model enables future systematic studies of PTBT in various solvent mixtures, in particular electrolytes, for the optimizations of modern Li/S batteries.

DY 11: Granular Matter and Contact Dynamics

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

DY 11.1 Mon 15:30 H19

Measuring the coarsening dynamics of ferromagnetic granular networks under impact of a vertical magnetic field — Matthias Biersack[1], Oksana Bilous[2], Pedro Sanchez[2], Sofia Kantorovich[2], and •Reinhard Richter[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Computational Physics, University of Vienna, 1090 Vienna, Austria

We are exploring in experiments the aggregation process in a shaken granular mixture of glass and magnetized steel beads, occuring in a horizontal vessel after the shaking amplitude is suddenly decreased. Then the magnetized beads form a transient network that coarsens in time into compact clusters, following a viscoelastic phase separation [1]. A homogeneous magnetic field oriented parallel to the system plane has been observed to "unknot" network structures orthogonal to the field [2]. Here we focus on the impact of a homogeneous magnetic field oriented in vertical direction. For certain field amplitudes we observe a three-phase state, namely mobile glass beads, a grid of isolated steel beads and the coarsening network. Our results demonstrate that via dipole-dipole repulsion the field reduces the mobility of isolated steel beads, thus hindering the growth of the networks. The experimental results are compared with those of numerical simulations.

[1] A. Kögel, et al. *Soft Matter*, 14 (2018) 1001.

[2] P. A. Sánchez, J. Miller, S. S. Kantorovich, R. Richter, *J. Magn. Magn. Mater*, 499 (2019) 166182.

DY 11.2 Mon 15:45 H19

Dynamic light scattering from single macroscopic particles — •Philip Born and Lisa Dossow — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

Here we present a methodology to extract information from the light intensity fluctuations that arise from motion of single granular particles. We first describe the experimental setup for dynamic light scattering measurements and the associated theoretical framework required to isolate contributions from the translational motion and from the rotational motion to the intensity autocorrelation function [1]. We subsequently present an approach to extract the angular velocity and the translational speed of the granular particles from the intensity autocorrelation. The approach is applied to a small ensemble of granular particles in an hour-glass-like experiment to determine the granular temperature with a dynamic light scattering measurement. The results indicate the next steps to be taken to eventually develop a thermometer for fluidized granular media based on dynamic light scattering.

[1] L. Dossow, R. Kessler, M. Sperl & P. Born, Dynamic light scatter-

ing from single macroscopic particles. Applied Optics, 60(32), 10160-10167 (2021).

DY 11.3 Mon 16:00 H19

Structural Analysis of Disordered Dimer Packings — •Esma Kurban and Adrian Baule — School of Mathematical Sciences, Queen Mary University of London, Mile End Road, London E1 4NS, UK

Jammed disordered packings of non-spherical particles show significant variation in the packing density as a function of particle shape for a given packing protocol. Rotationally symmetric elongated shapes such as ellipsoids, spherocylinders, and dimers, e.g., pack significantly denser than spheres over a narrow range of aspect ratios, exhibiting a characteristic peak at aspect ratios of $\alpha_{\max} \approx 1.4 - 1.5$. However, the structural features that underlie this non-monotonic behaviour in the packing density are unknown. Here, we study disordered packings of frictionless dimers in three dimensions generated by a gravitational pouring protocol in LAMMPS. Focusing on the characteristics of contacts as well as orientational and translational order metrics, we identify a number of structural features that accompany the formation of maximally dense packings as the dimer aspect ratio α is varied from the spherical limit. Our results highlight that dimer packings undergo significant structural changes as α increases up to $\alpha_{\max}$ manifest in the reorganisation of the contact configurations between neighbouring dimers, increasing nematic order, and decreasing local translational order. Remarkably, for $\alpha > \alpha_{\max}$ our metrics remain largely unchanged, indicating that the peak in the packing density is related to the interplay of structural rearrangements for $\alpha < \alpha_{\max}$ and subsequent excluded volume effects with unchanged structure for $\alpha > \alpha_{\max}$.

15 min. break

DY 11.4 Mon 16:30 H19

The role of the particle aspect ratio in the discharge of a narrow silo — •Bo Fan[2,4], Tivadar Pongó[1,2], Dariel Hernández-Delfin[1,5], János Török[3], Ralf Stannarius[6], Raúl Cruz-Hidalgo[1], and Tamás Börzsönyi[2] — [1]Universidad de Navarra, Pamplona, Spain — [2]Wigner Research Centre for Physics, Budapest, Hungary — [3]Budapest University of Technology and Economics, Budapest, Hungary — [4]Wageningen University, Wageningen, The Netherlands — [5]Basque Center for Applied Mathematics, Bilbao, Spain — [6]Otto von Guericke University, Magdeburg, Germany

The time evolution of silo discharge is investigated for different granular materials made of spherical or elongated grains in laboratory experiments and with discrete element model (DEM) calculations. For spherical grains, we confirm the widely known typical behavior with constant discharge rate (except for initial and final transients). For elongated particles with aspect ratios between $2 < L/d < 6.1$, we find a peculiar flow rate increase for larger orifices, especially in the last third of the discharge process. While the flow field is practically homogeneous for spherical grains, it has strong gradients for elongated particles with a fast-flowing region in the middle of the silo surrounded by a stagnant zone. For large enough orifice sizes, the flow rate increase is connected to a gradual change in the character of the flow field, including a shrinkage of the stagnant zone and an increase in both the packing fraction and flow velocity near the silo outlet.

DY 11.5 Mon 16:45 H19

Excitation of Platonic bodies on a vibrating plate analyzed with smart IMUs — •Torsten Trittel, Dmitry Puzyrev, Niklas Dieckmann, and Ralf Stannarius — Otto-von-Guericke Universität Magdeburg

For the investigation of granular gases, i.e. large ensembles of macroscopic particles that interact via frequent mutual collisions, an initial or permanent excitation of the ensembles is prerequisite. Typically, this excitation is realized by one or more vibrating plates (container walls). We investigate such a mechanical excitation of different Platonic bodies, e.g. icosahedra and cubes, and compare their dynamics with that of spherical particles. In earlier experiments with mechanically excited rods [1], the dynamic data were extracted from a huge amount of stereoscopic video data. This procedure is very complicated and time consuming. To overcome this problem, we equipped our particles with small IMUs (inertial measurement units) that are typically used for motion tracking [2]. From acceleration and rotation data, it is straightforward to calculate the rotational and translational energies of each jump. We present distributions of the energies on individual degrees of freedom and determine the efficiency of the excitation depending on vibration parameters. Finally, we compare the experimental findings with results obtained from numerical simulations.

[1] T. Trittel et al., Mechanical excitation of rodlike particles by a vibrating plate, Phys. Rev. E 95, 062904, (2017)

[2] M. Zenker, Dynamik platonischer Körper bei mechanischer Anregung, BA, Magdeburg (2021)

DY 11.6 Mon 17:00 H19

Rare Fluctuations in Sheared 2D LJ Fluids — •Daniel Dernbach and Jürgen Vollmer — Institut für Theoretische Physik, Universität Leipzig, Brüderstr. 16, D-04103 Leipzig, Germany

A distinguishing feature of sheared particulate flows are very large fluctuations in the dissipation, i.e. the product of the local velocity gradient and the local shear stress. At times, it even takes negative values (rare fluctuations). Surprisingly, the probability of rare fluctuations vanishes close to jamming [1], a far-from-equilibrium critical point where fluctuations are expected to be large.

Here, we compare this setting to the motion of classical fluids with attractive, elastic interactions. Specifically, we consider the transition from fluid to plastic flow in a two-dimensional (2D) Lennard-Jones (LJ) fluid subjected to a Nosé-Hoover thermostat.

Close to its critical rigidity transition this time-reversible sheared dynamics also features a drop of the probability of rare fluctuations. We will scrutinize the analogies and differences between the emergence of rare fluctuations in irreversible particulate flow and in time-reversible classical dynamics.

[1] Rahbari, Saberi, Park, Vollmer, Nat. Commun. 8, 11 (2017)

DY 11.7 Mon 17:15 H19

Granular Gases of Mixtures of Rods in Microgravity — •Kirsten Harth[1,2], Dmitry Puzyrev[3], Torsten Trittel[3], and Ralf Stannarius[3] — [1]Fachbereich Technik, TH Brandenburg, Brandenburg an der Havel, Deutschland — [2]MARS und MRTM, Otto von Guericke Universität Magdeburg, Deutschland — [3]Institut für Physik und MARS, Otto von Guericke Universität Magdeburg, Deutschland

Granular gases consist of macroscopic particles in erratic motion, rarely colliding among each other. They are a comparatively simple, yet illustrative example of a non-equilibrium dynamical system. Numerous theoretical and numerical studies deal with their dynamics, however, the realization of 3D experiments is rare. It usually requires microgravity. Typical experiments are either performed under continuous external energy supply or they consider the process of collective kinetic energy decay by dissipation (granular cooling). It has been recently shown that both ensembles of rods and spheres follow the scaling predicted by Haff in 1983, however, with stark quantitative disagreement with the theory.

Here, we consider a bidisperse ensemble of 2 types of rods in a cuboid container. We track their positions and rotations in 3D. Expererimental data will be compared to validated numerical simulations of frictional rods under similar conditions. We extract kinectic energies in individual degrees of freedom and other statistical quantities.

DY 11.8 Mon 17:30 H19

Pauling Structures in tribocharged Granular Media — Jan Haeberle, Matthias Sperl, and •Philip Born — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

Crystal-like arrangements of granular particles had been studied in the past for their mechanical properties or as a model system to study structure formation of non-equilibrium systems. These studies were limited to the formation of either hcp or fcc densest arrangements of monodisperse spheres. However, in most situations the hard core and the frictional contacts of the granular particles stabilize less dense disordered packings. Here we show that binary packings of granular particles with strong tribocharging spontaneouisly take BCC-like packing structures under suitable conditions [1]. We use a version of the bond-order parameter which is robust against noise to identify crystalline structures x-ray tomography reconstructions [2]. The observed BCC-like packing structures formed in incommensurate containers are, to large extent, in agreement with the prediction of Pauling's rules for ionic crystals, i.e. equilibrium structures of thermal ions.

[1] J. Haeberle, J. Harju, M. Sperl and P. Born, "Granular ionic crystals in a small nutshell", Soft Matter 15, 7179-7186 (2019).

[2] J. Haeberle, M. Sperl and P. Born, "Distinguishing noisy crystalline structures using bond orientational order parameters", EPJ E

42, 1-7 (2019).

DY 11.9 Mon 17:45 H19

Visualization of flow dynamics for Poly-dispersed dense granular suspension in various sections of pipe — •Himanshu P Patel and Günter K Auernhammer — Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Straße 6, D-01069 Dresden, Germany

The study of flow dynamics in non-Newtonian media with polydispersed dense granular suspension, e.g., slurry, mud, concrete, still lacks quantification on the flow parameters linked to shear induced particle migration and insight about flow at center and at wall in closed pipes.

We developed transparent granular system that is a granular suspension of particles suspended in non-Newtonian media (particle volume fractions of 30% to 48%) [1]. The non-Newtonian granular system has yield stress and plastic viscosity and is well index matched. The rheological characteristics of the model system is tunable through its composition of additives.

We analyze gravity-assisted continuous flow of millimetric sized particles. We perform tracking of flow at different sections of pipe. The flow analysis revels understanding on the relaxation of such flow and the development of velocity profile within the length of pipe, we observe this using camera at entry and exit of pipe and later a 3D setup to observe flow at near end of pipe. This gives quantitative values into the particle migration to understand the effect of polydispersity and particle flow.

[1] Auernhammer, Günter K., et al., Materials & Design (2020):108673

DY 12: Focus Session: Nonlinear Dynamics of Nanomechanic Oscillators

Time: Monday 15:30–17:45 Location: H20

Invited Talk DY 12.1 Mon 15:30 H20

A phononic frequency comb from a single resonantly driven nanomechanical mode — •Eva Weig — Department of Electrical and Computer Engineering, Technical University of Munich

Doubly-clamped nanostring resonators excel as high Q nanomechanical systems enabling room temperature quality factors of several 100,000 in the 10 MHz eigenfrequency range. Dielectric transduction via electrically induced gradient fields provides an integrated control scheme while retaining the large mechanical quality factor. Dielectrically controlled nanostrings are an ideal testbed to explore a variety of dynamical phenomena ranging from multimode coupling to coherent control. Here I will focus on the nonlinear dynamics of a single, resonantly driven mode. The broken time reversal symmetry gives rise to the squeezing of the string's fluctuations. As a result of the high mechanical Q factor, the squeezing ratio is directly accessible from a spectral measurement. It is encoded in the intensities of the two spectral peaks arising from the slow dynamics of the system in the rotating frame. For stronger driving, an onset of self-sustained oscillation is observed which leads to the generation of a nanomechanical frequency comb. The effect is a consequence of a resonantly induced negative effective friction force induced by the drive. This is the first observation of a frequency comb arising solely from a single mode and a single, resonant drive tone.

DY 12.2 Mon 16:00 H20

Fluctuations and strong nonlinear effects in nanomechanical resonators — •Fan Yang[1], Mengqi Fu[1], Yuxuan Jiang[2], and Elke Scheer[1] — [1]University of Konstanz, Konstanz, Germany — [2]Anhui University, Hefei, China

Membrane resonators are ideal model systems to investigate nonlinear dynamics. Membrane resonators operated in the nonlinear regime, far beyond the Duffing regime exhibit unusual dynamic behavior, including localized overtones of spatial modulation [1], parametric flexural mode coupling, and persistent response [2]. Our research focusing on revealing the microscopic origins, their characterization, local control, exploring the universality and fluctuations [3] of the nonlinear state.

[1] Yang, Fan, et al. "Spatial modulation of nonlinear flexural vibrations of membrane resonators." Physical review letters 122.15 (2019): 154301.

[2]Yang, Fan, et al. "Persistent Response in an Ultrastrongly Driven Mechanical Membrane Resonator." Physical Review Letters 127.1 (2021): 014304.

[3]Yang, Fan, et al. "Mechanically Modulated Sideband and Squeezing Effects of Membrane Resonators" Physical Review Letters 127 (18), 184301.

DY 12.3 Mon 16:15 H20

Tuning nonlinear damping in graphene nanoresonators by parametric-direct internal resonance — •Ata Keşkekler[1], Oriel Shohani[2], Martin Lee[1], Herre van der Zant[1], Peter Steeneken[1], and Farbod Alijani[1] — [1]TU Delft, Delft, The Netherlands — [2]Ben-Gurion University of Negev, Beersheba, Israel

Micro/Nano-mechanical systems are utilized in many technologies and often have been used for their sensing capabilities. An ideal framework for sensitive nanomechanical devices is 2-D materials, and especially graphene, due to its exceptional mechanical, electrical and thermal properties. By their atomically thin nature, these systems are fundamentally nonlinear. In addition to their geometric nonlinearities, graphene membranes have shown nonlinear energy decay mechanisms. Nonlinear damping in these devices is a fundamental limitation to their sensing capabilities yet its full understanding is an open question. Among different dissipation mechanisms, an important factor that is hypothesized to affect damping properties of graphene nanodrums is the intermodal couplings. In this work, we study the nonlinear dynamics of a nanomechanical graphene resonator near its internal resonance condition to amplify the intermodal effects and uncover the physics between nonlinear damping and mode coupling. We observe a massive increase in damping in the vicinity of internal resonance that is followed by a bifurcation causing a dramatic increase of amplitude and resonance frequency. Our study opens up a route towards utilizing modal interactions and parametric resonance to realize resonators with engineered nonlinear dissipation over wide frequency range.

Invited Talk DY 12.4 Mon 16:30 H20

From period-doubling bifurcations to time crystals and coherent Ising machines — •Oded Zilberberg[1,2], Toni L. Heugel[2], Jan Košata[2], Javier del Pino[2], R. Chitra[2], and Alexander Eichler[2] — [1]Department of Physics, University of Konstanz, 78464 Konstanz, Germany — [2]Department of Physics, ETH Zürich, CH-8093 Zürich, Switzerland

Networks of coupled parametric resonators (parametrons) hold promise for parallel computing architectures. These are classical systems with period-doubling bifurcations, where the logic information is stored in oscillation modes of the system. Such networks similarly realize the physics of so-called discrete time crystals (DTCs). The latter are a many-body state of matter whose dynamics are slower than the forces acting on it. I will report on our theoretical and experimental work on parametron networks, their relation to DTCs and their potential application for the realization of coherent Ising machines.

DY 12.5 Mon 17:00 H20

Sideband and noise squeezing effects in nonlinear mechanical membrane resonators — •Mengqi Fu[1], Fan Yang[1], Yuxuan Jiang[2], and Elke Scheer[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Anhui University, Hefei, China

The nonlinearity of a mechanical system has been shown to squeeze the noise by redistributing it in two conjugates of the observables under certain conditions and therefore provides a way to break the sensing limit of mechanical systems. In this work, we develop a novel method to characterize the noise squeezing of a nonlinear mechanical system by the frequency response of the low-frequency modulation based on a suspended silicon nitride (Si-N) membrane ($\sim$ 500 nm thickness) structure [1]. We first demonstrate an antiresonance effect between the "quasi modes" of the nonlinear mechanical system in the sideband spectra through low-frequency two-tone probing measurements. Then a direct connection between the antiresonance frequency and the noise squeezing factor of the system can be established to characterize the noise squeezing factor in a simple and robust method.

[1] F. Yang et at., Phys. Rev. Lett., 127, 184301 (2021).

Invited Talk DY 12.6 Mon 17:15 H20

2D membranes in motion — •Herre van der Zant — Kavli Institute of Nanoscience, Department of Quantum Nanoscience, Delft University of Technology, The Netherlands

Atomically thin membranes are ideal building blocks for nanoelectromechanical systems (NEMS) because of their unique mechanical properties and their low mass. We make membranes by transferring atomically thin layers on top of silicon oxide substrates that are prepatterned with circular or rectangular holes. The suspended membranes are characterized by a laser interferometer set-up that gives access to information on the dynamics in the frequency- and time-domain. The setup is equipped with a moveable x-y stage so that the membrane motion can be visualized; the nonlinear response of the motion is used to extract the mechanical parameters including the Young's modulus. Recently, it has become clear that nanomechanics can also probe thermodynamic properties such as thermal conductivity, specific heat, and thermal expansion [Dynamics of 2D material membranes, 2D Materials 8 (2021) 042001]. Specifically, phase transitions are typically accompanied by abrupt changes in the specific heat, resulting in accompanying changes in the strain of the material which are measured via mechanical resonances. In this way, we have detected the Néel temperature of antiferromagnetic $FePS_3$ membranes, their magnetic anisotropy and studied the nonlinear coupling between magnetic and elastic properties.

DY 13: Big Data and Artificial Intelligence (joint session SOE/DY)

Time: Monday 17:45–18:15 Location: H18

DY 13.1 Mon 17:45 H18

Revealing interactions between HVDC cross-area flows and frequency stability with explainable AI — •Sebastian Pütz[1,2], Benjamin Schäfer[3], Dirk Witthaut[1,2], and Johannes Kruse[1,2] — [1]Forschungszentrum Jülich, Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE), 52428 Jülich, Germany — [2]Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany — [3]Karlsruhe Institute of Technology, Institute for Automation and Applied Informatics (IAI), 76344 Eggenstein-Leopoldshafen, Germany

The energy transition introduces more volatile energy sources into the power grids. In this context, power transfer between different synchronous areas through High Voltage Direct Current (HVDC) links becomes increasingly important. Such links can balance volatile generation by enabling long-distance transport or by leveraging their fast control behavior. Here, we investigate the interaction of power imbalances - represented through the power grid frequency - and power flows on HVDC links between synchronous areas in Europe. We use explainable machine learning to identify key dependencies and disentangle the interaction of critical features. Our results show that market-based HVDC flows introduce deterministic frequency deviations, which however can be mitigated through strict ramping limits. Moreover, varying HVDC operation modes strongly affect the interaction with the grid. In particular, we show that load-frequency control via HVDC links can both have control-like or disturbance-like impacts on frequency stability.

DY 13.2 Mon 18:00 H18

From sample management to workflow integration: Semantic research data management in glaciology. — •Florian Spreckelsen[1], Daniel Hornung[1], and Johannes Freitag[2] — [1]IndiScale Gmbh, Göttingen — [2]Alfred Wegener Institute, Helmholtz Centre for Polar and Marine Research, Bremerhaven

Organizing data from a diversity of sources, from acquisition to publication, can be a tough challenge. We present implementations with the flexible open-source research data management toolkit CaosDB in the glaciology department at the Alfred Wegener Institute (AWI) in Bremerhaven. CaosDB is used in a diversity of fields such as turbulence physics, legal research, animal behavior and glaciology. CaosDB links research data, makes it findable and retrievable, and keeps data consistent, even if the data model changes.

At AWI, CaosDB keeps track of ice core samples and to whom samples are loaned for analyses. It made possible additional features such as: A revision system to track all changes to the data and the sample state at the time of analysis. Automated gathering of information for the publication in FAIR-DO meta-data repositories, e.g. Pangaea. Tools for storing, displaying and querying geospatial information and graphical summaries of all analyses performed on each ice core. Automatic data extraction and refinement into data records in CaosDB to minimize manual users interaction. A state machine which guarantees certain workflows, simplifies development and can be extended to trigger additional actions upon transitions.

We demonstrate how CaosDB simplifies semantic data in science.

DY 14: Invited Talk Sabine Klapp

Time: Tuesday 9:30–10:00 Location: H18

Invited Talk DY 14.1 Tue 9:30 H18

Non-Markovian Brownian systems: from single-particle thermodynamics to collective behavior — •Sabine Klapp — Institut fuer Theoretische Physik, TU Berlin, Hardenbergstrasse 36, 10623 Berlin

Recently, the dynamical behavior and the thermodynamics of stochastic systems involving time-delay or, more generally, memory effects has become a focus of growing interest. Indeed, memory is essentially omnipresent in many complex fluids and biological systems, but may also arise, e.g., due to delayed feedback protocols or sensorial delay in active systems. The theoretical description of such systems is still challenging due to the non-Markovian nature of the underlying Langevin equations, particularly in the case of discrete time delays. Here we present, first, recent research for Brownian particles subject to feedback with discrete or distributed time delay. We discuss peculiar thermodynamic features, such as delay-induced heat production, and the theoretical treatment based on the introduction of auxiliary variables with non-reciprocal coupling. Considering an ensemble of delayed Brownian particles we demonstrate the occurrence of new phases resembling active particles. Our second focus lies on systems with fractional Brownian motion (fBm). fBM is a well-established model for anomalous diffusion, where non-Markovianity arises through the noise correlation function. We discuss strategies how to treat this system thermodynamically and the role of memory for the collective behavior.

DY 15: Delay and Feedback Dynamics

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

DY 15.1 Tue 9:30 H19

Emergence of collective motion in two-dimensional colloidal systems with delayed feedback — •Robin A. Kopp and Sabine H. L. Klapp — ITP, TU Berlin, Berlin, Germany

In recent years, delayed feedback in colloidal systems has become an active and promising field of study [1], key topics being history dependence and the manipulation of transport properties. Here we study the dynamics of a two-dimensional colloidal suspension, subject to time-delayed feedback. To this end we perform overdamped Brownian dynamics simulations, where the particles interact through a Weeks-Chandler-Andersen potential. Furthermore, each particle is subject to a Gaussian, repulsive feedback potential, that depends on the difference of the particle position at the current time, and at an earlier time. We observe and quantitatively study the emergence of collective motion characterized by a nonzero mean velocity and provide a possible explanation combining single-particle and mean-field-like effects. Studying the corresponding one-particle system we obtain an understanding of the history dependence and the long-time behavior, in particular a nonzero stationary constant velocity state of the deterministic problem that translates to a constant average velocity magnitude in the stochastic system. By studying the mean square displacement we are able to point out how delayed feedback affects diffusion in the one-particle and the interacting system differently.

[1] S. A. M. Loos, S. Hermann, and S. H. L. Klapp, Entropy **23**, 696 (2021)

DY 15.2 Tue 9:45 H19

The role of the polarization dephasing time for stabilizing coupled nanolasers — •Aycke Roos[1], Stefan Meinecke[1], and Kathy Lüdge[2] — [1]Technische Universität Berlin - Institut für Theoretische Physik, Hardenbergstraße 36, 10623 Berlin — [2]Technische Universität Ilmenau - Institut für Physik, Fachgebiet Theoretische Physik 2, 98684 Ilmenau

As a prototypical model for on-chip laser networks, mutually coupled nanolasers attract attention in laser physics and dynamics. In the regime of small cavity lifetimes the carrier polarization essentially influences the dynamics of such lasers. We investigate the emission dynamics of two coupled lasers, modeled by Maxwell-Bloch type laser equations (class-C laser), and predict ways to optimize their stability, i.e., maximize their locking range. We find that tuning the cavity lifetime to the same order of magnitude as the dephasing time of the microscopic polarization yields optimal operation conditions, which allow for wider tuning ranges than usually observed in conventional semiconductor lasers. We present the steady state solutions and numerically characterize the emission dynamics via the underlying bifurcation structure. The dephasing time is found to be a crucial parameter, which impacts the observed dynamics in the parameter space spanned by frequency detuning, coupling strength and coupling phase.

DY 15.3 Tue 10:00 H19

Frequency combs and localized states in time-delayed Kerr-Gires-Tournois interferometers — •Thomas G. Seidel[1,2], Julien Javaloyes[2], and Svetlana V. Gurevich[1,2] — [1]Institute for Theoretical Physics & Center for Nonlinear Science (CeNoS), University of Münster, Schlossplatz 2, 48149 Münster, Germany — [2]Dpt. de Física, Universitat de les Illes Balears & IAC-3, Campus UIB, E-07122 Palma de Mallorca, Spain

We study theoretically the formation of phase-locked temporal localized states (TLSs) and frequency combs. Our system consists in an optically injected Fabry-Perot micro-cavity containing a Kerr medium that is coupled to an external cavity. Using a first-principles model based on delay algebraic equations (DAEs) and applying a combination of direct numerical simulations and path continuation methods, we disclose sets of multistable dark and bright TLSs coexisting on their respective bistable homogeneous backgrounds. We show that the detuning of the injection with respect to the micro-cavity resonance controls the region of existence of TLSs and its change can lead to a period-doubling route to chaos. Understanding the influence of the system parameters on physical mechanisms such as group delay dispersion and third order dispersion do not appear so obvious in the DAE model. Therefore, we transform the DAE into a real order parameter equation by using a rigorous multiple time scale analysis applied at the onset of bistability. The normal form given by a real Ginzburg-Landau equation and the full DAE model exhibit excellent quantitative agreement in both one- and two-parameter bifurcation diagrams.

DY 15.4 Tue 10:15 H19

Dynamics of square waves in a vertical external-cavity delayed Kerr-Gires-Tournois interferometer — •Elias R. Koch[1], Thomas G. Seidel[1,2], Julien Javaloyes[2], and Svetlana V. Gurevich[1,2] — [1]Institute for Theoretical Physics & Center for Nonlinear Science (CeNoS), University of Münster, Schlossplatz 2, 48149 Münster, Germany — [2]Dpt. de Física, Universitat de les Illes Balears & IAC-3, Campus UIB, E-07122 Palma de Mallorca, Spain

We study theoretically the mechanisms of square wave (SW) formation in a monomode micro-cavity, containing a nonlinear Kerr medium coupled to a long external feedback cavity under continuous wave injection. Employing a first-principle delay-algebraic equation (DAE) model in the long delay limit, we provide a simple analytical approximation of the SW's plateau intensities and the bifurcation points limiting the range of existence of the SWs. Using a combination of path-continuation techniques and direct numerical simulations, we show that depending on the system parameters SWs can exhibit homoclinic snaking leading to the formation of complex-shaped multistable SW solutions. Beyond that, more complex SW dynamics can be identified, including a period doubling route to chaos. The results obtained from the full DAE model and the simple analytical approximation are in excellent agreement. Furthermore, we demonstrate that SWs can be used as a platform to host other structures and we show that robust multiple bound states consisting of localized pulses can be formed on the SW plateaus.

DY 16: Active Matter 2 (joint session DY/BP/CPP)

Time: Tuesday 10:00–13:00 Location: H18

DY 16.1 Tue 10:00 H18

Density fluctuations in bacterial binary mixtures — •Silvia Espada Burriel, Victor Sourjik, and Remy Colin — Max Planck Institute for Terrestrial Microbiology, Karl-von-Frisch-strasse 10, 35043 Marburg & Center for Synthetic Microbiology (SYNMIKRO), Karl-von-Frisch-strasse 14, 35043 Marburg

In wild environments, bacteria are found as mixtures of motile and sessile species, which interact physically and chemically to give rise to complex community organization. Very little is understood of the role of physical interactions in these processes: Numerical works on dry active matter and experiments on colloidal systems have shown that the activity of the active particles may affect the spatial distribution of passive particles with which they are mixed. However, the physical behavior of binary mixtures of bacteria remains largely unexplored. In our study, we present a novel phenomenon in which non-motile bacteria form large density fluctuations when mixed with motile bacteria, distinct from the aforementioned behaviors. We systematically explored the phase diagram of the mixtures in experiments combining microfluidics, fluorescence (confocal) microscopy, quantitative image analysis and parameter tuning by genetic engineering. Our experimental results show that the emergence of these large density fluctuations of the non-motile cells in presence of motile cells is controlled by hydrodynamic interactions between the motile and non-motile cells and by the sedimentation of the non-motile cells, possibly because it breaks the systems symmetry.

DY 16.2 Tue 10:15 H18

Pulsating Active Matter — •Yiwei Zhang and Etienne Fodor

— 0 Av. de la Faiencerie, 1511 Luxembourg

Active matter features the injection of energy at individual level keeping the system out of equilibrium, which leads to novel phenomenologies without any equilibrium equivalents. So far, most active matter models assign a velocity to each particle, whilst we herein consider a system of pulsating soft particles where the activity sustains particles' periodic deformation instead of spatial displacement. At sufficiently high density, we reveal the existence of wave propagation independent of any particle migration, and derive the corresponding phase diagram. We study the character of phase transitions, and investigate the underlying physical mechanisms, using both particle-based simulations and hydrodynamic analysis.

DY 16.3 Tue 10:30 H18

Long-Range Nematic Order in Two-Dimensional Active Matter — •Benoît Mahault[1] and Hugues Chaté[2,3] — [1]MPIDS, 37077 Göttingen, Germany — [2]SPEC, CEA-Saclay, 91191 Gif-sur-Yvette, France — [3]CSRC, Beijing 100193, China

Studies of active matter continue to flourish, exploring more and more complex situations in an increasingly quantitative manner. Evidence has accumulated that shows active matter exhibits properties that are impossible in thermal equilibrium or even in driven systems. In spite of all this progress, important fundamental questions remain open. Such a long-standing issue is whether true long-range nematic order can emerge in two space dimensions. In this talk, we will present theoretical and numerical results obtained from minimal models of self-propelled polar particles aligning nematically. Our study shows that the orientational order emerging from such systems is quasi-long-ranged beyond the scale associated to induced velocity reversals, which is typically extremely large and often cannot even be measured. On scales where particle motion is ballistic, nematic order appears truly long-range. A hydrodynamic theory for this de facto phase is derived, and we show that its structure and symmetries differ from conventional descriptions of both polar flocks and active nematics. Our analysis of this field theory predicts π-symmetric propagative sound modes and the scaling form of space-time fluctuations. Finally, numerical results confirm the theory and allow us to estimate all scaling exponents.

DY 16.4 Tue 10:45 H18

Collective behavior of repulsive chiral active particles with non-reciprocal couplings — •Kim L. Kreienkamp and Sabine H. L. Klapp — Technische Universität Berlin, Germany

Mixtures of chiral active particles [1] as well as non-reciprocal systems [2] show intriguing collective behavior like pattern formation and traveling waves. The combination of both – non-reciprocal couplings in mixtures of chiral active particles – promises a rich variety of collective dynamics.

Here, we investigate how non-reciprocal couplings and naturally occurring repulsive interactions due to finite particle sizes affect the collective behavior in a mixture of two species of particles. We analyze the effects due to non-reciprocity and finite size individually as well as their interplay based on a field description of the system in terms of the particle concentration and director field, measuring the overall orientation of particles at a certain position.

We derive the field equations under the mean-field assumption by coarse-graining microscopic Langevin equations for individual chiral particles, which are modeled as self-propelling circle swimmers with soft repulsive forces, comprising the finite size effects. Particles of the two species rotate with different intrinsic frequencies and align with near-by particles. Focusing on non-reciprocity, we use a non-mutual alignment between the particles.

[1] D. Levis and B. Liebchen, Phys. Rev. E 100, 012406 (2019)

[2] M. Fruchart, R. Hanai, P. B. Littlewood, and V. Vitelli, Nature 592, 363-369 (2021)

DY 16.5 Tue 11:00 H18

Memory-induced chirality in self-freezing active droplets — •Aritra K. Mukhopadhyay[1], Kai Feng[2], José Carlos Ureña Marcos[1], Ran Niu[2], Qiang Zhao[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany. — [2]Huazhong University of Science and Technology, 430074 Wuhan, China.

We experimentally realize and numerically model a new type of self-propelled droplet swimmer which exhibits chiral motion due to self-induced memory effects without requiring any explicit symmetry breaking caused by specific droplet geometries or complex environments. The droplets are composed of a binary polymer mixture that solidifies over time, simultaneously emitting certain polymers into their environment. A spontaneous asymmetry of the emitted polymer concentration along the stationary droplet surface induces Marangoni flows which cause the droplet to initially self-propel ballistically. However, the emitted polymers diffuse slowly and form long-lived trails with which the droplet can self-interact in the course of time and this leads to a dynamical transition from ballistic to chiral motion. The droplets persistently exhibit chiral motion with the same handedness until at even later times a second transition occurs when the droplets confine themselves leading to self-trapping over the timescale of our experiments and simulations. Our results exemplify a new route to realizing synthetic active particles whose dynamics can be controlled via the pronounced self-induced memory effects.

15 min. break

DY 16.6 Tue 11:30 H18

Role of advective inertia in active nematic turbulence — •Colin-Marius Koch and Michael Wilczek — Theoretical Physics I, University of Bayreuth, Bayreuth

Suspensions of active agents with nematic interactions can exhibit complex dynamics such as mesoscale turbulence. Continuum descriptions for such systems are inspired by the hydrodynamic theory of liquid crystals and feature an advective nonlinearity which represents inertial effects. The typically low Reynolds number of such active flows raises the question whether and under which conditions the active stresses present in these systems can excite inertial flows. To address this question, we investigate mesoscale turbulence in a two-dimensional model for active nematic liquid crystals. In particular, we compare numerical simulations with and without nonlinear advection and frictional damping of the flow field. Studying the nondimensionalized equations of motion, we find that inertia can trigger large-scale motion even for small microscopic Reynolds numbers if the active forcing is sufficiently large and the Ericksen number is sufficiently low. Performing a spectral analysis of the energy budget, we identify an inverse energy transfer caused by inertial advection, whose impact is small in comparison to active forcing and viscous dissipation but accumulates over time. We additionally show that surface friction, mimicked by a linear friction term, dissipates the transported energy and suppresses the large-scale motion. We conclude that, without an a priori knowledge of model parameters matching experiments, including inertia and friction may be necessary for consistent modeling of active nematic turbulence.

DY 16.7 Tue 11:45 H18

Pumping in active microchannels — •Goncalo Antunes[1,2,3], Paolo Malgaretti[1,2,3], Siegfried Dietrich[2,3], and Jens Harting[1,4] — [1]Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien (IEK–11), Forschungszentrum Jülich, Erlangen, Germany — [2]Max–Planck–Institut für Intelligente Systeme, Stuttgart, Germany — [3]Universität Stuttgart, Stuttgart, Germany — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany

Much attention is currently being given to the problem of manipulating fluids at the microscale, with successful applications to fields such as 3D fabrication and biomedical research. Often micropumps are a fundamental component of these microfluidic systems. An intriguing technique to manipulate fluid flows in a channel is diffusioosmosis. Fluid flow is obtained upon imposing an inhomogeneous concentration of some solute, which generates flow in a boundary layer around the channel walls. This inhomogeneity is the result of a spatially inhomogenous production rate of solute inside the channel.

We show that a solute-producing, corrugated, active channel can act as a micropump even when it is fore-aft symmetric. This result is obtained by coupling the Stokes equation with an advection-diffusion equation for the solute concentration, which we solve analytically in the limit of thin, weakly-corrugated channels. Lattice Boltzmann simulations further support the existence of the symmetry-breaking. Our calculations are also valid for left-right asymmetric channels, and provide a tool to optimize the pumping rate of an active microchannel by tuning its shape or its solute production rate.

DY 16.8 Tue 12:00 H18

Active Refrigerators Powered by Inertia — •Lukas Hecht[1], Suvendu Mandal[1], Hartmut Löwen[2], and Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, D-64289 Darmstadt, Germany — [2]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-

Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

We present the operational principle for a refrigerator which uses inertial effects in active Brownian particles (ABPs) to locally reduce the (kinetic) temperature by two orders of magnitude below the environmental temperature. This principle requires two ingredients: First, we need the feature of inertial ABPs to undergo motility-induced phase separation into coexisting phases with different (kinetic) temperatures and second, a mechanism which localizes the dense phase in the targeted cooling domain is required.

Here, we exploit the peculiar but so-far unknown shape of the phase diagram of inertial ABPs to initiate motility-induced phase separation in the targeted cooling domain only. Remarkably, active refrigerators operate without requiring isolating walls separating the cooling domain from its environment. This feature opens the route towards using active refrigerators to systematically absorb and trap substances such as toxins or viruses from the environment.

DY 16.9 Tue 12:15 H18

The influence of motility on bacterial accumulation in a microporous channel — •Christoph Lohrmann[1], Miru Lee[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institute for Theoretical Physics, Georg-August-Universität Göttingen, 37073 Göttingen, Germany

Swimming microorganisms are often encountered in confined geometries where also an external flow is present, e.g. in filters or inside the human body. To investigate the interplay between microswimmer motility and external flows, we developed a model for swimming bacteria based on point coupling to an underlying lattice Boltzmann fluid. Random reorientation events reproduce the statistics of the run-and-tumble motion of the bacterium E. coli. We present the application of the model to the study of bacterial dynamics in a channel with a single cylindrical obstacle. In accordance with experimental measurements, simulations show asymmetric accumulation behind the obstacle only when the bacteria are active and an external flow is present.

Lee, Miru *et al.*, *Soft Matter* **17**, 893-902 (2021)

DY 16.10 Tue 12:30 H18

Inertial dynamics of an active Brownian particle* — •Jonas Mayer Martins and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Active Brownian motion commonly assumes spherical overdamped particles. However, self-propelled particles are often neither symmetric nor overdamped yet underlie random fluctuations from their surroundings. Active Brownian motion has already been generalized to include asymmetric particles. Separately, recent findings have shown the importance of inertial effects for particles of macroscopic size or in low-friction environments. We aim to consolidate the previous findings into the general description of a self-propelled asymmetric particle with inertia. We derive the Langevin equation of such a particle as well as the corresponding Fokker-Planck equation. Furthermore, a formula is presented that allows to reconstruct the hydrodynamic resistance matrix of the particle by measuring its trajectory. Numerical solutions of the Langevin equation show that, independent of the particle's shape, the noise-free trajectory at zero temperature starts with an inertial transition phase and converges to a circular helix. We discuss this universal convergence with respect to the helical motion that many microorganisms exhibit.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – Project-ID 433682494 - SFB 1459

DY 16.11 Tue 12:45 H18

Stochastic motion under active driving due to inverted dry (solid) friction — •Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

It has become common to describe the motion of actively driven or self-propelled objects using a driving force of constant magnitude. We assume that this driving force always acts along the current velocity direction. Moreover, we consider objects featuring a nonpolar axis, along which driving and propagation occur [1].

In that case, spontaneous symmetry breaking decides on the heading of propagation, that is, "forward" or "backward" along the nonpolar axis. Stochastic effects may reverse the velocity and thus the direction of the driving force.

As it turns out, active driving under these circumstances corresponds to inverted dry (solid) friction of the Coulomb type. Corresponding tools of theoretical analysis can thus be adopted, mapping the velocity spectrum to the one of a quantum-mechanical harmonic oscillator subject to a repulsive delta potential. In this way, the diffusion coefficient can be calculated analytically. We evaluate velocity and displacement statistics. Outward propagating displacement maxima emerge under increased active driving. The trajectories feature pronounced cusps when velocity reversals occur.

Our results should apply, for instance, to certain types of vibrated nonpolar rods and swimming bacteria that may reverse their propagation direction.

[1] A. M. Menzel, submitted.

DY 17: Invited Talk Bernhard Mehlig

Time: Tuesday 10:30–11:00 Location: H19

Invited Talk DY 17.1 Tue 10:30 H19

Caustics in turbulent aerosols — •Bernhard Mehlig — University of Gothenburg

Turbulent aerosols are suspensions of heavy particles in a turbulent fluid – such as water droplets in the turbulent air of a cumulus cloud, or dust grains in the turbulent gas around a growing star. The analysis of such highly non-linear and multi-scale problems poses formidable challenges. Experiments resolving the particle dynamics have only recently become possible, and direct numerical simulations of such systems are still immensely difficult.

Here I describe a different approach, to analyse the dynamics of turbulent aerosols in terms of synthetic turbulence models, using methods from non-equilibrium statistical physics and dynamical-systems theory. Although the models are highly idealised, their analysis has led to significant progress in understanding the mechanisms determining the particle dynamics. As an example I discuss the formation of mathematical catastrophes in the phase-space dynamics of turbulent aerosols, akin to caustics in geometrical optics. I describe where and how often these singularities form, and I explain their physical significance. I conclude with a discussion of successes and limitations of this statistical approach, and with a summary of open questions.

DY 18: Nonlinear Dynamics 1: Synchronization and Chaos (joint session DY/SOE)

Time: Tuesday 11:15–12:45 Location: H19

DY 18.1 Tue 11:15 H19

Stable Poisson chimeras in networks of two subpopulations — •Seungjae Lee and Katharina Krischer — Technical University of Munich, Garching, Germany

In this talk, we introduce recent results on dynamical and spectral properties of chimeras in two-population network based on Kuramoto order parameter and Lyapunov stability analysis. In particular, we address two qualitatively different dynamics of incoherent oscillator populations according to the given initial conditions, and which led to the classification of Poisson and non-Poisson chimera states. We numerically calculate the Lyapunov exponents and covariant Lyapunov vectors to determine the spectral properties of the chimera states, and then expound the classification of the Lyapunov exponents. Our stability analysis also confirms that the chimera states of Kuramoto-Sakaguchi phase oscillators in two-population networks are neutrally stable in many directions. Furthermore, we demonstrate that two *perturbations* of the phase model that reflect more realistic situations render Poisson chimeras stable. These models consider a nonlocal intra-population network and Stuart-Landau planar oscillators with amplitude degrees of freedom, respectively. Both these 'perturbations' might be considered a heterogeneity of the phase model and give rise to an asymptotically attracting Poisson chimera in two-population networks.

DY 18.2 Tue 11:30 H19

On rational reactions - and other ones - of overloaded magnetic gears — •Ingo Rehberg and Stefan Hartung — Universität Bayreuth

Experiments exploring the coupling of two rotating spherical magnets reveal a cogging-free coupling for two specific angles between the input and output rotation axes. The striking difference between these two phase-locked modes of operation is the reversed sense of rotation of the driven magnet. For other angles, the cogging leads to a more complex dynamical behaviour. The experimental results can be understood by a mathematical model based on pure dipole-dipole interaction, with the addition of adequate friction terms [1].

Like all magnetic couplings, the setup contains intrinsic overload protection. The dynamic answer of the gear with cogging to an overload shows a plethora of modes of the driven magnet.

[1] Dynamics of a magnetic gear with two cogging-free operation modes, Stefan Hartung & Ingo Rehberg, Archive of Applied Mechanics 91, 1423-1435 (2021).

DY 18.3 Tue 11:45 H19

Heteroclinic units acting as pacemakers: Entrained dynamics for cognitive processes — •Bhumika Thakur and Hildegard Meyer-Ortmanns — School of Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Heteroclinic dynamics is a suitable framework for describing transient and reproducible dynamics such as cognitive processes in the brain. We demonstrate how heteroclinic units can act as pacemakers to entrain larger sets of units from a resting state to hierarchical heteroclinic motion that is able to describe fast oscillations modulated by slow oscillations, features which are observed in brain dynamics. The entrainment range depends on the type of coupling, the spatial location of the pacemaker and the individual bifurcation parameters of the pacemaker and the driven units. Noise as well as a small back-coupling to the pacemaker facilitate synchronization. Units can be synchronously entrained to different temporal patterns, depending on the selected path in the hierarchical heteroclinic network. These locally generated temporal sequences of information items can be transferred over a spatial grid by entrainment to the pacemaker dynamics. Such spatiotemporal patterns are believed to code information in brain dynamics. Depending on the number and location of pacemakers on two-dimensional grids, synchronization can be maintained in the presence of a large number of resting state units and mediated via target waves when the pacemakers are concentrated to a small area of such grids. In view of brain dynamics, our results indicate a possibly ample repertoire for coding information in temporal patterns.

DY 18.4 Tue 12:00 H19

Suppression of quasiperiodicity in circle maps with quenched disorder — •David Müller-Bender[1], Johann Luca Kastner[1], and Günter Radons[1,2] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Institute of Mechatronics, 09126 Chemnitz, Germany

We show that introducing quenched disorder into a circle map leads to the suppression of quasiperiodic behavior in the limit of large system sizes. Specifically, for most parameters the fraction of disorder realizations showing quasiperiodicity decreases with the system size and eventually vanishes in the limit of infinite size, where almost all realizations show mode-locking. Consequently, in this limit, and in strong contrast to standard circle maps, almost the whole parameter space corresponding to invertible dynamics consists of Arnold tongues.

Details can be found in the preprint D. Müller-Bender, J. L. Kastner, and G. Radons, Suppression of quasiperiodicity in circle maps with quenched disorder, arXiv:2204.09392 [nlin.cd] (2022).

DY 18.5 Tue 12:15 H19

Reservoir Computing and Nonlinear Dynamics — •Ulrich Parlitz — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Göttingen, Germany

We discuss the interrelation between reservoir computing (RC) and nonlinear dynamics (NLD). On the one hand, the performance of RC can be characterized and improved by concepts from NLD such as generalized synchronization and delay embedding. On the other hand, RC can be used to predict and control dynamical systems, including hybrid architectures that employ physically informed machine learning. Various aspects of this mutual relationship between RC and NLD are illustrated using low-dimensional and spatially extended chaotic dynamical systems.

DY 18.6 Tue 12:30 H19

Chameleon attractors in deterministic and stochastic Lorenz-63 systems — •Reik V. Donner[1,2], Tommaso Alberti[3], and Davide Faranda[4] — [1]Hochschule Magdeburg-Stendal, Magdeburg, Germany — [2]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [3]National Institute for Astrophysics, Rome, Italy — [4]LSCE, Université Paris-Saclay, Gif-sur-Yvette, France

The dynamical chaacteristics of a trajectory on a chaotic or stochastic attractor undergo marked changes when successively eliminating the low-frequency variability components and focusing on the fast fluctuations only, motivating the new concept of Chameleon attractors. Here, we study the time scale dependent instantaneous and average fractal characteristics of partial sums of dynamical modes identified by means of empirical mode decomposition for the Lorenz-63 system and two stochastic versions thereof with additive and multiplicative noise as obtained by exploiting recurrences in phase space using extreme value theory. While the average fractal dimensions converge to the expected values as more and more low-frequency modes are included, we find an excess dimension larger than 3 for higher frequency modes below the Lyapunov time scale resulting from the stochastic components.

DY 19: Many-Body Quantum Dynamics 2 (joint session DY/TT)

Time: Tuesday 11:30–13:00 Location: H20

DY 19.1 Tue 11:30 H20

Disorder-free localization transition in a two-dimensional lattice gauge theory — •Nilotpal Chakraborty[1], Markus Heyl[1,2], Petr Karpov[1], and Roderich Moessner[1] — [1]Max Planck Institute for physics of complex systems, Dresden — [2]University of Augsburg, Augsburg

While the nature of the quantum localization transition (QLT) is still debated for conventional many-body localization, here we provide the first comprehensive characterization of the QLT in two dimensions (2D) for a disorder-free case. Disorder-free localization can appear in homogeneous 2D LGTs such as the U(1) quantum link model (QLM) due to an underlying classical percolation transition fragmenting the system into disconnected real-space clusters. Building on the percolation model, we characterize the QLT in the U(1) QLM through a detailed study of the ergodicity properties of finite-size real- space clusters via level-spacing statistics and localization in configuration space. We argue for the presence of two regimes - one in which large finite-size clusters effectively behave non-ergodically, a result naturally accounted for as an interference phenomenon in configuration space and the other in which all large clusters behave ergodically. As one central result, in the latter regime we claim that the QLT is equivalent to the classical percolation transition and is hence continuous. Utilizing this equivalence we determine the universality class and critical behaviour of the QLT from a finite-size scaling analysis of the percolation problem.

DY 19.2 Tue 11:45 H20

Quantifying local memory in disordered systems across the ETH-MBL transition — •Sebastian Wenderoth and Michael Thoss — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg

Thermalization decribes the process of a system reaching thermal equilibrium with its environment. The asymptotic state solely depends on a few macroscopic parameters of the environment. Hence, the information about the initial state is lost during the process. Many-body localized systems fail to thermalize due to the absence of transport, and thus, some information about the initial state is retained in local observables at all times.

Based on the time-evolution of a subsystem, we present a concept which can be used to quantify the influence of the initial state on local observables. Using this approach, we investigate local memory in the XXZ Heisenberg spin chain with random local disorder, a paradigmatic model exhibiting a transition from thermalizing to localized dynamics. We discuss the loss of local information and identify different delocalization mechanisms.

DY 19.3 Tue 12:00 H20

Dynamically Induced Exceptional Phases in Quenched Interacting Semimetals — •Carl Lehmann[1], Jan Carl Budich[1], and Michael Schüler[2] — [1]TU Dresden, Dresden, Germany — [2]Paul Scherrer Institute, Villigen, Switzerland

We report on the dynamical formation of exceptional degeneracies in basic correlation functions of nonintegrable one- and two-dimensional systems quenched to the vicinity of a critical point. Remarkably, fine-tuned semimetallic points in the phase diagram of the considered systems are thereby promoted to topologically robust non-Hermitian (NH) nodal phases emerging in the coherent time evolution of a dynamically equilibrating system. Using nonequilibrium Greens function methods within the conserving second Born approximation, we predict observable signatures of these NH nodal phases both in equilibrated spectral functions and in the nonequilibrium dynamics of single-particle density matrix functions.

DY 19.4 Tue 12:15 H20

Nontrivial damping of quantum many-body dynamics — •Tjark Heitmann[1], Jonas Richter[2], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]Department of Physics, University of Osnabrück, Germany — [2]Department of Physics and Astronomy, University College London, UK

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. While these predictions rely on random-matrix arguments and typicality, they can only be verified for a specific physical situation by comparing to the actual solution or measurement. Crucially, it also remains unclear how frequent and under which conditions counterexamples to the typical behavior occur. Here, we discuss 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. This suggestion has consequences for the time dependence of correlation functions. We substantiate our theoretical arguments by large-scale numerical simulations of charge transport in the extended Fermi-Hubbard model with nearest-neighbor interactions as perturbations to the integrable reference system.

DY 19.5 Tue 12:30 H20

Effect of electron-electron interaction on the spectral statistics in circular sector graphene billiards — •Xianzhang Chen[1,2] and Liang Huang[1] — [1]Lanzhou Center for Theoretical Physics, and Key Laboratory for Magnetism and Magnetic Materials of MOE, Lanzhou University, Lanzhou, Gansu 730000, China — [2]Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, F-67000 Strasbourg, France

The spectral statistics is a fundamental issue in quantum chaos and has been used widely as a measure to probe the complexity of the underlying quantum systems. In this work, we adopt the one-orbital mean-field Hubbard model to investigate the effect of many-body interactions on the spectral statistics of circular sector graphene billiards. It is found that the spectral statistics are insensitive to the Hubbard interaction U for most of the energy ranges, except for energies around the Dirac point. We choose two representative systems, whose spectral statistics follow Poisson and Gaussian orthogonal ensemble (GOE) when $U = 0$, respectively. As U increases, for both cases, the spectral statistics moves toward GOE. However, after passing a critical value U_c, the spectral statistics turns back toward Poisson as U is increased further, due to the emerging gap and henceforth distinct behaviors of the quasiparticles. In addition, the energies above and below the Dirac point may exhibit different spectral statistics. These results uncover the intriguing connection between Hubbard interaction and the spectral statistics in graphene sector billiards. A physical picture is provided to understand these effects.

DY 19.6 Tue 12:45 H20

Anisotropy-mediated localization — •Ivan Khaymovich — Nordic Institute for Theoretical Physics, Stockholm, Sweden

Recently, the standard picture of Anderson localization transition in d-dimensional long-range (e.g. dipolar) systems has been argued due to several reported counterintuitive examples of (at least power-law) localization beyond the convergence of the perturbation theory. In addition, wave-function spatial decay rates obey a "mysterious" duality [1] mapping different powers 'a' of power-law bending symmetrically around the critical point a=d.

In my talk, I address this intriguing question, present a general approach applicable to all such models, and uncover the role of correlations and the origin of the above duality [2]. The phenomenon of the correlation-induced localization [2] is just the very peak of the iceberg in this field. Therefore I will focus on the effects of anisotropy [3] in dipolar system and show the reentrant localization governed by the anisotropy parameter given by the tilt of an electric field. Note that the range of systems is also not limited by the dipolar systems, but includes also the Weyl semimetals, ultracold atoms, Rydberg excitations in the optical traps and many others.

Literature: [1] X. Deng, V. E. Kravtsov, G. V. Shlyapnikov and L. Santos, Phys. Rev. Lett. 120, 110602 (2018). [2] P. Nosov, I. M. Khaymovich, V. E. Kravtsov, Correlation-induced localization Phys. Rev. B 99, 104203 (2019) [arXiv:1810.01492] [3] X. Deng, A. L. Burin, I. M. Khaymovich, Anisotropy-driven localization transition in quantum dipoles [arXiv:2002.00013]

DY 20: Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)

Time: Tuesday 11:30–13:00 Location: H38

Invited Talk DY 20.1 Tue 11:30 H38

How X-rays can reveal waters mysteries — •Katrin Amann-Winkel — Max-Planck-Institut für Polymerforschung, Mainz, Germany — Johannes Gutenberg Universität Mainz, Institut für Physik, Mainz, Germany — Stockholm University, Department of Physics, Stockholm, Sweden

Water is ubiquitous and the most important liquid for life on earth. Although the water molecule is seemingly simple, various macroscopic properties of water are most anomalous, such as the density maximum at 4°C or the divergence of the heat capacity upon cooling. Computer-simulations suggest that the anomalous behaviour of ambient and supercooled water could be explained by a two state model of water. An important role in this ongoing discussion plays the amorphous forms of water [1]. Since the discovery of two distinct amorphous states of ice with different density (high- and low density amorphous ice, HDA and LDA) it has been discussed whether and how this phenomenon of polyamorphism at high pressures is connected to the occurrence of two distinct liquid phases (HDL and LDL). X-ray scattering experiments on both supercooled water [2] and amorphous ice [3] are of major importance for our understanding of water. In my talk I will give an overview on our recent experiments on supercooled water and amorphous ices. [1] K. Amann-Winkel et al., Waters controversial glass transition, Rev. Mod. Phys. 88, (2016) [2] K.H. Kim, et al., SCIENCE 358, 1589 (2017) [3] K.H. Kim, et al., SCIENCE 370, 6519, 978 (2020)

DY 20.2 Tue 12:00 H38

Electrostatic Shielding Behavior of Keggin Anions in Aqueous Solution — •Thomas Tilger and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Natural colloidal dispersions have accompanied mankind in the form of blood or milk ever since. Besides this, artificial systems have gained a significant importance for our daily life during the last decades.

Therefore, it is of special interest to gain an understanding of which interparticle forces govern the stability of colloidal dispersions and how this stability can be tailored. In electrolyte solutions, the classical DLVO theory describes these interactions. Whilst this description provides a good agreement with experimental data for 1:1 electrolytes, larger deviations appear for systems of higher valency. For a detailed examination of the van der Waals and electrostatically dominated regimes, we directly measure the forces between colloidal silica particles in aqueous solutions by the colloidal probe AFM (atomic force microscopy) technique.

Varying the concentration of monovalent salts and acids allows us to demonstrate the transition from the double layer to the van der Waals dominated regime and to determine the pH dependence of the colloidal probes double layer potential. Similar measurements for phosphotungstic (PTA, a 1:3 system) and silicotungstic acid (STA, a 1:4 system) - both nanometer-sized anions of the Keggin type - can still be described with the DLVO theory, but reveal significant deviations between the calculated and measured ionic strengths.

DY 20.3 Tue 12:15 H38

Influence of the imbibition of colloids through the morphology of porous CNF layers — •Constantin Harder[1,2], Marie Betker[1,3], Alexakis E. Alexakis[3], Andrei Chumakov[1], Benedikt Sochor[1], Elisabeth Erbes[1,4], Marc Gensch[1,2], Qing Chen[1], Calvin Brett[1,3], Jan Rubeck[1], Matthias Schwartzkopf[1], Eva Malmström[3], Daniel Söderberg[3], Peter Müller-Buschbaum[2,5], and Stephan V. Roth[1,3] — [1]DESY, 22607 Hamburg, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, 10044 Stockholm, Sweden — [4]Institute for X-ray Physics, Goettingen University, 37077 Goettingen, Germany — [5]MLZ, TU München, 85748 Garching, Germany

Functionalization of porous materials in terms of optical, chemical, and mechanical properties is readily achieved by applying colloidal layers. Our goal is to functionalize porous cellulose nanofibril (CNF) templates by applying tailored core-shell colloids with specific surface properties. The colloidal layer formation influencing the surface properties can be tuned by the deposition conditions and subsequent annealing. Therefore, we applied colloidal inks (poly(butyl methacrylate) and poly(sobrerol methacrylate) in aqueous dispersion) with different glass transition temperatures T_g as the colloidal layers on the CNF templates. During the deposition, the colloids partially enter the CNF layer to fill the CNF voids and remain on the CNF surface, leading to complex drying processes. The morphology of the mixed CNF / colloidal thin film changes when T_g of the colloids is exceeded.

DY 20.4 Tue 12:30 H38

Elastic core-shell materials and their deformational behavior — Jannis Kolker[1], •Lukas Fischer[2], Andreas M. Menzel[2], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Elastic materials consisting of an inner part, a core, and an outer part, a shell, of possibly different material properties can be found from planetary scales down to the colloidal microscale. We here describe a situation amenable to analytical theory, namely the linear elastic deformation of a spherical core-shell system in response to an equatorial load in form of a force line density [1]. The relevance of this setup lies in, e.g., functionalized microgel particles absorbed to fluid-fluid interfaces or macroscopic illustrative show-and-tell objects.

Situations of different elastic properties and sizes of core and shell are analyzed to study their influence on the deformational response of the whole system. For example, tuning the two Poisson ratios allows to adjust the relative degree of oblate or prolate deformations and change in volume between core and shell. Due to the overall spherical shape and the two-component structure, the stress and strain distributions become rather inhomogeneous. Using different core and shell materials in colloidal microgel particles allows for inner functionalization while simultaneously adjusting the outer wetting properties.

[1] J. Kolker, L. Fischer, A. M. Menzel, H. Löwen, *J. Elasticity*, in press.

DY 20.5 Tue 12:45 H38

Effective Thomas-Fermi screening approach and wetting transition at charge/metal interfaces — •Alexander Schlaich[1,2], Dongliang Jin[1,3], Lyderic Bocquet[4], and Benoit Coasne[1] — [1]Univ. Grenoble Alpes, CNRS, LIPhy, Grenoble, France — [2]Stuttgart Center for Simulation Science, Universität Stuttgart, Germany — [3]Institut fur Theoretische Physik, Technische Universitat Wien, Austria — [4]Laboratoire de Physique de l'Ecole Normale Supérieure, CNRS, Université PSL, Sorbonne Université, Sorbonne Paris Cité, Paris, France

At the nanometer scale the commonly employed image charge approach to obtain the electrostatic interactions close to a metallic interface breaks down due to the finite screening in any real metal. We develop an effective approach that allows dealing with any real metal using the Thomas-Fermi formalism. [1]

We find a microscopic picture based on the Gibbs-Thomson equation for capillary freezing of an ionic liquid. An unprecedented wetting transition is found upon switching the confining medium from insulating to metallic. The wetting behavior at imperfect metals raises new challenging questions on the complex behavior of charged systems in the vicinity or confined within surfaces.

[1] A. Schlaich, D. Jin, L. Bocquet & B. Coasne, Nat. Mater. 1 (2021).

DY 21: Invited Talk Dirk Brockmann (joint session SOE/DY)

Time: Wednesday 9:30–10:15 Location: H11

Invited Talk DY 21.1 Wed 9:30 H11

The Corona Data Donation Project - When Citizens Collaborate to Fight a Pandemic — •Dirk Brockmann — Humboldt University of Berlin, Berlin, Germany

In response to the COVID-19 pandemic we launched the Corona Data Donation Project in April 2020. In this citizen science project participants donate physiological data on heart rate, sleep and physical activity measured by smart watches, fitness trackers and wearable devices on a daily bases. With more than 500,000 donors the project is the largest data donation project worldwide. Initially conceived as a tool for real-time syndromic surveillance of the Covid-19 pandemic and as a monitoring tool, it has evolved into a large scale experimental and exploratory technological framework that continues to reveal a number of fascinating insights concerning Covid-19 related topic such has Long-Covid, the effects of vaccination, sleeping patterns but also insights with broader applications. The project now hosts physiological time-series that span over two years of over 200,000 individuals. I will discuss the promises and discoveries of citizen science and wearable devices from the perspective of digital epidemiology and illustrate what role "physics"-thinking plays in projects like this.

DY 22: Active Matter 3 (joint session BP/CPP/DY)

Time: Wednesday 9:30–12:30 Location: H16

DY 22.1 Wed 9:30 H16

Collective foraging of microrobots trained by reinforcement learning — •Robert C. Löffler[1], Emanuele Panizon[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Department of Quantitative Life Science, International Centre for Theoretical Physics, Trieste, Italy

From bacteria to mammals, collective behavior can be observed on all scales in nature. It is generally driven by the benefit to individuals when cooperating with others. However, the exact motivation of individuals to participate is challenging to investigate, as biological creatures are complex systems theirself. At the same time engineers seek to create collective groups of autonomous systems to perform dedicated tasks by cooperation.

Here we present an experimental model system of feedback-controlled microswimmers which are trained with multi agent reinforcement learning in an actor-critic scheme. A group of active particles is situated in a 2D environment containing a virtual food source which is changing position over time. Despite being rewarded individually for being inside the food source, particles show cohesive collective motion forming flocks and swirls. This is driven by the benefit of social information and collision avoidance, resulting in faster migration to a relocated food source. Understanding those mechanisms behind the emergence of collective behavior is of biological interest as well as to understand human crowd behavior and to design future robotic systems.

DY 22.2 Wed 9:45 H16

Collective response of microrobotic swarms to external threats — •Chun-Jen Chen[1] and Clemens Bechinger[1,2] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]Centre for the Advanced Study of Collective Behaviour, Universität Konstanz, 78464 Konstanz, Germany

Many animal species organize within groups to achieve advantages compared to being isolated. Such advantages can be found e.g. in collective responses which are less prone to individual failures or noise and thus provide better group performance. Inspired by social animals, here we demonstrate with a swarm of microrobots made from programmable active colloidal particles (APs) that their escape from a hazardous area can originate from a cooperative group formation. As a consequence, the escape efficiency remains almost unchanged even when half of the APs are not responding to the threat. Our results not only confirm that incomplete or missing individual information in robotic swarms can be compensated by other group members but also suggest strategies to increase the responsiveness and fault-tolerance of robotic swarms when performing tasks in complex environments.

DY 22.3 Wed 10:00 H16

Soft robots powered by magnetically driven active particles — •Hongri Gu and Clemens Bechinger — Fachbereich Physik, University of Konstanz, Germany

Active matter describes systems of a large number of self-driving particles that convert surrounding energy into active motion. Many of the emergent behaviors resemble life-like behaviors in nature. However, it is still unclear how one can utilize such active collective motions for engineering and robotic applications. In this talk, we would like to bridge the research fields of active matter and soft robots by designing soft machines powered by active matter. The main objective is to investigate the general interactions between swarm active particles and soft structures and use this knowledge to design a new type of soft robots that are driven by swarm active particles. To facilitate the investigation, we built a highly customizable fabrication process for magnetic composite soft structures at mesoscales based on two-step micromolding. We also built a modular magnetic actuation system based on rotating permanent magnets. This new experimental platform has an enormous design space for magnetic soft matters with the capability to tune individual system parameters. By carefully designing these parameters, it is possible to precisely tune the local magnetic, elastic, and hydrodynamic interactions between active particles and soft structures. This new type of soft machine can potentially take advantage of the robust dynamic states of the active matter, which can recover their functions from extreme mechanical deformations.

DY 22.4 Wed 10:15 H16

Microswimmers in viscosity gradients — •Sebastian Ziegler[1], Maxime Hubert[1], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Division of Physical Chemistry, Ruder Bošković Institute Zagreb, Croatia

Regions of variant viscosity are ubiquitous in both inanimate systems as well as in living systems. It is therefore of great interest to understand the effect of viscosity gradients on the mobility of both passive particles as well as on active systems. We firstly study a system of passive spheres and provide a general expression for the asymptotic mobility matrix in small viscosity gradients. We apply this result to linear viscosity gradients, where we unveil the existence of radially constant flows and elaborate on the effect of asymmetry of the particle position within the finite-size gradient, which hitherto has not been considered.

These results are subsequently applied to bead-spring microswimmers as model systems for self-propelling active matter. In contrast to the common approach of prescribing the stroke of the swimmer, we here employ a force-based swimmer model, allowing for an adaption of the swimming stroke to the environment, and reveal the rich viscotactic properties of such a microswimmer. We also construct a simple swimmer inspired by the Chlamydomonas algae and compare the viscotactic behavior of the biological swimmer to ours.

15 min. break

DY 22.5 Wed 10:45 H16

Noisy pursuit of active Brownian particles — •Segun Goh, Roland G. Winker, and Gerhard Gompper — IBI-5, Forschungszentrum Jülich, 52425 Jülich, Germany

Many biological and artificial agents are not only motile, but also capable of adjusting their motion based upon information gathered from their environment. This study considers sensing of a target and as a consequence reorientation of the direction of self-propulsion, which enables active pursuit. Specifically, an active Brownian particle is employed as a model agent to investigate pursuit dynamics in two dimensions, for both stationary as well as moving targets. We discuss how

the interplay between intrinsic persistent self-propulsion and active reorientation by sensing gives rise to unexpected complex behaviors. In particular, the noise plays a pivotal role with both positive and negative influences on the success of pursuit. Numerical simulations and analytical calculations reveal that strong motility results in overshooting of the target, while pursuers cannot approach the target effectively at low Péclet numbers. Moreover, we propose a strategy to sort active pursuers according to their motility and reorientation capability by employing particular target trajectories.

DY 22.6 Wed 11:00 H16

Rheotaxis of the ciliate — •Takuya Ohmura[1], Yukinori Nishigami[2], and Masatoshi Ichikawa[3] — [1]Biozentrum, University of Basel, Switzerland — [2]Research Institute for Electronic Science, Hokkaido University, Japan — [3]Department of Physics, Kyoto University, Japan

Rheotaxis, a property of organisms to move against an external flow, has a crucial role to stay in living environment. For instance, freshwater fishes in rivers swim upstream to avoid being swept away to the sea. Interestingly, recent studies reported that not only fish but also swimming cells show rheotaxis. We elucidated the rheotaxis of the ciliate, Tetrahymena, a well-known single-celled freshwater microorganism swimming by cilia [1]. While that microorganism doesn*t have a sensor to detect flow direction and micrometer-sized particles are swept away downstream in a viscous flow, what dynamics underlie the rheotaxis of the ciliate? Our experiments revealed that the ciliate slid upstream along a wall, which indicates that the cells receive rotational torque from shear flow to align swimming orientation. To evaluate the shear torque, we performed a numerical simulation with a hydrodynamic model swimmer adopting cilia dynamics in a shear flow. The result suggests that the ciliate automatically slides upstream by using cilia-stalling mechanics.

[1] T. Ohmura, et al., Science Advances, 7(43), eabi5878 (2021).

DY 22.7 Wed 11:15 H16

Analytical study of active semiflexible ring polymer — •Christian A. Philipps, Gerhard Gompper, and Roland G. Winkler — Forschungszentrum Jülich, Jülich, Germany

Nature provides a variety of active matter systems, with self-propelled agents consuming internal energy or extracting it from their vicinity for locomotion [1]. Examples on the cellular level are self-propelled semiflexible actomyosin ring-like filaments driven by myosin motors in the cytoskeleton. We present a theoretical study of an active ring polymer [2] with tangential propulsion applying the continuous Gaussian semiflexible polymer model [3]. By a normal-mode expansion, the ring polymer conformational and dynamical properties, emerging by the homogeneous active force, and its interplay with rigidity are determined. Remarkably, the ring conformations are unaffected by activity for any rigidity. In contrast to linear filaments, the center-of-mass motion is independent of propulsion. However, activity strongly influences the internal dynamics with an activity enhanced diffusive for the flexible and a ballistic regime for the semiflexible ring polymer. Furthermore, a dominant rotational mode over several orders of magnitude in time emerges for high activities, which implies a rotational motion of the entire ring polymer. [1] R. G. Winkler, G. Gompper, J. Chem. Phys. 153, 040901 (2020); [2] M. Mousavi, R. G. Winkler, G. Gompper, J. Chem. Phys. 150, 064913 (2019); [3] T. Eisenstecken, G. Gompper, R. G. Winkler, Polymers 8, 304 (2016).

DY 22.8 Wed 11:30 H16

Dynamical Renormalization Group approach to the collective behavior of natural swarms — Andrea Cavagna[1], Luca Di Carlo[1], Irene Giardina[1], Tomas Grigera[1,3], •Giulia Pisegna[1,2], and Mattia Scandolo[1] — [1]Sapienza Università di Roma, Roma IT — [2]Max Planck Institute for Dynamics and Self-Organization, Goettingen DE — [3]IFLYSIB, La Plata, Argentina

Recent data on strongly correlated biological systems showed the validity of scaling laws as one of the fundamental traits of collective behaviour. Experiments on natural swarms of insects unveiled traces of critical dynamics, with inertial features and a dynamical critical exponent z=1.2. To rationalize this evidence, we develop an inertial active field theory in which the velocity is coupled to its generator of internal rotations, namely the spin, through a mode-coupling interaction. We study its near-critical regime with a one-loop Renormalization Group approach under the assumption of incompressibility. The presence of friction in the dynamics of the spin rules a paramount crossover between two fixed points: the unstable underdamped fixed point with z=1.3 and the stable overdamped fixed point with z=1.7, where dissipation takes over. We show how finite-size systems with weak dissipation, such as swarms, can actually exhibit the critical dynamics of the unstable fixed point thus providing a theoretical result which is in fair agreement with experimental data.

15 min. break

DY 22.9 Wed 12:00 H16

Dynamics and rheology of active suspensions in viscoelastic media — •Akash Choudhary[1], Sankalp Nambiar[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Nordita, KTH Royal Institute of Technology and Stockholm University, Stockholm 10691, Sweden

Active suspensions are systems of motile organisms or active motors that are driven out of equilibrium through self-propulsion. This localized energy-work conversion imparts rich phenomenology and anomalous macroscale properties that are in stark contrast to passive suspensions and polymeric fluids. Motivated by the ubiquitous microbial systems in biological fluids, we analyse the impact of non-Newtonian fluids on the rheological response of active suspensions to steady shear flows.

We first study the suspension at an individual scale and show that elongated pushers (representative of *E. coli*) and pullers (*C. reinhardtii*) exhibit diverse orbital dynamics in a viscoelastic fluid. We find that the active stresses not only modify the Jeffery orbits, well-known for viscous fluids, but microswimmers can even resist flow-induced rotation and align themselves at an angle with the flow. To analyze the impact of such behavior on the bulk rheological response, we study an ensemble of a dilute suspension of such swimmers in the presence of stochastic noise from bacterial tumbling and rotary diffusion. In comparison to Newtonian media, the polymeric elastic stresses substantially and non-monotonically amplify the swimmer-induced viscosity, in particular, the superfluid transition of pusher solutions.

DY 22.10 Wed 12:15 H16

Intercellular transport in *Chara corallina* — •Florian von Rüling[1], Anna Alova[2], Alexander Bulychev[2], and Alexey Eremin[1] — [1]Otto von Guericke University Magdeburg, Germany — [2]Moscow, Russia

We explore the kinetics of the intercellular transport between the giant cells of characean algae. The transport involves advection via cytoplasmic streaming and diffusion through the plasmodesmata, pores that penetrate the cell walls. Using fluorescent dye as a tracer, we measure the permeation through the node of tandem cells. The permeability is extracted from the experimental data using an advection-diffusion model. The current work is focused on the roles of cytoplasmic streaming and the nodal cells in the transport mechanism. To separate the diffusive permeation from the advective contribution, cyclosis was temporarily inhibited using action potentials. Streaming cessation results in dye accumulation in the vicinity of the node. The shape of regions with high dye concentration indicates that action potentials may induce closure of the plasmodesmata in central nodal cells.

DY 23: Complex Fluids and Soft Matter 1 (joint session DY/CPP)

Time: Wednesday 9:30–12:00 Location: H18

DY 23.1 Wed 9:30 H18

Writing in Water — •Thomas Palberg and Nadir Möller — Institut für Physik, Johannes Gutenberg Universität Mainz

Writing is an ancient cultural technique, typically performed by leaving some trace in or on a solid surface. We here explore the possibilities of leaving the trace in a liquid medium close to a surface and obtain lines or letters with high contrast and durability. Ion exchange (IEX) resin beads are used as mobile proton or hydroxyl ion sources. Moving them across the substrate in low-salt water, leaves a pH trace. Added autonomously swimming particles are able to follow this trace, mimicking hunter and prey dynamics or mate tracing, but without leaving a visible testimony. Written lines are realized by adding larger amounts of micron-sized passive particles, which settle to the like-charged substrate. Being phoretically drawn to or repelled from the pH traces, they form a well-visible trail behind the source. Trails of cationic IEX are white on black, those of anionic IEX are black on white. Their diffusive fading is slowed by continued phoretic flows and trails are stable up to hours. Sources moving autonomously just scribble. Sources propelled straight by gravity leave high-contrast lines. Deliberate tilting sequences for the substrate, then, facilitate writing.

DY 23.2 Wed 9:45 H18

Composition Dependent Instabilities in Mixtures With Many Components — •Filipe Thewes, Matthias Krüger, and Peter Sollich — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

Understanding the phase behavior of mixtures with many components is a key step towards a physics-based description of intracellular compartmentalization. We study the instabilities of a model where the interactions as quantified by the second virial coefficients are taken as random Gaussian variables. Using tools from free probability theory we obtain the spinodal curve and the nature of instabilities for an arbitrary distribution of components, thus lifting the drastic simplification of uniform composition that has been made in earlier work. We illustrate our results with examples and show that, by controlling the density of only a few components, one can systematically change the nature of instabilities and achieve demixing for realistic scenarios, which appeared to be ruled out by previous studies. Inspired by these results, we introduce an additive model taking into account also deterministic interactions. We show how this systematic interaction leads to a competition between different forms of instabilities that can be tuned by controlling the model parameters. Since most experimental protocols for complex mixtures rely on tuning either the composition or systematic interactions, we expect our results to significantly extend the range of mixtures that can be treated within the mean-field model.

DY 23.3 Wed 10:00 H18

Phase behaviour of mixtures of hard spheres and hard rods — •Poshika Gandhi[1], Joeri Opdam[2], Anja Kuhnhold[1], Tanja Schilling[1], and Remco Tuinier[2] — [1]Institute of Physics, Albert-Ludwigs-University Freiburg, Germany — [2]Institute for Complex Molecular Systems, Eindhoven University of Technology, The Netherlands

Phase behaviours of complex mixtures are challenging to predict. A binary mixture of hard spherocylinders (HSC) and hard spheres (HS) is one such system. As rod-like particles have large excluded volume, a free volume theory (FVT) can be used to gain insights into demixing phenomenon and phase stability.

Vliegenthart *et al*[1] modified an existing FVT for binary mixtures of HS to accommodate HSC. This FVT works well for the needle limit, i.e., weak excluded volume interactions between HSC. It, however, predicts the phase boundaries at too low HSC concentrations. Opdam *et al*[2] showed that by incorporating excluded volume interactions between the depletants even in the reservoir improves the FVT significantly.

We used the new FVT to predict phase boundaries of colloidal mixtures and compared them to MC simulations. The results show that accounting for all the excluded volumes of all the components may be pivotal in understanding phase behaviour of colloidal mixtures [3].

[1] G. A. Vliegenthart et al., J. Chem. Phys., **111**, 4153 (1999).
[2] J. Opdam, et al., J. Chem. Phys., **154**, 204906 (2021)
[3] J. Opdam, et al., Phys. Chem. Chem. Phys., **24**, 11820 (2022)

DY 23.4 Wed 10:15 H18

Markov State Modelling of Self Assembling Colloidal Systems — •Salman Fariz Navas and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Many colloidal particle systems display self-assembly phenomena yielding, e.g., clusters or gel-like materials. The current project focuses on the use of phase space discretization techniques towards developing a coarse-grained description of self-assembly processes in colloidal systems.

Specifically, we develop a corresponding Markov State Model from particle-resolved Brownian Dynamics simulations, wherein the Markov states are the various local structural configurations present in the system and the Markovian process describing the stochastic transition of particles from one structure to the other.

The specific self-assembly problem studied here involves the aggregation of colloidal particles with field-induced multipolar interactions [1]. We use bond orientational order parameters and the coordination number as parameters to define the discrete states. The number of particles in the largest cluster in the system (n) is used as a parameter to quantify the progress of the overall aggregation. Transition probability matrices (TPM) between the different states are then computed for each value of n. Information regarding relaxation times and pathways relevant to the aggregation process are extracted by analyzing changes in the TPM elements.

[1] Florian Kogler, Orlin D. Velev, Carol K. Hall and Sabine H. L. Klapp, Soft Matter 11, 7356 (2015)

DY 23.5 Wed 10:30 H18

Repulsion of topological defects in quasi-2D liquid crystal films — •Kirsten Harth[1,2] and Ralf Stannarius[3] — [1]Fachbereich Technik, TH Brandenburg, Brandenburg an der Havel, Deutschland — [2]MARS und MRTM, Otto von Guericke Universität Magdeburg, Deutschland — [3]Institut für Physik und MARS, Otto von Guericke Universität Magdeburg, Deutschland

The dynamics of topological defects is of interest, e.g., in phase transitions, cosmology or structural organization of colloids and active matter. Liquid crystals are a straightforward system allowing optical characterization of defect motion. As anisotropic fluids, they are characterized by orientational order, introducing long-range elastic forces, in addition to liquid-like fluidity with viscosity coefficients related to, e.g., the local shear flow directions respective to the local orientational field. This causes intriguing effects and must not be neglected.

The comparison of recent exeriments [1,2] in free-standing smectic C films to theoretical and numerical predictions [2,3] leaves a number of questions unanswered. A proper consideration of flow coupling and / or of an anistropy of the elastic constants in a simulation with realistic boundary conditions may solve the issues. We explain why elastic anisotropy is particularly important here. Experimental and numerical data are compared to elucidate the effect of elastic constants and flow on the repeulsion dynamics.

[1] A. Missaoui, et al., PR Research 2 013080 (2020). [2] R. Stannarius, K. Harth, PRL 117 157801 (2016). [3] e.g. X. Tang, J. V. Selinger, Soft Matter 13 5481 (2017) ; Soft Matter, 15 587 (2019)

15 min. break

DY 23.6 Wed 11:00 H18

Incipient motion for 3d geometries — •Dominik Geyer, Paolo Malgaretti, Othmane Aouane, and Jens Harting — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Cauerstr. 1, 91058 Erlangen, Germany

The incipient motion describes the threshold conditions between erosion and sedimentation. This natural process is relevant for a broad field of natural and industrial processes, for example, cell detachment, cleaning of surfaces, and transportation in pipelines. Our interest is in the incipient motion of a single particle on non-trivial geometries. The crucial parameter for describing incipient motion is the so-called Shields number which is the ratio between viscous forces and buoyancy. Interestingly, the incipient motion has been reported at values of the Shields number much smaller than unity ($\theta \simeq 10^{-2}$) hence questioning whether the proposed Shields number is indeed capturing the relevant physical phenomena. In order to critically discuss this aspect, we per-

form lattice Boltzmann simulations of a solid particle on a substrate consisting of solid spheres taking into account the local fluid velocity and the particle size. Our numerical data will allow us to calculate the effective viscous force acting on the particle and hence to propose possible corrections to the Shields number which can better account for the experimental and numerical data.

DY 23.7 Wed 11:15 H18

Phase behaviour in a mono-layer colloidal membrane — •Léa Beaules, Anja Kuhnhold, and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Kosterlitz-Thouless-Halperin-Nelson and Young (KTHNY) theory predicted that the melting of a purely 2D hard disk system would be defect-mediated and occur via two continuous transitions: from the solid to the intermediate hexatic phase and, from the hexatic to the fluid phase. Since then phase behaviour of this system as well as closely related systems have been extensively investigated and debated, showing that the hexatic-liquid transition is of first order for purely hard system [1]. Additionally, upon increasing interaction range or adding dispersity in the system the transition can become continuous or the hexatic phase can vanish [2].

However a large number of real systems can be more accurately approximated as a quasi-2D system that exhibits out of plane interactions, e.g. biological membranes; therefore understanding their role in the phase behaviour is important. Thus to extend our understanding of these systems, we use Monte-Carlo simulations to study an infinite mono-layer membrane of hard rod-like particles. We investigate how the orientational degree of freedom of the rods, and the range of their out of plane interactions affect the phase behaviour of the system.

[1] E. P. Bernard and W. Krauth, Phys. Rev. Lett. **107**, p. 155704 (2011).

[2] Y.-W. Li and M. P. Ciamarra, Phys. Rev. E **102**, p. 062101 (2020).

DY 23.8 Wed 11:30 H18

Particle-resolved topological defects of smectic colloidal liquid crystals in 2d confinement — •René Wittmann[1], Paul A. Monderkamp[1], Louis B. G. Cortes[2,3], Dirk G. A. L. Aarts[3], Frank Smallenburg[4], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine Universität Düsseldorf, Germany — [2]School of Applied and Engineering Physics, Cornell University, USA — [3]Department of Chemistry, Physical and Theoretical Chemistry Laboratory, University of Oxford, UK — [4]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, France

We present a general classification scheme [1] of the intrinsic structure of smectic colloidal liquid crystals in two spatial dimensions, dictated by the interplay between the intrinsic layering and the externally imposed boundary structure. Thereby, we demonstrate that topological defects emerge in the form of spatially extended grain-boundaries, which are characterized by coexisting nematic and tetratic orientational order. We examine these intriguing topological properties on the particle scale by means of Monte-Carlo simulations, fundamental-measure-based density functional theory and real-space microscopy of colloidal rods. The structural details agree on a quantitative level. In particular, we analyze the typical shape of grain-boundary networks in a large range of polygonal confinements [1] and the stability of different competing topological states in nontrivial domains with additional interior boundaries [2].

[1] P. A. Monderkamp et al., Phys. Rev. Lett. 127, 198001 (2021).

[2] R. Wittmann et al., Nat. Commun. 12, 623 (2021).

DY 23.9 Wed 11:45 H18

Structure of nematic hard rod tactoids — •Anja Kuhnhold[1] and Paul van der Schoot[2] — [1]University of Freiburg, Freiburg, Germany — [2]Eindhoven University of Technology, Eindhoven, The Netherlands

Droplets of ordered phases of anisotropic particles take on specific shapes and internal structures. Compared to droplets of spherical particles, tactoids are elongated with cusp-like tips. Several parameters dictate the overall shape and structure: density of the system, elastic constants of the particles, anchoring strength, interfacial tension, and volume of the tactoid. [1]

We compare Monte Carlo simulation results of hard rod tactoids in a bath of spherical ghost particles to predictions from a scaling theory. We focus on small tactoids where the macroscopic scaling description might break down. We find that smaller tactoids have a more uniform director field than larger tactoids. Also, the segment density increases towards the tactoid tips in agreement with the theory. In addition, we find further density modulations when the average density increases.

Besides, we test the effect of an aligning field on the shape and structure of the tactoids and find that the director field becomes more uniform and the aspect ratio increases, but not to a vast extent. [2]

[1] P. Prinsen, P. van der Schoot, EPJ E **13**, 35 (2004).

[2] A. Kuhnhold, P. van der Schoot, JCP **156**, 104501 (2022).

DY 24: Stochastic Thermodynamics and Information Processing

Time: Wednesday 9:30–11:15 Location: H19

DY 24.1 Wed 9:30 H19

Optimising Energetics in Field Theories: Pareto Front and Phase Transitions — •Atul Tanaji Mohite and Etienne Fodor — University of Luxembourg, Department of Physics and Materials Science, L-1511, Luxembourg

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 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 minimise average stochastic work, which we apply to cases with either conserved or non-conserved scalar order parameter in the weak noise regime. Moreover, we formulate a numerical multi-optimization problem to simultaneously optimize the mean and fluctuations of stochastic 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 theories at a minimal energy cost, with the potential to be deployed to a broad class of systems.

DY 24.2 Wed 9:45 H19

Replica-Symmetry Breaking for Ulam's problem — •Phil Krabbe[1], Hendrik Schawe[2], and Alexander K. Hartmann[1] — [1]Institute of Physics, University of Oldenburg, Germany — [2]LPTM, CY Cergy Paris Université, France

For a given sequence $X = x_1, x_2, \ldots, x_n$ of numbers, an increasing subsequence (IS) is a subset of l elements $i(1) < i(2) < \ldots < i(l)$ such that $x_{i(1)} < x_{i(2)} < \ldots < x_{i(l)}$. The longest increasing subsequences (LIS) problem, i.e. to maximise l, was considered numerically first by S. Ulam and is a well studied topic. Here we consider the length l as an energy and study the canonical ensemble of ISs controlled by temperature parameter T, which includes the LIS for $T \to 0$. We extended our algorithm from [1] such that we can draw ISs in perfect equilibrium in polynomial time. This allows us to study large sequences with up to $n = 8192$ numbers.

We studied the IS numerically [2] for sequences X being permutations of integers. As measurable quantities, we analysed the mean energy, the specific heat C and and the overlap q between the drawn ISs. Our exact-sampling results indicate that the IS exhibits in the thermodynamic limit a complex energy landscape in the spirit of Replica Symmetry Breaking, characterised by a broad distribution $P(q)$ of overlaps and a hierarchical organization of the configuration space.

[1] P. Krabbe, H. Schawe and A.K. Hartmann, Phys. Rev. E **101**, 062109 (2020)

[2] A.K. Hartmann, *Big Practical Guide to Computer Simulations*, World Scientific (2015)

15 min. break

DY 24.3 Wed 10:15 H19

Optimality of nonconservative driving for finite-time pro-

cesses with discrete states — •Benedikt Remlein and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

An optimal finite-time process drives a given initial distribution to a given final one in a given time at the lowest cost as quantified by total entropy production. We prove that for a system with discrete states this optimal process involves nonconservative driving, i.e., a genuine driving affinity, in contrast to the case of a system with continuous states. In a multicyclic network, the optimal driving affinity is bounded by the number of states within each cycle. If the driving affects forward and backwards rates nonsymmetrically, the bound additionally depends on a structural parameter characterizing this asymmetry [1]. [1] B. Remlein and U. Seifert, Phys. Rev. E 103, L050105 (2021)

DY 24.4 Wed 10:30 H19

Phase shift in periodically driven non-equilibrium systems: Its identification and a bound — •Julius Degünther, Timur Koyuk, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Time-dependently driven stochastic systems form a vast and manifold class of non-equilibrium systems used to model important applications on small length scales such as bit erasure protocols or microscopic heat engines. One property that unites all these quite different systems is some form of lag between the driving of the system and its response. For periodic steady states, we quantify this lag by introducing a generalized phase difference. We prove two tight bounds for this generalized phase difference, which provide upper limits to the lag such systems can yield. The first and most general bound depends only on the relative speed of the driving. The second more detailed bound takes additional information about the rates into account. We show that both bounds can be saturated by an appropriate choice of parameters.

DY 24.5 Wed 10:45 H19

Thermodynamic inference in partially accessible Markov networks: A unifying perspective from transition-based waiting time distributions — •Jann van der Meer, Benjamin Ertel, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

The inference of thermodynamic quantities from the description of an only partially accessible physical system is a central challenge in stochastic thermodynamics. A common approach is coarse-graining, which maps the dynamics of such a system to a reduced effective one. While coarse-graining states of the system into compound ones is a well studied concept, recent evidence hints at a complementary description by considering observable transitions and waiting times. We consider waiting time distributions between two consecutive transitions of a partially observable Markov network and their ratios to quantify irreversibility and entropy production. We formulate criteria whether this entropy estimator provides a lower bound or recovers the full physical entropy production. Additionally, we derive estimators for the topology of the network, i.e., the presence of a hidden cycle, its number of states and its driving affinity. From a different perspective, our results can be condensed into a fluctuation theorem for an equivalent semi-Markov process. This mathematical perspective provides a unifying framework to compare our and known estimators. The correct version of time-reversal is crucial to clarify the relationship of formal versus physical irreversibility. Numerical calculations illustrate our exact results and estimate the quality of our bounds.

DY 24.6 Wed 11:00 H19

Geometric Brownian Information Engine — •Debasish Mondal, Rafna Rafeek, and Syed Yunus Ali — Department of Chemistry, Indian Institute of Technology Tirupati, Andhra Pradesh, India

We design a geometric Brownian information engine by considering over-damped Brownian particles inside a 2-D monolobal confinement with irregular width. Under such detention, particles experience an effective entropic potential which has a logarithmic form. We employ a feedback control protocol as an outcome of error-free position measurement. We reposition the centre of the confinement to the feedback site (x_f) instantaneously when the position of the trapped particle crosses the measurement distance (x_m) for the first time. Then, the particle is allowed to thermal relaxation. We find the exact analytical value of the upper bound of extractable work as $(\frac{5}{3} - 2ln2)k_BT$. We introduce a constant force G downwards to the transverse coordinate. G tunes the entropic contribution in the effective potential and hence the standard deviation (σ) of the probability distribution. The upper bound of the achievable work shows a cross-over from $(\frac{5}{3} - 2ln2)k_BT$ to $\frac{1}{2}k_BT$ when the system changes from an entropy dominated regime to energy dominated one. Compared to an energetic analogue, the loss of information during the relaxation process is higher in the entropy-dominated region, which accredits the less value in achievable work. We recognize that the extracted work is maximum when $x_f = 2x_m$ with $x_m \sim 0.6\sigma$, irrespective of the extent of the entropic limitation. The average displacement increases with growing entropic control and is maximum when $x_m \sim 0.81\sigma$.

DY 25: General Session to the Symposium: Interplay of Substrate Adaptivity and Wetting Dynamics from Soft Matter to Biology (joint session CPP/DY)

Time: Wednesday 9:30–11:15 Location: H39

DY 25.1 Wed 9:30 H39

Adaptive two capacitor model to describe slide electrification in moving water drops — •Pravash Bista[1], Amy Z. Stetten[1], William S.Y Wong[1], Hans-Jürgen Butt[1], and Stefan A.L. Weber[1,2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Johannes Gutenberg University, Department of Physics, Staudingerweg 10, 55128 Mainz, Germany

Slide electrification is a contact-charge separation where neutral water drops slide over a neutral hydrophobic surface, accumulating and leaving behind a net charge. The accumulated drop charge for successive sliding drops decreases and eventually reaches a steady state. On hydrophobic and hydrophilic mixed surfaces, even a polarity flipping of drop charge depending on a drop rate was observed. Here, we describe this effect in terms of a voltage generated at the three-phase contact line. This voltage moves charges between capacitors, one formed by the drop combined with the solid surface and one on the solid-surface. By introducing an adaptation of the voltage upon water contact, we can model drop charge experiments on different surfaces, including more exotic ones with drop-rate-dependent charge polarity. Thus, the adaptive two capacitor model enables new insights into the molecular details of the charge separation mechanism.

DY 25.2 Wed 9:45 H39

Memory effects of PNiPAAm brushes in different atmospheres — •Simon Schubotz, Marisa Fischer, Jens-Uwe Sommer, Petra Uhlmann, Andreas Fery, and Günter Auernhammer — Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany

Some polymer brushes show a co-nonsolvency effect: They collapse in a mixture of two good solvents at some specific mixing ratio. In contrast to previous studies we concentrate on partial wetting of co-nonsolvent polymer brushes, i.e., on the dynamics of a three-phase contact line moving over such brushes.

We found that Poly(N-isopropylacrylamide) (PNiPAAm) brushes experiences a memory effect when consecutively depositing drops at the same position. Previously deposited drops adapt the brush and changes the wetting behavior (advancing contact angle) of subsequent drops.

We measure water drops in an ethanol-saturated atmosphere on PNiPAAm brushes. The measurements show that the memory effect is strongly effected by an ethanol-enriched atmosphere. At the three-phase contact line, due to evaporation from the drop, the composition of the atmosphere and probably also the brush will transition from an ethanol-rich state to a water-enriched state. Thus, the brush might pass through the co-nonsolvency regime. On large time scales the ethanol enriched gas phase and the water drop will become mixtures of ethanol and water. We present strategies to counter this mixing effect.

DY 25.3 Wed 10:00 H39

Fast contact lines on soft solids — •Hansol Jeon[1,2] and Stefan Karpitschka[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August-Universität Göttingen, Göttingen, Germany

When a droplet is resting on a soft surface, the capillary forces deform the surface into a sharp wetting ridge. The amplitude of the wetting ridge is determined by elasto-capillary length, but the angles by which the interfaces meet at the ridge tip only depend on the balance of surface tensions, the so-called Neumann balance. For moving contact lines, dissipation in the wetting ridge leads to viscoelastic braking. In recent literature, various effects that could alter Neumann balance and viscoelastic braking have been suggested, ranging from free, extractable oligomers to point forces emerg-ing from bulk viscoelasticity. We visualize moving wetting ridges at high spatio-temporal resolution and determine the tip geometry for various liquids and PDMS substrates. We observe an increase of the ridge opening angle at large speeds, even for very mild deformations caused by the low surface tension of a fluorinated oil. We also find no significant change in ridge rotation and opening angle for gels with different fractions of crosslinked and free chains, nor for different bulk rheological properties. These findings highlight the need for a non-trivial surface constitutional relation that is different from the bulk.

DY 25.4 Wed 10:15 H39

Mixed grafted homopolymer and diblock copolymer functional brush layers upon humidity alterations: nanoscale morphology and transformations — •Apostolos Vagias[1], Theodore Manouras[2], Eleftherios Koufakis[2,3], Peixi Wang[4], Marcell Wolf[1], Fabian A. C. Apfelbeck[4], Sigrid Bernstorff[5], Maria Vamvakaki[2,3], and Peter Müller-Buschbaum[1,4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — [2]Foundation for Research and Technology (F.O.R.T.H.) Hellas, Institute of Electronic Structure and Laser,700 13 Heraklion, Crete, Greece — [3]Department of Materials Science and Technology, University of Crete, 700 13 Heraklion, Crete, Greece — [4]Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, 85748 Garching, Germany — [5]Elettra Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy

Using in situ grazing-incident small-angle X-ray scattering (GISAXS) measurements during water vapor uptake, we study the nanostructure morphology in the dry state, during vapor swelling and in the fully swollen state, for thin (<100nm) films of poly(2-(dimethylamino)ethyl methacrylate) (PDMAEMA) and poly(fluoroalkyl methacrylate) (POFPMA) homopolymer and PDMAEMA-b-POFPMA block copolymer dual functional, bactericidal and antifouling, brushes. Our surface energy and swelling studies, stress on the role alkyl chain length, charged groups and brush topology in morphology, for the brush functionality.

DY 25.5 Wed 10:30 H39

Steering droplets on substrates with periodic wettability patterns and deformations — •Josua Grawitter and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Straße des 17. Juni 135, 10623 Berlin

Droplets are set in motion on substrates with a spatio-temporal wettability pattern as generated, for example, on light-switchable surfaces. To study such cases, we implement the boundary-element method to solve the governing Stokes equations for the fluid flow field inside and on the surface of a droplet and supplement it by the Cox*Voinov law for the dynamics of the contact line. Our approach reproduces the relaxation of an axisymmetric droplet in experiments, which we initiate by instantaneously switching the uniform wettability of a substrate quantified by the equilibrium contact angle.

First, we investigate a droplet on substrates with planar-wave-like wettability profile by varying the speed an wave length of the pattern. When the profile moves slowly, it moves the droplet moves steadily forward. Above a critical pattern speed the droplet performs steady oscillations, the effective (time-averaged) velocity of which decreases with the square of the pattern speed.

Second, we investigate a droplet on substrates which deform periodically according to a planar-wave profile. We analyze the effective velocity again as a function of wave speed and length and investigate specifically the influence of curvature changes on droplet motion.

DY 25.6 Wed 10:45 H39

Spontaneous charging affects the motion of sliding drops — Xiaomei Li[1], Pravash Bista[1], Rüdiger Berger[1], Steffen Hardt[2], Holger Marschall[3], Hans-Jürgen Butt[1], and •Stefan A.L. Weber[1,4] — [1]MPI for Polymer Research, Ackermannweg 10, Mainz, Germany — [2]Institute for Nano- and Microfluidics, Technische Universität Darmstadt, Darmstadt, Germany — [3]Computational Multiphase Flows, Technische Universität Darmstadt, Darmstadt, Germany — [4]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany

The motion of water drops on surfaces is still far from being fully understood. Previous understanding is that drop motion is dictated by viscous dissipation and activated dynamics at the contact line. To accurately measure the forces experienced by moving drops, we imaged their trajectory when sliding down a tilted surface, and applied the relevant equations of motion [1]. We found that drop motion on low-permittivity substrates is substantially influenced by electrostatic forces. Our findings confirm that electrostatics must be taken into consideration for the description of the motion of water, aqueous electrolytes and ethylene glycol on hydrophobic surfaces. Our results are relevant for improving the control of drop motion in many applications, including printing, microfluidics, water management and triboelectric nanogenerators. [1] Li, X. et al. Spontaneous charging affects the motion of sliding drops. Nat. Phys. (2022).

DY 25.7 Wed 11:00 H39

Dynamic mesoscopic model for two-component compound drops — •Jan Diekmann and Uwe Thiele — Westfälische Wilhelms-Universität, Münster, Deutschland

We consider a mesoscopic model for two immiscible fluids forming two-layer liquid films or compound drops on a rigid solid substrate. The earlier macroscale description [1,2] is connected to our mesoscopic approach (building on [3]) via consistency conditions. Thereby we relate macroscale and mesoscale versions of the Young and Neumann relations at the liquid 1/solid/gas and liquid 1/liquid 2/gas contact lines, respectively. Furthermore, we employ the mesoscale model to investigate selected dewetting and coarsening processes for physically realistic parameters. The steady compound drops emerging from the time simulations are related to bifurcation scenarios determined via macroscale and mesoscale descriptions.

[1] L. Mahadevan, M. Adda-Bedia, and Y. Pomeau. "Four-phase merging in sessile compound drops". In: J. Fluid Mech. 451 (2002), pp. 411-420. [2] M. J. Neeson et al. "Compound sessile drops". In: Soft Matter 8 (2012), pp. 11042-11050. doi: 10.1039/c2sm26637g. [3] A. Pototsky et al. "Morphology changes in the evolution of liquid two-layer films". In: J. Chem. Phys. 122 (2005), p. 224711. doi: 10.1063/1.1927512. [4] Uwe Thiele et al. "Equilibrium contact angle and adsorption layer properties with surfactants". In: Langmuir 34.24 (2018), pp. 7210-7221.

DY 26: Critical Phenomena and Phase Transitions

Time: Wednesday 10:00–11:30 Location: H20

DY 26.1 Wed 10:00 H20

Percolation properties of the Ising spin glass in two dimensions — •Lambert Münster and Martin Weigel — Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

Cluster representations provide a framework to study critical phenomena from the geometrical perspective of percolation. Due to frustration the common Fortuin-Kasteleyn cluster representation of ferromagnets is not well suited to describe the spin-glass transition [1,2]. The order parameter of this transition is the overlap which is naturally defined with respect to two replicas. In the present work we hence study a two-replica cluster representation [3] of the two-dimensional Ising spin glass by performing Monte Carlo simulations at low temperatures. Our data is consistent with the existence of a zero-temperature percolation transition in agreement with the zero-temperature spin-glass transition in two dimensions. The overlap is proportional to the difference in density of the two largest clusters.

[1] V. Cataudella, G. Franzese, M. Nicodemi, A. Scala, and A. Coniglio, Phys. Rev. Lett. **72**, 1541, (1994).
[2] H. Fajen, A. K. Hartmann, and A. P. Young, Phys. Rev. E **102**, 012131, (2020).
[3] J. Machta, C. M. Newman, and D. L. Stein, J. Stat. Phys. **130**, 113, (2008).

DY 26.2 Wed 10:15 H20

Replica-symmetry breaking for directed polymers in correlated random media — •Alexander K. Hartmann — Institute of Physics, University of Oldenburg

The phase-space behavior of complex system can often be described by *replica-symmetry breaking* (RSB), as introduced by Giorgio Parisi for mean-field Ising spin glasses [1] and highlighted by the Nobel price 2021. Numerically, spin glasses and related problems are notoriously hard to study, such that models exhibiting RSB have been treated so far only for small sizes. Here, directed polymers on 1+1 dimensional lattices at temperature T are considered [2]. New ensembles with correlations of the disorder as well as fractal patterning are introduced [3]. This model allows for direct sampling in perfect thermal equilibrium for large system sizes of $N = L^2 = 32768 \times 32768 \approx 10^9$ sites. Fluctuations of the free energy and transverse extension are obtained and compared with the standard uncorrelated ensemble. The phase-space structure is studied via the distribution of overlaps, hierarchical clustering methods and analysis of ultrametricity. One ensemble shows a simple behavior like a ferromagnet. The other two ensembles exhibit indications for multiple RSB. In total, the present model ensembles offer convenient numerical access to comprehensively studying complex RSB-like behavior.
[1] G. Parisi, Phys. Rev. Lett. **43**, 1754 (1979)
[2] A. K. Hartmann, Big Practical Guide to Computer Simulations, World-Scientific, Singapore (2015)
[3] A. K. Hartmann, Euro. Phys. Lett. **137**, 41002 (2022)

DY 26.3 Wed 10:30 H20

Interplay of disorder and flat band geometry for generalized Lieb models in 3D with correlated order — •Jie Liu[1], Carlo Danieli[2], Jianxin Zhong[1], and Rudolf A. Römer[1,3,4] — [1]School of Physics and Optoelectronics, Xiangtan University, Xiangtan 411105, China — [2]MPI-PaKS, Nöthnitzer Strasse, Dresden, Germany — [3]Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom — [4]CY Advanced Studies and LPTM (UMR8089 of CNRS), CY Cergy-Paris Université, F-95302 Cergy-Pontoise, France

Uniform Anderson disorder in generalized 3D Lieb models gives rise to the existence of bounded mobility edges and destroys the macroscopic degeneracy of the compactly-localized states. We now introduce correlated order such that this degeneracy remains and the compactly-localized states are preserved. We obtain the energy-disorder phase diagrams via transfer matrix methods, computing the localization lengths and via sparse-matrix direct diagonalization, using r-value energy-level statistics. For suitably large disorders, we can finite-size scale both quantities and identify mobility edges with critical properties close to the standard Anderson transition in 3D. Intriguingly, the survival of the compactly-localized states lead to seemingly diverging mobility edges. For small disorder, however, a change from extended to localized behavior can be found upon decreasing disorder — leading to an unconventional "inverse Anderson" behavior.

DY 26.4 Wed 10:45 H20

Anomalous collective dynamics of auto-chemotactic populations — Jasper van der Kolk[1], •Florian Rasshofer[1], Richard Swiderski[1], Astik Haldar[2], Abhik Basu[2], and Erwin Frey[1,3] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 Munich, Germany — [2]Theory Division, Saha Institute of Nuclear Physics, HBNI, 1/AF Bidhannagar, Calcutta 700 064, West Bengal, India — [3]Max Planck School Matter to Life, Hofgartenstraße 8, 80539 Munich, Germany

While the role of local interactions in non-equilibrium phase transitions is well studied, a fundamental understanding of the effects of long-range interactions is lacking. In particular, we ask the question how long-ranged interactions can alter the universal behaviour close to an absorbing state. As a model system, we study the critical dynamics of reproducing agents subject to auto-chemotactic interactions and limited resources.

A renormalization group analysis reveals distinct scaling regimes for fast (attractive or repulsive) interactions; for slow signal transduction the dynamics is dominated by a diffusive fixed point. Further, we present a novel nonlinear mechanism that stabilizes the continuous transition against the emergence of a characteristic length scale due to a chemotactic collapse.

DY 26.5 Wed 11:00 H20

Population Annealing Monte Carlo Using the Rejection-Free n-Fold Way Update Applied to a Frustrated Ising Model on a Honeycomb Lattice — •Denis Gessert[1,2], Martin Weigel[1,3], and Wolfhard Janke[2] — [1]Centre for Fluid and Complex Systems, Coventry University, Coventry, CV1 5FB, United Kingdom — [2]Institut für Theoretische Physik, Leipzig University, Postfach 100920, 04009 Leipzig, Germany — [3]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Population annealing (PA) is a Monte Carlo method well suited for problems with a rough free energy landscape such as glassy systems. PA is similar to repeated simulated annealing, with the addition of a resampling step at each temperature. While a large population may to some extent compensate for imperfect equilibration, it is clear that PA must fail if almost no spins are flipped during equilibration.

This is the case in systems with a phase transition at a very low temperature where a high Metropolis rejection rate makes sampling phase space near infeasible. To overcome this slow-down we propose a combination of the PA framework with the rejection-free “n-fold way” update and achieve an exponential speed-up at low temperatures as compared to Metropolis.

To test our method we study the Ising model with competing ferromagnetic ($J_1 > 0$) nearest and antiferromagnetic ($J_2 < 0$) next-to-nearest neighbor interactions on a honeycomb lattice. As T_c becomes arbitrarily small when approaching the special point $J_2 = -J_1/4$ with $T_c = 0$ we consider this a good choice to test the efficacy of our method.

DY 26.6 Wed 11:15 H20

Critical behavior of the three-state random-field Potts model in three dimensions — Manoj Kumar[1], Varsha Banerjee[2], Sanjay Puri[3], and •Martin Weigel[1] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi – 110016, India — [3]School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067, India.

Enormous advances have been made in the past 20 years in our understanding of the random-field Ising model, and there is now consensus on many aspects of its behavior at least in thermal equilibrium. In contrast, little is known about its generalization to the random-field Potts model which has a number of important experimental realizations. Here we start filling this gap with an investigation of the three-state random-field Potts model in three dimensions. Building on the success of ground-state calculations for the Ising system, we use a recently developed approximate scheme based on *graph-cut methods* to

study the properties of the zero-temperature random fixed point of the system that determines the zero and non-zero temperature transition behavior. We find compelling evidence for a continuous phase transition. Implementing an extensive finite-size scaling (FSS) analysis, we determine the critical exponents and compare them to those of the random-field Ising model.

DY 27: Networks: From Topology to Dynamics (joint session SOE/BP/DY)

Time: Wednesday 10:15–12:45 Location: H11

DY 27.1 Wed 10:15 H11

Modeling tumor disease and sepsis by networks of adaptively coupled phase oscillators — •Eckehard Schöll[1,2,3], Jakub Sawicki[2], Rico Berner[1,4], and Thomas Löser[5] — [1]Institut für Theoretische Physik, TU Berlin, Germany — [2]Potsdam Institute for Climate Impact Research — [3]Bernstein Center for Computational Neuroscience Berlin — [4]Institut für Physik, HU Berlin — [5]Institut LOESER, Wettiner Straße 6, 04105 Leipzig

In this study, we provide a dynamical systems perspective to the modelling of pathological states induced by tumors or infection. A unified disease model is established using the innate immune system as the reference point. We propose a two-layer network model for carcinogenesis and sepsis based upon the interaction of parenchymal cells (organ tissue) and immune cells via cytokines, and the co-evolutionary dynamics of parenchymal, immune cells, and cytokines [1]. Our aim is to show that the complex cellular cooperation between parenchyma and stroma (immune layer) in the physiological and pathological case can be functionally described by a simple paradigmatic model of phase oscillators. By this, we explain carcinogenesis, tumor progression, and sepsis by destabilization of the healthy state (frequency synchronized), and emergence of a pathological state (multifrequency cluster). The coupled dynamics of parenchymal cells (metabolism) and nonspecific immune cells (reaction of innate immune system) are represented by nodes of a duplex layer. The cytokine interaction is modeled by adaptive coupling weights. [1] Sawicki, J., Berner, R., Löser, T., and Schöll, E., Frontiers Netw. Physiology 1,730385 (2022), arXiv:2106.13325v2.

DY 27.2 Wed 10:45 H11

Analysis of the Football Transfer Market Network — •Tobias Wand — WWU Münster — CeNoS Münster

Football clubs buy and sell players for millions of Euros and until Covid, their combined transfer values were growing steadily at an impressive rate. Instead of analysing their aggregated transfer activities, one can take a look at the topology of the network of player transfers: complex networks have already been used in various sciences [1] including research on sports [2] and provide a novel approach to investigate the football transfer market network and in particular the impact of Covid on football clubs.

[1] G. Caldarelli and A. Vespignani, "Large Scale Structure and Dynamics of Complex Networks". World Scientific Publishing, 2007.

[2] Arriaza-Ardiles et al. "Applying graphs and complex networks to football metric interpretation". Human Movement Science 57, 2018.

DY 27.3 Wed 11:00 H11

Variability in mesoscale structure inference using stochastic blockmodels — •Lena Mangold and Camille Roth — CNRS (Paris) / Centre Marc Bloch (Berlin)

Characterising the mesoscale structure of networks, in terms of patterns variously called communities, blocks, or clusters, has represented both a central issue and a key instrument in the study of complex systems. Clearly, distinct methods designed to detect different types of patterns may provide a variety of answers to the mesoscale structure. Yet, even multiple runs of a given method can sometimes yield diverse and conflicting results, posing challenges of model and partition selection. As an alternative to forcing a global consensus from a distribution of partitions (i.e. choosing one among many by maximising some objective), recent work has emphasised the importance of exploring the variability of partitions. Here we examine how a specific type of mesoscale structure (e.g. assortative communities or core-periphery) may be linked with more or less inconsistency in resulting partitions. We focus on Stochastic blockmodels (SBMs), initially proposed in mathematical sociology and increasingly used to infer mesoscale structure with a relatively general definition of similarity between nodes in the same group, and whose stochastic nature lends itself to the exploration of disagreement within populations of partitions. In particular, we generate families of synthetic networks in which we plant different types of mesoscale structures and explore the transitions between consensus and dissensus in the landscape of partitions over multiple SBM runs.

DY 27.4 Wed 11:15 H11

Extracting signed relations from interaction data — •Georges Andres, Giona Casiraghi, Giacomo Vaccario, and Frank Schweitzer — ETH Zürich, Chair of Systems Design, Switzerland

Social relations influence human interactions and hence, help to explain individual behaviours. Moreover, humans perceive patterns of signed relations, either positive (e.g., friendship) or negative (e.g., enmity), and adapt to them. Data about signed relations are rare, despite their importance for understanding phenomena at the community level. Interaction data is, however, more abundantly available, for example, about proximity or communication events. Interactions and relations change on different time scales; interactions are more volatile and evolve faster than relations. Using this, I will present an ensemble-based approach to infer pair-wise signed relations from interaction data and consequently construct a signed network from them. By studying different datasets on interactions and relations, e.g. between students, I will further evaluate the quality of the inferred networks. Subsequently, I will study the presence of structural balance in the studied communities, describing the cognitive dissonance ensuing from particular triadic constellations of signed relations. Bearing similarities to frustrations in spin systems, structural balance can now be analysed solely from interaction data thanks to the presented method, a task which was previously out of reach.

DY 27.5 Wed 11:45 H11

Disentangling homophily, community structure and triadic closure in networks — •Tiago Peixoto — Central European University, Vienna, Austria

Network homophily, the tendency of similar nodes to be connected, and transitivity, the tendency of two nodes being connected if they share a common neighbor, are conflated properties in network analysis, since one mechanism can drive the other. Here we present a generative model and corresponding inference procedure that is capable of distinguishing between both mechanisms. Our approach is based on a variation of the stochastic block model (SBM) with the addition of a triadic closure dynamics, and its inference can identify the most plausible mechanism responsible for the existence of every edge in the network, in addition to the underlying community structure itself, based only on the final observation of the network. We show how the method can evade the detection of spurious communities caused solely by the formation of triangles in the network, and how it can improve the performance of link prediction when compared to the pure version of the SBM without triadic closure.

[1] Tiago P. Peixoto, Disentangling homophily, community structure and triadic closure in networks, Phys. Rev. X 12, 011004 (2022)

DY 27.6 Wed 12:15 H11

Evolving networks towards complexity: an evolutionary optimization approach — Archan Mukhopadhyay and •Jens Christian Claussen — University of Birmingham, UK

Complexity measures for graphs have been proposed and compared [1,2] widely, but the question how to mathematically define complexity is less clear as for text strings where Lempel-Ziv and Kolmogorov complexity provide clear approaches. In complexity science, the notion of complexity implies distinction from regular structures (lattices) as well as from random structures (here: random graphs). This however has not lead to any constructive definition. Complexity measures therefore typically assess artefacts of complexity (in some cases quite successfully). Here we present a complementary computational approach: we utilize each complexity measure as a fitness function of an evolutionary algorithm, and investigate the properties of the resulting networks. The goal is a better understanding of the existing complexity measures, and to shed some light on (artificial) network evolution: what evolutionary goals lead to complexity?

DY 28: Extreme Events, Glasses and Miscellaneous

Time: Wednesday 11:15–13:00 Location: H19

DY 28.1 Wed 11:15 H19

Symmetries and zero modes in sample path large deviations — •Timo Schorlepp[1], Tobias Grafke[2], and Rainer Grauer[1] — [1]Institute for Theoretical Physics I, Ruhr-University Bochum, Bochum, Germany — [2]Mathematics Institute, University of Warwick, Coventry, United Kingdom

Sharp large deviation estimates for stochastic differential equations with small noise, based on minimizing the Freidlin-Wentzell action functional under appropriate boundary conditions, can be obtained by integrating certain matrix Riccati differential equations along the large deviation minimizers or instantons, either forward or backward in time. Previous works in this direction often rely on the existence of isolated minimizers with positive definite second variation. By adopting techniques from field theory and explicitly evaluating the large deviation prefactors as functional determinant ratios using Forman's theorem, we extend the approach to general systems where degenerate submanifolds of minimizers exist. The key technique for this is a boundary-type regularization of the second variation operator. This extension is particularly relevant if the system possesses continuous symmetries that are broken by the instantons. We find that removing the vanishing eigenvalues associated with the zero modes is possible within the Riccati formulation and amounts to modifying the initial or final conditions and evaluation of the Riccati matrices. We apply our results in multiple examples including a dynamical phase transition for the average surface height in short-time large deviations of the one-dimensional Kardar-Parisi-Zhang equation with flat initial profile.

DY 28.2 Wed 11:30 H19

Diffusivity dependence of the transition path ensemble — Lukas Kikuchi, Ronojoy Adhikari, and •Julian Kappler — DAMTP, Cambridge University, Cambridge, UK

Transition pathways of stochastic dynamical systems are typically approximated by instantons. Here we show, using a dynamical system containing two competing pathways, that at low-to-intermediate temperatures, instantons can fail to capture the most likely transition pathway. We construct an approximation which includes fluctuations around the instanton and, by comparing with the results of an accurate and efficient path-space Monte Carlo sampling method, find this approximation to hold for a wide range of temperatures. Our work delimits the applicability of large deviation theory and provides methods to probe these limits numerically.

DY 28.3 Wed 11:45 H19

Sampling Rare Event Energy Landscapes via a Birth-Death Process — •Benjamin Pampel[1], Simon Holbach[2], Lisa Hartung[2], and Omar Valsson[1,3] — [1]Max-Planck-Institute für Polymerforschung, Ackermannweg 10, 55128 Mainz — [2]Institut für Mathematik, Johannes Gutenberg-Universität Mainz, Staudingerweg 9, 55099 Mainz — [3]Department of Chemistry, University of North Texas, Denton, TX, USA

We investigate a novel sampling algorithm that augments Langevin dynamics with birth-death moves. This is a modification of a previously proposed algorithm [arXiv:1905.09863] that provides an approximation of a stochastic birth-death process for a particle-based implementation. The method connects multiple parallel Langevin dynamics simulations of the same system with a birth-death scheme to facilitate global sampling according to the equilibrium distribution. We investigate the algorithm theoretically, implement it into a custom molecular simulation code, and test it via numerical simulations. We also examine the behavior of the algorithm under change of parameters. In this process, we observe the desired sampling for all tested systems. We find that the performance of the method is independent of the intrinsic time scales and barriers of the system, which is favorable for systems with processes on long time scales.

DY 28.4 Wed 12:00 H19

MD simulations of partially frozen water in silica nanopores — •Sebastian Kloth and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

The properties of confined water are of enormous importance in nature and technology. In particular, the effects of partial freezing on structure and dynamics is highly relevant for, e.g. geology, cryopreservation and our understanding of the glass transition of water [1]. A powerful tool to study structural and dynamical properties of confined liquids are MD simulations [2]. We use this method to gain a better understanding of the effect of partial crystallization on the properties of confined water. A series of silica confinements with and without an artificially frozen crystalline core were prepared and the remaining liquid water layer was analyzed. Dynamics and structures of liquid layers with various thicknesses and their temperature dependencies are determined and compared to those with interfacial layers in the absence of a frozen crystalline core. We show that partial crystallization has substantial effects on the properties of confined water. Additionally the simulation results are used to calculate spectral densities of water dynamics for comparison with results of experimental studies. In particular, we explore which model for the functional form of the spectral density should be used in NMR spin-lattice relaxation studies on the dynamics of completely liquid or partially frozen water in nanopores.
[1] Cerveny, S. et al., Chem. Rev., **2016**, *116* (13) 7608-7625
[2] Horstmann, R. et al., Langmuir, **2022**, 10.1021/acs.langmuir.2c00521

DY 28.5 Wed 12:15 H19

Driven aging dynamics on sparse networks — •Benedikt Johannes Grüger[1], Diego Tapias[1], and Peter Sollich[1,2] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Department of Mathematics, King's College London, London WC2R 2LS, UK

We investigate the interaction of two paradigmatic ways of being out of equilibrium, aging and driving, in simple models of glassy dynamics. We specifically consider the Bouchaud model, where a system jumps between the numerous minima of a rough energy landscape in configuration space. As the temperature decreases, the system undergoes a dynamical phase transition, at which the relaxation time diverges. With an additional field, we then drive the system by biasing its dynamics towards higher/lower jumping activity. We investigate the spectrum of the (biased) master operator in that framework, using a population dynamics algorithm based on cavity theory that allows us to deduce statements about the thermodynamic limit. Combining this with extensive diagonalization we identify novel regimes in the bias-temperature phase diagram that are distinguished by the occurrence of different kinds of eigenvector localization and are linked to the existence of a spectral gap. We also present methodological advances in the form of novel strategies for operating the population dynamics algorithm.

DY 28.6 Wed 12:30 H19

Moiré-pattern evolution couples rotational and translational friction at crystalline interfaces — •Xin Cao[1], Andrea Silva[2,3], Emanuele Panizon[4], Andrea Vanossi[2,3], Nicola Manini[5], Erio Tosatti[2,3,4], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]CNR-IOM, Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, c/o SISSA, Via Bonomea 265, 34136, Trieste, Italy — [3]International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy — [4]The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34151 Trieste, Italy — [5]Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy

We experimentally and theoretically study the rotational dynamics and depinning of two-dimensional colloidal crystalline clusters on periodically corrugated surfaces under well-controlled torques. We demonstrate that the traversing of locally commensurate areas of the moiré pattern through the edges of clusters, which is hindered by potential barriers during cluster rotation, eventually controls its rotational depinning. The experimentally measured depinning thresholds as a function of cluster size strikingly collapse onto a universal theoretical curve which predicts a superlow-static-torque state for large clusters. We further reveal a cluster-size-independent rotation-translation depinning transition when lattice-matched clusters are driven jointly by a force and a torque. Our work provides guidelines to the design of nanomechanical devices that involve rotations on atomic surfaces.

DY 28.7 Wed 12:45 H19

Accurate dynamics from memory in chemical reactions with

small copy numbers — •Moshir Harsh and Peter Sollich — Institut für Theoretische Physik, Georg-August-Universität Göttingen

Chemical reactions in the regime of small copy numbers of species such as *gene* regulation or *protein* interaction networks show large fluctuations, making mean field solutions as given by mass action kinetics unreliable. Accurate calculations of the one and two-time quantities of these stochastic processes remain a challenging problem; numerical solutions to the master equation or stochastic simulations can be deployed, but these are computationally intensive and do not allow likelihood inference from dynamical trajectories.

Here, we present a method that captures the fluctuations beyond mean field using self-consistently determined *memory*: by integrating information from the past we can systematically improve our approximation for the dynamics of chemical reactions. This memory is not added ad-hoc, but can be shown to arise naturally by considering the effective action of the Doi-Peliti field theory of chemical reactions. The effective action is treated perturbatively but we can self-consistently resum a very large class of diagrams resulting in a stable expansion. We demonstrate this method and its accuracy on single and multi-species binary reactions across a range of parameter values. We show how this approach also opens a route to making inferences from experimentally measured dynamics.

DY 29: Invited Talk Eric Bertin

Time: Wednesday 12:00–12:30 Location: H18

Invited Talk DY 29.1 Wed 12:00 H18

Derivation of a continuum description of sheared jammed soft suspensions from particle dynamics — •Eric Bertin, Nicolas Cuny, and Romain Mari — Univ. Grenoble Alpes, CNRS, LIPhy, 38000 Grenoble, France

Jammed soft suspensions exhibit a rich phenomenology under deformation, including the existence of a yield stress and non-monotonous stress relaxations. Starting from the microscopic particle dynamics, we derive using a set of approximations a continuum description in terms of the macroscopic stress tensor (or more precisely, its traceless part) for given applied time-dependent deformations. The coefficients appearing in this equation are expressed in terms of the packing fraction and of particle-level parameters. This constitutive equation rooted in the microscopic dynamics qualitatively reproduces a number of salient features of the rheology of jammed soft suspensions, including the presence of yield stresses for both the shear component of the stress and the normal stress difference. Time-dependent protocols like the relaxation after a preshear are also considered, showing that a stronger preshear eventually leads to a more relaxed stress. This new methodology opens avenues for future developments, and involves physically more transparent approximations than the Mode Coupling approach.

DY 30: Energy Networks (joint session SOE/DY)

Time: Wednesday 12:45–13:15 Location: H11

DY 30.1 Wed 12:45 H11

Revealing drivers and risks for power grid frequency stability with explainable AI — •Benjamin Schäfer[1], Johannes Kruse[2,3], and Dirk Witthaut[2,3] — [1]Institute for Automation and Applied Informatics, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]Forschungszentrum Jülich, Institute for Energy and Climate Research-Systems Analysis and Technology Evaluation (IEK-STE), Jülich, Germany — [3]Institute for Theoretical Physics, University of Cologne, Köln, Germany

The transition to a sustainable energy system is challenging for the operation and stability of electric power systems as power generation becomes increasingly uncertain, grid loads increase, and their dynamical properties fundamentally change. At the same time, operational data are available at an unprecedented level of detail, enabling new methods of monitoring and control. To fully harness these data, advanced methods from machine learning must be used.

Here, we present explainable artificial intelligence (XAI) as a tool to quantify, predict, and explain essential aspects of power system operation and stability in three major European synchronous areas. We focus on the power grid frequency, which measures the balance of generation and load and thus provides the central observable for control and balancing. Combining XAI with domain knowledge, we identify the main drivers and stability risks, while our model and open dataset may enable further XAI research on power systems.

DY 30.2 Wed 13:00 H11

Cascading Failures and Critical Infrastructures in Future Renewable Power Systems — Franz Kaiser[1,2], Johannes Kruse[1,2], •Philipp C. Böttcher[1], Martha Maria Frysztacki[3], Tom Brown[3,4], and Dirk Witthaut[1,2] — [1]IEK-STE Forschungszentrum Jülich, Jülich, Germany — [2]THP Uni Köln, Köln, Germany — [3]KIT-IAI, Karlsruhe, Germany — [4]Institut für Energietechnik TU Berlin, Berlin, Germany

The world's power systems are undergoing a rapid transformation, shifting away from carbon-intensive power generation to renewable power sources. As a result, there is a growing importance of long-distance power transmission, while the intrinsic system inertia provided by thermal power plants decreases. This poses several challenges to the system such as accelerated dynamics and thus a higher control effort for transmission system operators. These developments make power grids more vulnerable to cascading failures, which may result in a splitting of the grid and eventually in a large-scale blackout. While large blackouts are rare but devastating events, several smaller splits were observed in recent years.

In this work, we use the state of the art open energy system model PyPSA to generate future energy systems and assess the risk of cascading failures and systems splits in the European power grid for different carbon reduction targets. We determine the likelihood of dangerous splits and discuss mitigation strategies.

DY 31: Active Matter 4 (joint session DY/BP/CPP)

Time: Wednesday 15:00–17:30 Location: H18

DY 31.1 Wed 15:00 H18

Clusters and fractals in non-reciprocally interacting colloids — •Sebastian Fehlinger and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Non-reciprocal interactions are widespread in nature. For the specific case of a binary mixture of passive particles, 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 based on phoretically interacting binary colloidal mixtures [1,2].

The focus of the present work is to understand the many body behaviour of active molecules. Using particle based simulations and continuum theory, we find that non-reciprocal attractions in a binary mixture of non-motile particles can destabilize the uniform disordered phase and lead to clusters which grow in time. Surprisingly, for a wide parameter range, the clusters only grow up to a certain size such that coarsening is arrested. We attribute this to an effective screening effect which hinges on the characteristic spatiotemporal organization of the two species within the clusters. In addition, remarkably, in a different parameter regime, we find porous macroclusters featuring significant holes and a fractal dimension which differs from the one expected for conventional diffusion limited aggregation.

[1]F. Schmidt et al. J. Chem. Phys. 150, 094905 (2019)
[2]J. Grauer et al. Nat. Commun. 12, 6005 (2021).

DY 31.2 Wed 15:15 H18

Analysis of transient dynamics of bioconvection in swimming algae — •Alexander Jarosik, Florian von Rüling, and Alexey Eremin — Otto-von-Guericke Universität, Magdeburg, Germany

Swimming unicellular algae Chlamydomonas reinhardtii exposed to light form intricate hydrodynamic instability patterns called bioconvection. High-density plumes of cells are formed in the top layer, descend to the container's bottom, and rise again to the top. This instability arises from coupling between the gyro- and phototactic behaviour of the cells, their physical properties and the flow. In this work, we analyse the microswimmer's dynamics as a function of the cell density, confinement of the environment and light. The transient behaviour of the plume formation is analysed using the Continuous Wavelet Transformation (CWT). We demonstrate that the plume formation can be controlled by local illumination.

DY 31.3 Wed 15:30 H18

Optimal turbulent transport in microswimmer suspensions — •Henning Reinken[1], Sabine H. L. Klapp[1], and Michael Wilczek[2] — [1]Technische Universität Berlin — [2]Universität Bayreuth

Microwsimmer suspensions, a paradigmatic example of an active fluid, self-organize into complex spatio-temporal flow patterns, including regular vortex lattices and mesoscale turbulence. This work investigates the transport properties of these suspensions by tracking the diffusive motion of passive tracers in the turbulent flow. We apply a continuum model for the effective microswimmer velocity field [1,2], where the dynamics is governed by the competition between relaxation to a regular vortex lattice and destabilization by nonlinear advection. Varying the strength of nonlinear advection, we observe two qualitatively different regimes of flow transport that we distinguish with the help of the dimensionless Kubo number K, which compares different time scales. Right above the transition to turbulence, the flow field evolves very slowly ($K \gg 1$) and the spatial vortex structures lead to dominant trapping effects. In contrast, for large advection strength, much faster dynamics ($K \ll 1$) leads to transport properties completely determined by the temporal correlations of the flow. In between ($K \approx 1$), we observe a regime of optimal transport, where the diffusion coefficient reaches a maximum.

[1] Reinken, Klapp, Bär, Heidenreich, Phys. Rev. E **97**, 022613 (2018)
[2] James, Bos, Wilczek, Phys. Rev. Fluids **3**, 061101(R) (2018).

DY 31.4 Wed 15:45 H18

Interfacial activity dynamics of confined active droplets — •Prashanth Ramesh[1,2], Babak Vajdi Hokmabad[1], Arnold J.T.M. Mathijssen[3], Dmitri O. Pushkin[4], and Corinna C. Maass[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization — [2]University of Twente — [3]University of Pennsylvania — [4]University of York

Active emulsions exhibit a complex hydrodynamic mode spectrum driven by chemical advection-diffusion instabilities. We study such an active emulsion consisting of oil droplets that dynamically solubilize in a supramicellar aqueous surfactant solution. It has been predicted that the interaction with self-generated chemical fields leads to multistable higher-mode flow fields and chemorepulsive phenomena. To investigate such chemodynamic effects, we study cylindrical droplets pinned between the top and bottom surfaces of a microfluidic reservoir, such that they only produce pumping flows, while we simultaneously quantify the chemical concentration field and the hydrodynamic velocity field. With increasing droplet radius we observe: vortical structures generated by the droplet migrating around the interface, bistability between a dipolar and quadrupolar flow mode, and, eventually, a transition to multipolar modes. We further measured flow fields by particle image velocimetry and compared them to a hydrodynamic model based on a Brinkman squirmer. A simultaneous quantification of the flow fields and oil-filled micelle distribution suggests that a local buildup of chemical products leads to a saturation of the surface, which affects the propulsion mechanism and eventually suppresses all activity.

DY 31.5 Wed 16:00 H18

Hydrodynamics and fluctuations in bacterial models — •Subhadip Chakraborti — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Motivated by a biological example of the persistent motion of bacteria, we propose two one-dimensional models of active lattice gases with hardcore interactions. Using macroscopic fluctuation theory (MFT), we analytically derive hydrodynamics for those models and calculate two density-dependent transport coefficients – the bulk-diffusion coefficient and the conductivity, and verify the Einstein relation (ER) by comparing the ratio of those transport coefficients with subsystem number fluctuation. The first model consisting of particles with competing mechanisms of short and long-range hopping obeys the Einstein relation, and exhibits, in the limit of infinite range hopping, upon tuning density (or activity), a 'superfluid' transition from a finitely conducting state to an infinitely conducting one. Interestingly, the bulk-diffusion coefficient remains constant throughout. The diverging conductivity induces 'giant' number fluctuations in the system. In the second model, consisting of hardcore run and tumble particles with persistent motion in one direction decided by an associated spin variable until the direction of spin is reversed, we perform a similar calculation and find that the Einstein relation is violated. This analytic framework could be useful for a better understanding of the collective behavior of many biological systems such as bacterial colonies and other multicellular aggregates, in the context of dynamics and transport properties.

15 min. break

DY 31.6 Wed 16:30 H18

Shearing an Active Glass — •Rituparno Mandal and Peter Sollich — Institut für Theoretische Physik, Göttingen, Germany

Recent experiments and simulations have revealed glassy features of cytoplasm, tissues and dense assemblies of self propelled colloids. This prompts the fundamental question of whether non-equilibrium (active) amorphous materials are essentially equivalent to their passive counterparts, or whether they can present qualitatively different behaviour. To tackle this challenge we investigate the yielding and mechanical behaviour of a model active glass former, a Kob-Andersen glass in two dimensions where each particle is driven by a constant propulsion force whose direction varies diffusively over time. Using extensive Molecular Dynamics simulations, we focus in particular on the effects of the intermittent dynamics in the regime of highly persistent activity and reveal a novel type of shear induced orientational ordering in the system.

DY 31.7 Wed 16:45 H18

Active motion with varying self propulsion — Lorenzo Caprini[1], Alexander R. Sprenger[1], Umberto M. B. Marconi[2], Hartmut Löwen[1], and •René Wittmann[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine Universität Düssel-

dorf, Germany — [2]School of Sciences and Technology, University of Camerino, Italy

Active Brownian Particles (ABPs), commonly perceived as the standard model for (dry) active motion, are characterized by a constant self-propulsion velocity along the direction of a unit vector which performs rotational diffusion. In nature, however, the swim velocity is usually not a constant in time and space. Here, we present a generic form of the equations of motion of active particles, which account for two aspects of varying self propulsion. First, we introduce a general stochastic process with fluctuating modulus of the self-propulsion vector, which defines a parental active model (PAM). We argue that the two well-known models of ABPs and Active Ornstein-Uhlenbeck Particles (AOUPs) emerge as limiting cases of the PAM [1], i.e., they are rather sisters than cousins. Second, we demonstrate that a position-dependent swim-velocity field can be consistently introduced for any self-propulsion mechanism [2]. Finally, we discuss the effects of varying self propulsion in external confinement [1,3] and predict the stationary probability distributions in terms of effective interactions [3].

[1] L. Caprini et al., J. Chem. Phys. 156, 071102 (2022).
[2] L. Caprini et al., Soft Matter, 18, 1412 (2022).
[3] L. Caprini et al., arXiv:2203.00603 (2022).

DY 31.8 Wed 17:00 H18

Perturbing the athermal jamming transition by activity — •Michael Schmiedeberg — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

By minimizing the interaction energy in a soft sphere system without crossing energy barriers the discontinuous athermal jamming transion can be observed at a packing fraction of about 0.64 in three dimensions [1]. We consider the jamming of active particles where the activity corresponds to a perturbation to the athermal jamming process. We find that due to the activity the transition becomes continuous and the transition packing fraction might occur at a different density [2]. The critical exponents agree to those of the universality class of directed percolation. As a consequence, athermal jamming of passive particles seems to be a (singular) limit of the jamming transition in an active system. Note that other perturbation like thermal fluctuations lead to a similar behavior [3]. Therefore, athermal active particles can be seen as a prototype system that leads to new insights how jamming with perturbations (as also studied in [2-5]) can be related to glassy dynamics.

[1] C.S. O'Hern et al., Phys. Rev. Lett. 88, 075507 (2002) and Phys. Rev. E 68, 011306 (2003).
[2] M. Maiti and M. Schmiedeberg, EPL 126, 46002 (2019).
[3] M. Maiti and M. Schmiedeberg, Scientific Reports 8, 1837 (2018); for 2D: Eur. Phys. J. E 42, 38 (2019).
[4] L. Milz and M. Schmiedeberg, Phys. Rev. E 88, 062308 (2013).
[5] S. Wilken et al., Phys. Rev. Lett. 127, 038002 (2021).

DY 31.9 Wed 17:15 H18

Non-equilibrium phase separation in mixtures of catalytically active particles: size dispersity and screening effects — •Vincent Ouazan-Reboul[1], Jaime Agudo-Canalejo[1], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK

Biomolecular condensates in cells are often rich in catalytically active enzymes. This is particularly true in the case of the large enzymatic complexes known as metabolons, which contain different enzymes that participate in the same catalytic pathway. One possible explanation for this self-organization is the combination of the catalytic activity of the enzymes and a chemotactic response to gradients of their substrate, which leads to a substrate-mediated effective interaction between enzymes. These interactions constitute a purely non-equilibrium effect and show exotic features such as non-reciprocity. Here, we analytically study a model describing the phase separation of a mixture of such catalytically active particles. We show that a Michaelis-Menten-like dependence of the particles' activities manifests itself as a screening of the interactions, and that a mixture of two differently sized active species can exhibit phase separation with transient oscillations. We also derive a rich stability phase diagram for a mixture of two species with both concentration-dependent activity and size dispersity.

DY 32: Invited Talk Stephan Weiss

Time: Wednesday 15:00–15:30 Location: H19

Invited Talk DY 32.1 Wed 15:00 H19

Large scale patterns in turbulent Rayleigh-Bénard convection — •Stephan Weiss — DLR Göttingen — MPI f. Dyn. & Self-Org.

Thermal convection is one of the most important heat transport mechanisms and the driving force behind large scale flows in geo- and astrophysics. It is mostly studied in the Rayleigh-Bénard (RB) setup, where a horizontal fluid layer is heated from below and cooled from above. RB convection is a model system not only to study transport phenomena in turbulent flows under strong driving, but also to study pattern formation as it exhibits regular laminar flow patterns under weak thermal driving. Turbulent RB convection is usually studied experimentally and numerically in containers of small aspect ratios between their lateral size (L) and their height (H). Rather recently, however, investigations have also focused on RB convection in laterally extended systems, as it was found that the time-averaged mean velocity resembles the laminar pattern under weak driving. In my talk I will first discuss some recent developments in the research of large scale patterns in RB convection. Then I will present our own results from volumetric spatially velocity measurements in a rectangular RB cell with a square horizontal cross-section and an aspect ratio $\Gamma = L/H = 16$. Via Lagrangian particle tracking, we have measured the velocity and acceleration of up to 300,000 fluorescent microspheres simultaneously and have calculated the entire three-dimensional velocity field with a resolution of about the Kolmogorov length. From these data, we can determine the large scale patterns, as well as their morphology and follow their slow temporal evolution.

DY 33: Invited Talk Anatoli Polkovnikov

Time: Wednesday 15:00–15:30 Location: H20

Invited Talk DY 33.1 Wed 15:00 H20

Detecting dynamical quantum phase transitions by string observables — •Anatoli Polkovnikov[1], Amit Dutta[2], and Souvik Bandyopadhyay[2] — [1]Boston University, Boston, USA — [2]IIT Kanpur, India

Dynamical quantum phase transitions (DQPT) were proposed as singularities developing in time following a quantum quench in the return amplitude or the Loschmidt echo. They have close connection with Fisher zeros of the partition function extended to imaginary temperatures (real time). Because the Loschmidt echo is hard to measure it is not easy to observe DQPT experimentally. In this talk I will explain how one can detect DQPT both as a function of time and as a function of quench amplitude in finite size string observables. These findings are in very good agreement with an experiment by J. Zhang et. al. Nature 551, 601 (2017) performed in a trapped ion simulator.

DY 34: Fluid Physics: Turbulence and Convection

Time: Wednesday 15:30–17:15 Location: H19

DY 34.1 Wed 15:30 H19

Ejection of marine microplastics by raindrops: A computational and experimental study — •Moritz Lehmann[1], Lisa Marie Oehlschlägel[2], Fabian Häusl[1], Andreas Held[2], and Stephan Gekle[1] — [1]Biofluid Simulation and Modeling - Theoretische Physik VI, Universität Bayreuth — [2]Umweltchemie und Luftreinhaltung, Technische Universität Berlin

Raindrops impacting water surfaces such as lakes or oceans produce myriads of tiny droplets which are ejected into the atmosphere at very high speeds. Here we combine computer simulations and experimental measurements to investigate whether these droplets can serve as transport vehicles for the transition of microplastic particles with diameters of a few tens of micrometers from ocean water to the atmosphere. Using the Volume-of-Fluid lattice Boltzmann method, extended by the immersed-boundary method, we performed more than 1600 raindrop impact simulations and provide a detailed statistical analysis on the ejected droplets. Using typical sizes and velocities of real-world raindrops, we simulate straight impacts with various raindrop diameters as well as oblique impacts. We find that a 4 mm diameter raindrop impact on average ejects more than 167 droplets. We show that these droplets indeed contain microplastic concentrations similar to the ocean water within a few millimeters below the surface. To further assess the plausibility of our simulation results, we conduct a series of laboratory experiments, where we find that microplastic particles are indeed contained in the spray. Based on our results and known data, we estimate the global relevance of this transport mechanism.

DY 34.2 Wed 15:45 H19

Transition between 2D and 3D rotating incompressible convection in direct numerical simulations — •Kevin Lüdemann and Andreas Tilgner — Institute of Astrophysics and Geophysics, Göttingen, Germany

Direct numerical simulations of an incompressible fluid with a Prandtl number of 0.7 are used to investigate differences between exact 2D and 3D convection. The fluid is rotating about a direction perpendicular to the direction of gravity (centrifugal gravity) and zonal flow is suppressed by horizontal walls in a container with an aspect ratio of 0.5. The convection is controlled by a Rayleigh number ranging from 10^4 to 10^9 and rotation is characterised by the Ekman number ranging from 10^{-1} down to 10^{-5}. Due to the Taylor-Proudman theorem, the convective flow will be restrained to the plane perpendicular to the direction of rotation at high rotation rates. This behaviour will break down once convective driving and therefore kinetic energy is large enough. Thermal transport and kinetic energy density show different scalings for the 2D and 3D flow. The stability theory of a vortex with elliptical streamlines is tailored to the geometry in order to explain the transition. Ultimately, a dependence of the Reynolds number on the Rossby number is found $\mathrm{Re} \propto \mathrm{Ro}^{-2}$ for small Rossby numbers. Both are based on the RMS velocity of the vortex.

15 min. break

DY 34.3 Wed 16:15 H19

The onset of non-Gaussian velocity gradient statistics in low-Reynolds number flows — •Maurizio Carbone[1] and Michael Wilczek[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]Theoretical Physics I, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

The Reynolds number prescribes the range of active scales involved in a turbulent flow. Stirring a fluid through a Gaussian forcing at vanishingly small Reynolds produces a multi-point Gaussian field, while flows at higher Reynolds exhibit non-Gaussianity, cascades, anomalous scaling and preferential alignments. Recent works (Yakhot and Donzis, Phys. Rev. Lett. 2017) showed that low-Reynolds flows exhibit features of high-Reynolds turbulence.

We address the onset of turbulent features in low-Reynolds flows by combining a perturbation theory of the full Navier-Stokes equations (Wyld, Ann. Phys. 1961) with the Lagrangian modelling of velocity gradients along fluid particle trajectories (Meneveau, Annu. Rev. Fluid Mech. 2011). We construct a stochastic model for the velocity gradient in which all the model coefficients follow directly from the Navier-Stokes equations. The associated Fokker-Planck equation for the single-time velocity gradient probability density admits analytic solutions which show the onset of non-Gaussianity: skewness, intermittency and preferential alignments arise in the gradients statistics as the Reynolds number increases. The results are in excellent agreement with direct numerical simulations of low-Reynolds flows.

DY 34.4 Wed 16:30 H19

Temporal large-scale intermittency and its impact on flow statistics — •Lukas Bentkamp[1,2] and Michael Wilczek[1,2] — [1]Theoretical Physics I, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth — [2]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen

Turbulent flows in three dimensions are characterized by the transport of energy from large to small scales, the so-called energy cascade. Since the small scales are the result of the nonlinear dynamics across the scales of the energy cascade, they are often thought of as universal and independent of the large scales. However, as famously remarked by Landau in 1959, sufficiently slow variations of the large scales should nonetheless be expected to impact small-scale statistics. Such variations, often termed large-scale intermittency, are almost inevitable in experiments and even in simulations, while differing from flow to flow.

Here we evaluate the impact of temporal large-scale fluctuations on velocity, velocity gradient, and acceleration statistics by introducing controlled variations of the energy injection rate into direct numerical simulations of turbulence. We find that slow variations can have a strong impact on flow statistics, amplifying the tails of the measured distributions. We also show that the stronger tails can be accounted for by superposing an ensemble of stationary flows such that the temporal variations of an appropriate flow measure such as the energy dissipation rate are matched. Overall, our work demonstrates that in order to ensure comparability of statistical results in turbulence, large-scale intermittency needs to be taken into account.

DY 34.5 Wed 16:45 H19

Towards an effective description of turbulent superstructures in simple shear flows — •Fabián Álvarez-Garrido and Michael Wilczek — Theoretical Physics I, University of Bayreuth, Bayreuth

Turbulent flows driven by large-scale forces such as convection, shear, or rotation may display large-scale coherent flows, namely turbulent superstructures, coexisting with fully developed turbulence on the small scales. A complete description of these flows involves innumerable de-

grees of freedom, yet turbulent superstructures seem to evolve according to a comparably lower-dimensional set of equations. In addition, despite the ubiquity of turbulent superstructures, their interplay with the smaller scales is not yet fully understood. We study a simple shear-driven flow, the three-dimensional Kolmogorov flow. The large scales in this flow feature the formation of large-scale vortex pairs. Moreover, the system exhibits permanent dynamics between states having a different number of vortex pairs. Employing amplitude equations, we characterize the dynamics of the large scales close to the onset of the vortex pairs. We show that the dynamics close to the onset correspond to the one of a two-dimensional flow. Furthermore, we show that far from the onset, the derived model captures the structure of the large-scale vortices. Based on data from direct numerical simulations, we introduce new stochastic terms to these amplitude equations to model the contribution of the small scales to the dynamics of the large ones. These modified amplitude equations can qualitatively reproduce the dynamics of these large-scale vortex pairs and shed light on the role of small-scale turbulence in the formation of turbulent superstructures.

DY 34.6 Wed 17:00 H19

3D simulation of convection patterns in dry salt lakes — •Lucas Goehring[1], Matthew Threadgold[2], Cédric Beaume[2], and Steve Tobias[2] — [1]Nottingham Trent University, Nottingham, UK — [2]University of Leeds, Leeds, UK

Salt deserts are some of the most extreme and beautiful landscapes in the world–flat silver-white crystalline plains covered with bizarre and seemingly unnatural shapes. The most prominent feature of these fantastic landscapes is a characteristic tiling of polygons, formed by ridges in the salt-encrusted surface, and always a few meters across. Recently, a dynamical model has been proposed to explain their formation as the surface expression of buoyancy-driven convection happening in the wet salty soil beneath the desert surface. Here, we present a 3D numerical model of the salt lake problem, where a fluid-saturated porous medium is subject to a constant surface evaporation, mimicking the conditions of a desert with an underground aquifer near the surface. We look in turn at the initial instabilities expected in this system, and how they will evolve in time into a dynamical steady state. In this we focus on identifying the patterns that develop in the model, and exploring how the surface flux of salinity depends on the driving parameters.

DY 35: Quantum Chaos and Coherent Dynamics

Time: Wednesday 15:30–18:00 Location: H20

DY 35.1 Wed 15:30 H20

THz-induced high-order harmonic generation and nonlinear transport in graphene — •Wenwen Mao[1], Angel Rubio[1,2], and Shunsuke A. Sato[3,1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), Flatiron Institute, 162 Fifth Avenue, New York, NY 10010, USA — [3]Center for Computational Sciences, University of Tsukuba, Tsukuba 305-8577, Japan

Employing the quantum master equation with phenomenological relaxation, we theoretically study the nonequilibrium dynamics of THz-induced high-order harmonic generation in graphene. We first performed fully dynamical simulation to investiget the high-order harmonic generation in graphene induced by THz laser fields. We found that the emitted harmonics is enhanced with the increase in the chemical potential, and this observation is consistent with the recent experiments. Then we introduce a quasi-static picture to develop the microscopic understanding of the THz-induced currents and the population distribution of conduction band in graphene from the viewpoint of a nonequilibrium picture of electron dynamics. The nonlinear electric conductivity of graphene is also investigated under static electric fields for various field strength and chemical potential shifts. The impact of electron temperature change is also investigated to compare with the thermodynamic model in the previous work.

DY 35.2 Wed 15:45 H20

Explicit expressions for stationary states of the Lindblad equation for a finite state space — •Bernd Michael Fernengel — Technische Universität Darmstadt, Darmstadt, Germany

The Gorini-Kossakowski-Sudarshan-Lindblad Equation describes the time evolution of the probabilities of and the coherences between the quantum mechanical states. It is often used to model open quantum systems. We give explicit 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 shows a continuous time evolution, which is interrupted by stochastic jumps. We discuss differences to the classical case and conditions, under which the Lindblad equation is asymptotically stable (also called 'relaxing').

DY 35.3 Wed 16:00 H20

Eigenstate entanglement in coupled kicked spin chains with chaotic dynamics — •Tabea Herrmann, Maximilian F. I. Kieler, and Arnd Bäcker — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

We study the behaviour of the eigenstate entanglement in two coupled quantum chaotic kicked spin chains in dependence on the coupling strength. It is demonstrated that a random matrix transition ensemble explains the transition from the uncoupled case to strong coupling. Remarkably, the numerical results can be described by an extended perturbation theory which was introduced for the case of two coupled chaotic one-body-systems.

DY 35.4 Wed 16:15 H20

Quantum chaos in microwave cavities with mixed dynamics — •Lennart Anderson and Andreas Wieck — Angewandte Festkörperphysik, Ruhr-Universität Bochum

Based on the analogy of the Schrödinger equation with Dirichlet boundary conditions and the Helmholtz equation for a flat resonator, it is possible to study the dynamical and statistical properties of quantum billiards experimentally in the quasi-classical limit. Billiards, i.e. dynamical systems in which a particle moves ballistically and gets reflected by hard walls, provide a very simple model system, since the entire dynamics only depends on the geometry of the boundary. We investigate Hamiltonian systems with divided phase space, i.e. systems enabling a continuous transition from completely regular to completely chaotic dynamics, like the mushroom billiard, introduced by L. Bunimovich, in the quantum regime. Generalizations of the mushroom billiard and further geometries, i.e. those ranging from convex to non-convex domains, are considered. We further discuss the experimental setup and the impact of parameters like the conductivity of the resonator.

15 min. break

DY 35.5 Wed 16:45 H20

NQCDynamics.jl: Nonadiabatic quantum classical dynamics in the Julia language — •James Gardner[1], Oscar A. Douglas-Gallardo[1], Wojciech G. Stark[1], Julia Westermayr[1], Svenja M. Janke[1,2], Scott Habershon[1], and Reinhard J. Maurer[1] — [1]Department of Chemistry, University of Warwick, United Kingdom — [2]Institute of Advanced Study, University of Warwick, United Kingdom

Accurate and efficient methods to simulate nonadiabatic and quantum nuclear effects in high-dimensional and dissipative systems are crucial for the prediction of chemical dynamics in the condensed phase. To facilitate effective development, code sharing, and uptake of newly developed dynamics methods, it is important that software implementations can be easily accessed and built upon. In this talk, I will present the NQCDynamics.jl package, which provides a Julia language framework for established and emerging methods for performing semiclassical and mixed quantum-classical dynamics in the condensed phase. The code provides several interfaces to existing atomistic simulation frameworks, electronic structure codes, and machine learning representations. In addition to the existing methods, the package enables the development and deployment of new dynamics methods for condensed phase quantum dynamics, which I will show using examples based on model Hamiltonians and full-dimensional ab-initio systems.

DY 35.6 Wed 17:00 H20

Metastability and quantum coherence-assisted sensing in interacting parallel quantum dots — •Stephanie Matern[1], Katarzyna Macieszczak[2], Simon Wozny[1], and Martin Leijnse[1] — [1]NanoLund and Solid State Physics, Lund University, Box 118, 22100 Lund, Sweden — [2]TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Ave., Cambridge CB3 0HE, United Kingdom

We study the transient dynamics of two interacting parallel quantum dots weakly coupled to macroscopic leads to gain access to the non-equilibrium transport properties. The stationary state current of this quantum system is known to be sensitive to perturbations much smaller than any other energy scale in the system, specifically compared to the system-lead coupling and the temperature. We show that this is due to a bistable point which leads to a regime in the dynamics where the system exhibits metastability and the dynamics is described as classical dynamics between two metastable phases. The competition of those two metastable phases explain the sensitive behaviour of the stationary current towards small perturbations. We show that this behaviour bears the potential of utilizing the parallel dot as charge sensor which makes use of the quantum coherence effects to achieve a high sensitivity that is not limited by temperature. We analyse the sensitivity in terms of the current signal to noise ratio and find that the parallel dots outperform an analogous single dot setup for a wide range of parameters.

DY 35.7 Wed 17:15 H20

Classical and Quantum Dynamics in Resonance Channels — •Jan Robert Schmidt, Arnd Bäcker, and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

In higher-dimensional Hamiltonian systems resonance channels play a prominent role for chaotic transport. It is typically slow due to Arnold diffusion, leading quantum mechanically to dynamical localization. Resonance channels widen as they approach the chaotic sea. We show that this geometry induces classically a drift. Quantum mechanically this leads to a transition from localization to delocalization if the drift is strong enough. This is quantified using a transition parameter depending on classical quantities only. Numerically this is confirmed for a 4D symplectic map.

DY 35.8 Wed 17:30 H20

Coupling in Optical Microcavity-Arrays — •Tom Rodemund and Martina Hentschel — Department of Physics, Technische Universität Chemnitz, Chemnitz, Germany

Optical microcavities capture light by total internal reflection in so-called whispering-gallery modes. Deformed disk-shaped microcavities, for example of Limaçon shape, allow one to keep high Q-factors while manipulating the far-field emission via the resonator geometry, thereby allowing for a wide range of applications from microlasers to sensors.

Coupling of several microdisk resonators enhances the possibilities to tame light considerably [1]. Depending on the number and distance of the coupled cavities, the far-field characteristics vary tremendously and can even be reversed [1]. Here, we investigate the underlying mechanisms. To this end we use phase-space methods and analyze the resonance wave functions in real space as well as the corresponding Husimi functions to characterize the coupling behavior. We employ ideas from ray-wave correspondence to deepen our insight by establishing a relation to the nonlinear light ray dynamics and its fingerprint in the Poincaré surface of section.

[1] J. Kreismann et al., Phys. Rev. Res. 1, 033171 (2019).

DY 35.9 Wed 17:45 H20

Time-dependent Redfield and Lindblad equations with effective time-dependent temperature — •Nikodem Szpak, Lukas Litzba, Eric Kleinherbers, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

For a quantum system coupled to environment we apply the first Markov approximation and write the Redfield equation at the first order in the system-environment coupling. Then, we evaluate the remaining time-dependent integral and approximate it uniformly for all times, temperatures and energies by one simple analytical function which corresponds to the Fermi-Dirac distribution with time-dependent effective temperature T(t). Thus, we obtain a new Redfield equation with time-dependent effective temperature. A consecutive approximation brings it to the Lindblad equation with time-dependent Lindblad operators whose time-dependence enters solely via T(t). The variation of the effective temperature T(t) reflects the sudden switch-on of the system-environment interaction at the beginning and becomes high at early times to eventually fall to the true environment temperature T. We discuss possible physical effects and their measurability in some simple examples.

DY 36: Quantum Coherence and Quantum Information Systems (joint session TT/DY)

Time: Thursday 9:30–12:30 Location: H22

DY 36.1 Thu 9:30 H22

Design of a granular aluminum Fluxonium qubit in a coplanar waveguide architecture — •Patrick Paluch, Martin Spiecker, Nicolas Gosling, Alexandru Ionita, Simon Günzler, Daria Gusenkova, Dennis Rieger, Ivan Takmakov, Francesco Valenti, Patrick Winkel, Wolfgang Wernsdorfer, and Ioan-Mihai Pop — Karlsruhe Institute of Technology

Fluxonium qubits are often embedded in rectangular waveguides which dilute the electric field and favor high coherence [1,2]. However, this configuration complicates in-situ flux gates and multi-qubit experiments. Here, we present a fluxonium qubit placed in a coplanar waveguide architecture with an integrated fast-flux coil, surrounded by a normal metal ground plane. The superinductor is made out of granular aluminum (grAl) [3] and the use of a comparably large silver ground plane potentially decreases the number of quasiparticles in the system via phonon trapping [4].

[1] Pop et al., Nature 508, 369 (2014)
[2] Somoroff et al., arXiv:2103.08578 (2021)
[3] Grünhaupt et al., Nat. Mater. 18, 816 (2019)
[4] Henriques et al., Appl. Phys. Lett. 115, 212601 (2019)

DY 36.2 Thu 9:45 H22

Gralmonium: Granular aluminum nano-junction Fluxonium qubit — •Dennis Rieger, Simon Günzler, Martin Spiecker, Patrick Paluch, Patrick Winkel, Lothar Hahn, Judith K. Hohmann, Andreas Bacher, Wolfgang Wernsdorfer, and Ioan M. Pop — Karlsruhe Institute of Technology, Germany

Mesoscopic Josephson junctions (JJs), consisting of overlapping superconducting electrodes separated by a nanometer thin oxide layer, provide a precious source of nonlinearity for superconducting quantum circuits and are at the heart of state-of-the-art qubits, such as the transmon and fluxonium. Here, we show that in a fluxonium qubit the role of the JJ can also be played by a lithographically defined, self-structured granular aluminum (grAl) nano-junction: a superconductor-insulator-superconductor (SIS) JJ obtained in a single layer, zero-angle evaporation. The measured spectrum of the resulting qubit, which we nickname gralmonium, is indistinguishable from the one of a standard fluxonium qubit. Remarkably, the lack of a mesoscopic parallel plate capacitor gives rise to an intrinsically large grAl nano-junction charging energy in the range of $10 - 100\,\mathrm{GHz}$, comparable to its Josephson energy E_J. We measure average energy relaxation times of $T_1 = 10\,\mu\mathrm{s}$ and Hahn echo coherence times of $T_2^{\mathrm{echo}} = 9\mu\mathrm{s}$. The exponential sensitivity of the gralmonium to the E_J of the grAl nano-junction provides a highly susceptible detector. Indeed, we observe spontaneous jumps of the value of E_J on timescales from milliseconds to days, which offer a powerful diagnostics tool for microscopic defects in superconducting materials.

DY 36.3 Thu 10:00 H22

Quantum dynamics of disordered arrays of interacting superconducting qubits: Signatures of quantum collective states — Mikhail Fistul, •Oliver Neyenhuys, Antonia Bocaz, and Ilya Eremin — Theoretische Physik III, Ruhr-Universität Bochum, Bochum 44801, Germany

We study theoretically the collective quantum dynamics occurring in various interacting superconducting qubits arrays (SQAs) in the presence of a spread of individual qubit frequencies. The interaction is

provided by mutual inductive coupling between adjacent qubits (short-range Ising interaction) or inductive coupling to a low-dissipative resonator (long-range exchange interaction). In the absence of interaction the Fourier transform of the temporal correlation function of the total polarization (z-projection of the total spin), i.e. the dynamic susceptibility $C(\omega)$, demonstrates a set of sharp small magnitude resonances corresponding to the transitions of individual superconducting qubits. We show that even a weak interaction between qubits can overcome the disorder with a simultaneous formation of the collective excited states. This collective behavior manifests itself by a single large resonance in $C(\omega)$. In the presence of a weak non-resonant microwave photon field in the low-dissipative resonator, the positions of dominant resonances depend on the number of photons, i.e. the collective ac Stark effect. Coupling of an SQA to the transmission line allows a straightforward experimental access of the collective states in microwave transmission experiments and, at the same time, to employ SQAs as sensitive single-photon detectors.

DY 36.4 Thu 10:15 H22

Heat transport and rectification in an ultrastrongly-coupled qubit-resonator system — •Luca Magazzu[1], Milena Grifoni[1], and Elisabetta Paladino[2] — [1]University of Regensburg — [2]University of Catania

Inspired by the recent experimental developments in the field of heat transport in the quantum regime, we consider a flux qubit coupled to a superconducting resonator as a composite open quantum system. The two elements of this open quantum Rabi system interact with two heat baths held at different temperatures. At the steady state, a heat current is established which is the result of photon exchanges between the system and the baths. Due to the geometry of the setup, the coupling to the heat baths is asymmetric. In turn this entails the presence of a preferred direction for the heat current, to a degree quantified by the heat rectification.

We calculate the heat current and rectification in different coupling regimes and considering a periodic driving applied to the qubit. The rectification displays the signatures of multi-photon processes that occur when the qubit-resonator coupling enters the nonperturbative regime

[1] A. Ronzani et al., Nat. Phys. 14, 991 (2018)
[2] J. Senior, A. Gubaydullin, B. Karimi, J. T. Peltonen, J. Ankerhold, J. P. Pekola, Commun. Phys. 3, 40 (2020)
[3] B. Bhandari, P. Andrea Erdman, R. Fazio, E. Paladino, and F. Taddei. Phys. Rev. B 103, 155434 (2021)
[4] L. Tesser, B. Bhandari, P. A. Erdman, R. Fazio, E. Paladino, F. Taddei, New J. Phys. 24, 035001 (2022)

DY 36.5 Thu 10:30 H22

Probing the coherence of superconducting Fluxmon qubits — •Benedikt Berlitz, Alexander Neumann, Alexander Bilmes, Jürgen Lisenfeld, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

The Fluxmon qubit combines a transmission line resonator with a DC-SQUID and offers wide control over the circuit's potential energy via two independently applied bias flux channels. This allows one to operate the qubit as a phase or flux qubit, provides means for fast single-shot qubit readout, and offers a path to characterize decoherence due to surface spins and tunneling defects in a wide frequency range. We will review the Fluxmon qubit design and fabrication, and present measurements of its potential energy landscape which demonstrate single- and double well qubit physics. Our time-resolved measurements confirm that the Fluxmon qubit's performance is strongly limited by microscopic sources of decoherence, which might render it a suitable detector for defect spectroscopy applications.

DY 36.6 Thu 10:45 H22

Mapping the positions of individual material defects in superconducting transmon qubits — •Alexander K. Händel, Benedikt Berlitz, Alexander Bilmes, Jürgen Lisenfeld, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

In superconducting quantum bits, material defects at the surface of circuit electrodes and the substrate constitute a major source of decoherence. In our experiment, we detect individual defects with a transmon qubit while tuning their resonance frequencies with applied static electric fields. We fabricated samples that feature on-chip gate electrodes that are placed close to the qubit island. By measuring the coupling strength of each detected defect to various electrodes, we are able to deduce the defect's position on the qubit chip. Our goal is to create two-dimensional maps of defect distribution over qubit electrodes. This will help to identify circuit components which contain majority of coherence-breaking defects and improve fabrication methods towards more coherent qubits.

15 min. break

DY 36.7 Thu 11:15 H22

Quantum memory based on spin donors in silicon — •Patricia Oehrl[1,2], Julian Franz[1,2], Florian Fesquet[1,2], Nadezhda Kukharchyk[1,2], Kirill G. Fedorov[1,2], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technologies (MCQST), Germany

Quantum memories are considered as key elements for the successful realization of quantum communication [1]. In order to allow for the connection of several quantum nodes into a quantum network without frequency conversion, several requirements have to be met such as frequency compatibility and connectability to the quantum system of choice. As superconducting quantum processors operate in the microwave regime, solid-state spin ensembles with their exceptional coherence times are promising candidates [2]. 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 present experimental results on the storage of coherent microwave states and their retrieval using a Hahn-echo type pulse sequence. In detail, we discuss the impact of the resonator design, the classical storage times and outline strategies towards storing quantum signals.

We acknowledge financial support from the Federal Ministry of Education and Research of Germany (project number 16KISQ036).

[1] H. J. Kimble, Nature **453**, 1023 (2008)
[2] C. Gezes *et al.*, Phys. Rev. X **4**, 021049 (2014)

DY 36.8 Thu 11:30 H22

Crystal electric field effects in yttrium orthosilicate doped with paramagnetic rare-earth ions — •Tim Hofmann, Andreas Bauer, Fabian Kessler, and Christian Pfleiderer — Chair for the Topology of Correlated Systems, Department of Physics, Technical University of Munich, Germany

Monoclinic yttrium orthosilicate Y_2SiO_5 doped with several ten ppm of rare-earth ions, such as Er^{3+}, Yb^{3+}, or Nd^{3+}, represents a candidate material for optical applications in quantum information technology. The amount of dopants directly influences key properties, such as the linewidth or the coherence time, and in turn precise control on the doping levels is essential. The quantitative determination of doping on ppm level is challenging when using conventional characterization techniques. Here, we report the magnetic characterization of rare-earth doped yttrium orthosilicate single crystals. We infer information from magnetization measurements at low temperatures down to 2 K for magnetic fields up to 14 T applied along the optical axes b, $D1$, and $D2$, exhibiting paramagnetic contributions characteristic of rare-earth ions. Distinct crystalline anisotropy and the substitution of yttrium on two magnetically inequivalent sites is observed, indicating the importance of crystal electric field effects for both the fundamental characterization and potential applications in quantum information technology.

DY 36.9 Thu 11:45 H22

Synchronized coherent charge oscillations in coupled double quantum dots — •Eric Kleinherbers[1], Philipp Stegmann[2], and Jürgen König[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

We study coherent charge oscillations in double quantum dots tunnel-coupled to metallic leads [1]. If two such systems are coupled by Coulomb interaction, there are in total six (instead of only two) oscillation modes of the entangled system with interaction-dependent oscillation frequencies. By tuning the bias voltage, one can engineer decoherence such that only one of the six modes, in which the charge oscillations in both double quantum dots become synchronized in antiphase, is singled out. We suggest to use waiting-time distributions and the $g^{(2)}$-correlation function to detect the common frequency and

the phase locking.
[1] E. Kleinherbers et al., Phys. Rev. B 104, 165304 (2021)

DY 36.10 Thu 12:00 H22

Electrically driven spin resonance with bichromatic driving — •Zoltán György[1], András Pályi[2], and Gábor Széchenyi[1] — [1]Institute of Physics, Eötvös University, H-1117 Budapest, Hungary — [2]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary

Electrically driven spin resonance (EDSR) is an established tool for controlling semiconductor spin qubits. Here, we theoretically study a frequency-mixing variant of EDSR, where two driving tones with different drive frequencies are applied, and the resonance condition connects the spin Larmor frequency with the sum of the two drive frequencies. Focusing on flopping-mode operation, we calculate the parameter dependence of the Rabi frequency and the Bloch-Siegert shift. A shared-control spin qubit architecture could benefit from this bichromatic EDSR scheme, as it enables simultaneous single-qubit gates.

DY 36.11 Thu 12:15 H22

Cavity-mediated superconductor-ferromagnet interaction — Andreas T. G. Janssønn, •Henning G. Hugdal, Arne Brataas, and Sol H. Jacobsen — Center for Quantum Spintronics, Department of Physics, NTNU, Norwegian University of Science and Technology, Trondheim, Norway

We present a microscopic theoretical analysis of interactions between a ferromagnet (FM) and superconductor (SC) mediated by photons in a cavity. This facilitates interactions over macroscopic distances, in contrast with extensively researched FM-SC proximity systems, and ensures there is no interfacial suppression of their respective order parameters. The spatial separation between the materials also means the FM and SC may be held at different temperatures, and has potential applications as a bridge in spintronic-superconducting circuitry. Specifically, we deduce the anisotropy field induced across the FM due to the presence of the SC when the system is subjected to a symmetry-breaking external field. Other quantities such as renormalized dispersion relations can also be deduced. The model is a modification and quantum mechanical extension of the principle presented in Janssøn et al. PRB 102, 180506(R) (2020).

DY 37: Invited Talk David Zwicker

Time: Thursday 9:30–10:00 Location: H20

Invited Talk DY 37.1 Thu 9:30 H20

Controlled and robust phase separation in cells — •David Zwicker — MPI for Dynamics and Self-Organization, Göttingen, Germany

Phase separation is a key process for the spatiotemporal organization of biomolecules in cells. In particular, phase separation explains how droplets can form spontaneously to create subcellular compartments. However, traditional theories of phase separation cannot explain how cells control these droplets robustly. To elucidate this, I will discuss how droplets interact with the elastic cellular environment and how cells use driven chemical reactions to control droplets. First, I will show how monodisperse emulsions form when droplets grow in a mesh that can break and re-arrange. We demonstrate that stiffness gradients cause elastic ripening, which biases droplets toward softer regions. These processes quantitatively explain experiments where oil droplets form in PDMS gels. The same physics applies to droplets interacting with the cytoskeleton in cells. In the second part, I will show how driven reactions control droplet size and position so that multiple droplets can coexist. Taken together, our models identify key physical processes that allow cells to control the phase separation of biomolecules.

DY 38: Complex Fluids and Soft Matter 2 (joint session DY/CPP)

Time: Thursday 10:00–11:30 Location: H18

DY 38.1 Thu 10:00 H18

Underscreening in the Restricted Primitive Model — •Andreas Härtel — Institute of Physics, University of Freiburg, Germany

Electric double layers occur where charges are screened by other charges, for instance, when charged surfaces of electrodes, colloids, or cells are exposed to electrolytes (mobile ions in a solvent). Increasing the concentration of mobile ions leads to more efficient screening, if concentrations are sufficiently low. At high concentrations, however, the screening by finite-sized ions becomes less efficient than those of point-like ions due to packing, an effect called underscreening. Some experiments report underscreening as a strong effect that follows some universal scaling [1], but the observation could not been explained by theoretical models yet. Conversely, independent theoretical studies actually ruled out the most important model for electrolytes of finite-sized ions as a candidate able to explain underscreening, namely the restricted primitive model [2]. In this talk I will discuss in which sense underscreening can and cannot be found in the restricted primitive model and in which sense the effect follows some universal scaling. I will support the discussion by recent theoretical results obtained from simulations and liquid state theories.

[1] Lee et al., Underscreening in concentrated electrolytes, Faraday Dicuss. 199, 239 (2017).

[2] Cats et al., Primitive Model Electrolytes in the Near and Far Field: Decay Lengths from DFT and Simulations, J. Chem. Phys. 154, 124504 (2021).

DY 38.2 Thu 10:15 H18

Reciprocal and nonreciprocal eigenmodes of viscoelastic fluids — •Juliana Caspers[1], Clemens Bechinger[2], Nikolas Ditz[2], Matthias Fuchs[2], Felix Ginot[2], Karthika Krishna Kumar[2], Luis Frieder Reinalter[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August Universität Göttingen, 37073 Göttingen, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Complex fluids such as wormlike micellar solutions are in general non-Markovian. In equilibrium, their behavior is often well approximated by a simple Maxwell model with one characteristic timescale [1]. Recoil experiments, after a colloidal probe has been sheared through the solvent, however, displayed a double-exponential relaxation [2]. We found excellent agreement of our measurements with a linear two-bath particle model. Depending on whether the optical trap which confines the probe is turned on or off, we find two sets of eigenmodes in our model, corresponding to either nonreciprocal (trap on) or reciprocal (trap off) forces. Using different recoil protocols as well as equilibrium mean square displacement measurements we confirmed the existence of these two different sets of timescales with experiments. Finally, for linear systems, we find a Volterra relation between two memory kernels, characterizing reciprocal and nonreciprocal forcing.

[1] F. Ginot, J. Caspers, M. Krüger, C. Bechinger. *Phys. Rev. Lett.* **128**, 028001 (2022)

[2] F. Ginot, J. Caspers, L. F. Reinalter, K. Krishna Kumar, M. Krüger, C. Bechinger. *arXiv:2204.02369* (2022)

DY 38.3 Thu 10:30 H18

Elastic Turbulence in von Kármán geometry — •Reinier van Buel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Elastic turbulence, occurring in viscoelastic fluid flow at vanishing Reynolds numbers, is an interesting flow state [1-4] and has been experimentally studied in the von Kármán geometry [1]. Elastic turbulence is especially appealing for the mixing of fluids on the micron scale, which is extremely challenging in Newtonian fluids where transport

relies on diffusion. Here, we present a fully three-dimensional numerical investigation of the von Kármán flow using the Oldroy-B model [4]. We observe a non-axisymmetric mode with four-fold symmetry that drives the flow instability towards elastic turbulence and compare it to results obtained from a linear stability analysis. By analyzing the velocity fluctuations and defining an order parameter, we identify a bistable flow state above a sub-critical transition, which switches between a weakly chaotic flow state and elastic turbulence and exhibits hysteretic behavior. Furthermore, we reveal a sharp increase in the flow resistance at the transition to elastic turbulence, which we attribute to the elastic contribution of the work performed at the open side surface of the flow. Finally, an analysis of the spatial and temporal velocity power spectra confirms the turbulent nature of the flow.

[1] A. Groisman and V. Steinberg, Nature **405**, 53 (2000).
[2] R. Buel, C. Schaaf, H. Stark, Europhys. Lett. **124**, 14001 (2018).
[3] R. Buel and H. Stark, Sci. Rep. **10**, 1-9 (2020).
[4] R. Buel and H. Stark, Phys. Fluids **34**, 4 (2022).

DY 38.4 Thu 10:45 H18

Coarsening dynamics of quasi 2D emulsions in free-standing smectic films — •Christoph Klopp, Torsten Trittel, and Ralf Stannarius — Institute for Physics, Otto von Guericke University Magdeburg, Germany

Hydrodynamic phenomena in thin films play a crucial role in biological systems, in nature and modern technology. Various experimental and theoretical studies explored, e.g., the motion of objects in quasi two-dimensional films [1], the merging of inclusions [2-4] and the structural change of emulsions during long-term observations. Here, we demonstrate and describe the coarsening dynamics of emulsions formed by smectic islands (flat circular regions) on liquid crystal bubbles in microgravity at the International Space Station (ISS). The smectic islands form polydisperse, disordered arrangements representing quasi 2D emulsions. We analyze the time evolution of these ensembles that proceed through direct island coalescence or the exchange of material through the background film (Ostwald ripening). Coarsening is ubiquitous in liquid emulsions and foams, and important for their stability. We compare our results with such systems and analyze the dominant process for the 2D coarsening dynamics.

Acknowledgements: This study was supported by NASA, DFG and DLR within the OASIS and OASIS-Co projects.

References: [1] A. Eremin et al., Phys. Rev. Lett., 107, 268301 (2011) [2] N. S. Shuravin et al., Phys. Rev. E, 99, 062702 (2019) [3] Z. H. Nguyen et al., Phys. Rev. Research, 3, 033143 (2021) [4] C. Klopp et al., Soft Matter 16 4607 (2020)

DY 38.5 Thu 11:00 H18

Phase transitions in the generalised chiral Lebwohl-Lasher model — •Philipp Elsässer and Anja Kuhnhold — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

The behaviour of liquid crystals can be described by using the Lebwohl-Lasher (LL) model, where unit vectors that resemble nematic directors are positioned on a simple cubic lattice. Due to the interaction potential, which favours parallel orientations, this model is well suited to analyse isotropic-nematic (IN) phase transitions.

There exist several extensions to this model with which its applicability can get further enhanced. We use two combined extensions to obtain the generalised chiral Lebwohl-Lasher model: We apply a generalisation to tune the sharpness of the potential, as in the work of Fish and Vink [1] and add a chiral term which is based on the work of Memmer et al. [2]. In this system we study the phase transition properties with the help of Monte Carlo simulations. To identify characteristic properties of the transitions, we apply finite-size scaling. This allows us to determine chirality-sharpness parameter pairs with which we can manipulate the nature of the transition between ordered and disordered states [3].

[1] J. M. Fish, R. L. C. Vink, PRE **81**, 021705 (2010).
[2] R. Memmer, O. Fliegans, PCCP **5**, 558 (2003).
[3] P. Elsässer, A. Kuhnhold, PRE **105**, 054704 (2022).

DY 38.6 Thu 11:15 H18

Systematic parametrization of non-Markovian dissipative thermostats for coarse-grained molecular simulations with accurate dynamics — •Viktor Klippenstein and Nico F. A. Van Der Vegt — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, 64287 Darmstadt, Germany

The Mori-Zwanzig theory, in principle, allows to derive an exact equation of motion for coarse-grained degrees of freedom based on the dynamics of an underlying fine-grained reference system.[1] Still, in practice the simultaneous representation of structural and dynamic properties in particle-based models poses a complicated problem, e.g. due to the non-linearity of the exact coarse-grained equation of motion.

A viable approximate approach is to start from a conservative coarse-grained force-field and to extend the standard Newtonian equation of motion used in molecular simulation with a linear generalized Langevin thermostat. We demonstrate how such a thermostat can be parametrized to correctly represent dynamic properties, both in a purely bottom-up approach[2,3] or by applying iterative optimization.[3] We consider the Asakura-Oosawa model as a test case.[3]

[1] V. Klippenstein, M. Tripathy, G. Jung, F. Schmid, and N. F. A. van der Vegt, The Journal of Physical Chemistry B 125, 4931 (2021).
[2] V. Klippenstein and N. F. A. van der Vegt, The Journal of Chemical Physics 154, 191102 (2021).
[3] V. Klippenstein and N. F. A. Van Der Vegt, The Journal of Chemical Physics under review (2022).

DY 39: Pattern Formation and Reaction-Diffusion Systems

Time: Thursday 10:00–12:15 Location: H19

DY 39.1 Thu 10:00 H19

Dynamics of tagged particles in a biased $A + A \to \emptyset$ system in one dimension : result for asynchronous and parallel updates — •Reshmi Roy[1], Parongama Sen[1], and Purusattam Ray[2] — [1]University of Calcutta, Kolkata, India — [2]IMSC, Chennai, India

We have studied dynamical features of tagged particles in one dimensional $A + A \to \emptyset$ system, where the particles A have a bias ϵ such that they move towards their nearest neighbour with the probability $0.5 + \epsilon$ and move in the opposite direction with probability $0.5 - \epsilon$ and annihilate on contact. We found that for $\epsilon > 0$ when asynchronous dynamics is used to update the system, probability distribution $\Pi(x, t)$ of the particles shows a double peak structure with a dip at $x = 0$ and it assumes a double delta form at very late time regime. For any $\epsilon > 0$, there is a crossover at time t^*, below which the particle motions are highly correlated, and beyond t^*, the particles move as independent biased walkers. When we use parallel updating rule, $\Pi(x, t)$ shows a non-Gaussian single peaked structure and the fraction of surviving particle $\rho(t)$ shows a $\ln t/t$ variation. For the deterministic point $\epsilon = 0.5$, we found that an isolated pair of particles, termed as dimers, can survive indefinitely in the system which is exclusive for parallel dynamics. When ϵ is made negative, $\Pi(x, t)$ becomes Gaussian as found in $\epsilon = 0$. A comparative analysis for the relevant quantities using asynchronous and parallel dynamics shows that there are significant differences for $\epsilon > 0$ while the results are qualitatively similar for $\epsilon < 0$.

Journal Ref: J. Phys. A: Math. Theor. 53, 155002 (2020), J. Phys. A: Math. Theor. 53, 405003 (2020), Physica A 97569, 125754 (2021).

DY 39.2 Thu 10:15 H19

Wrinkling in Curved Films — •Megha Emerse and Lucas Goehring — Nottingham Trent University, Nottingham, United Kingdom

Thin films or sheets exposed to external forces can become unstable to drastic shape changes, often forming regular or periodic patterns like wrinkles, folds, creases, etc. This can be distinctly observed when one tries to wrap a world map onto a globe since it is unachievable without creating any wrinkles. Wrinkling is a self-initiated process, spontaneously generating periodic structures out of a uniformly smooth surface and represents a pathway for simply creating regular surface topography. Here, we study thin elastic membranes that form complex wrinkle patterns when put on substrates where there is a mismatch in their inherent shape. Using 3D-printed moulds, we prepare elastic membranes with different curvatures, including cases of positive and negative Gaussian curvature, and shapes with two distinct principal curvatures. Through these, we experimentally investigate the depen-

dence of the amplitude and wavelength of the wrinkles that spontaneously form when these curved membranes are constrained by a flat fluid substrate. We also study how these properties change along the membrane, for example with distance from the film edges.

DY 39.3 Thu 10:30 H19

Exploring Bifurcations in Bose-Einstein Condensates via Phase Field Crystal Models — •Alina B. Steinberg[1], Fabian Maucher[2], Svetlana V. Gurevich[1,3], and Uwe Thiele[1,3] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Strasse 9, 48149 Münster, Germany — [2]Departament de Física, Universitat de les Illes Balears \& IAC-3, Campus UIB, E-07122 Palma de Mallorca, Spain — [3]Center of Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Corrensstrasse 2, 48149 Münster, Germany

To facilitate the analysis of pattern formation and phase transitions in Bose-Einstein condensates as well as to unravel analogies we present an explicit approximate mapping from the nonlocal Gross-Pitaevskii equation with cubic nonlinearity to a model of phase field crystal type. This approximation is valid close to the superfluid-supersolid phase transition and permits us to explore the phase transition through the corresponding bifurcation diagrams obtained via numerical path continuation. Additionally the effects of phenomenological higher order nonlinearities are considered. In passing we discuss the importance of localized states as an indicator of a first order character of the phase transition. A. B. Steinberg, F. Maucher, S. V. Gurevich and U. Thiele, Exploring Bifurcations in Bose-Einstein Condensates via Phase Field Crystal Models, http://arxiv.org/abs/2205.15194 (2022)

DY 39.4 Thu 10:45 H19

Phase Field Crystal model for particles with n-fold rotational symmetry in two dimensions — •Robert F. B. Weigel and Michael Schmiedeberg — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

We introduce a Phase Field Crystal (PFC) model for particles with n-fold rotational symmetry in two dimensions [1]. The n-fold symmetry of the particles corresponds to the one that can be realized for colloids with symmetrically arranged patches, with the patches being either attractive or repulsive.

Our approach is based on a free energy functional that depends on the reduced one-particle density, the strength of the orientation, and the direction of the orientation, where all these order parameters depend on the position. The functional is constructed such that for particles with axial symmetry (*i. e.* $n = 2$) the PFC model for liquid crystals [2] is recovered. We explain how both, repulsive as well as attractive patches, are described in our model.

We discuss the stability of the functional and explore phases that occur for $1 \leq n \leq 6$. In addition to isotropic, nematic, stripe, and triangular order, we also observe cluster crystals with square, rhombic, honeycomb, and even quasicrystalline symmetry.

[1] arXiv:2204.00051 [cond-mat.soft]
[2] H. Löwen, *J. Phys.: Condens. Matter* **22**, 364105 (2010)

15 min. break

DY 39.5 Thu 11:15 H19

Control-optimisation for spatiotemporal chaos in 2D excitable media through a genetic algorithm — •Marcel Aron[1,2,3], Thomas Lilienkamp[2,4], Stefan Luther[1,2,3,5], and Ulrich Parlitz[2,3,5] — [1]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Göttingen, Germany — [4]Computational Physics in den Life Sciences, Technische Hochschule Nürnberg, Nürnberg, Germany — [5]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen, Göttingen, Germany

The emergence of spatiotemporal chaos (i.e. fibrillation) in the cardiac muscle (an excitable medium) leads to loss of pumping function and sudden cardiac death. Clinically, such episodes are treated with high-energy electric shocks to control (terminate) the chaotic dynamics and restore a regular heart rhythm. However, high shock energies result in increased risk of tissue damage or worsening the overall prognosis. This motivates the search for alternatives, including periodic sequences of low-energy electric pulses of constant field strength, which has seen success in pre-clinical trials on pig hearts.

Here we show that non-uniform pulse energies and time intervals can be used to further optimise the control of spatiotemporal chaos in 2D simulations of homogeneous cardiac tissue. We use a simplified shock-application model and define control-performance metrics to employ a genetic algorithm in the search for more efficient control approaches.

DY 39.6 Thu 11:30 H19

The French flag problem revisited: Creating robust and tunable axial patterns without global signaling — •Stephan Kremser[1], Gabriel Vercelli[1,2], and Ulrich Gerland[1] — [1]Physics Department, Technical University of Munich — [2]MIT Microbiology Program, Massachusetts Institute of Technology

Wolpert's French flag problem conceptualizes the task of forming axial patterns with broad regions in multicellular systems. Wolpert described two different solutions to his problem, the balancing model and thresholding of a morphogen gradient, both of which require global, long-range signaling between cells. Since global signaling becomes challenging in large systems, we computationally explore alternative solutions, which use only local cell-cell signaling and are simple enough to potentially be implemented in natural or synthetic systems. We employ cellular automata rules to describe local signal processing logics, and search for rules capable of robust and tunable axial patterning with evolutionary algorithms. This yields large sets of successful rules, which however display only few types of different behaviors. We introduce a rule alignment and consensus procedure to identify patterning modules that are responsible for the observed behaviors. With these modules as building blocks, we then construct local schemes for axial patterning, which function also in the presence of noise and growth, and for patterns with a larger number of different regions. The regulatory logic underlying these modules could therefore serve as the basis for the design of synthetic patterning systems, and as a conceptual framework for the interpretation of biological mechanisms.

DY 39.7 Thu 11:45 H19

Coupling-Mediated Protein Waves in Mass-Conserved Pattern Forming Systems — •Benjamin Winkler[1], Sergio Alonso Muñoz[2], and Markus Bär[1,3] — [1]Physikalisch-Technische Bundesanstalt — [2]Universitat Politècnica de Catalunya — [3]TU Berlin

The formation of protein patterns inside biological cells is of crucial importance for their spatial organization, growth and division. In many cases these dynamics can be described by coupled, mass-conserving reaction-diffusion equations [Brauns et al., PRX, 2020]. Motivated by the question how the generation of cell polarity is influenced by membrane heterogeneity, we study the behavior of the coupled dynamics of two well-known, mass-conserved systems. System A is therein given by a simplified model [Mori et al., Biophys.J., 2008] for the emergence of cell polarity with a single pair of activated-inactivated proteins M and B. The inactive, fast-diffusing species (B) in the bulk of the cell becomes activated (M) when bound to the cell membrane. When endowed with a positive feedback on the membrane-mediated activation, the system exhibits inherent polarizability. System B is described by the Cahn-Hilliard equation, two membrane species demixing into a pattern of comparatively small, static droplets. We then consider a difference in interaction affinity for M with respect to the two phases of the cell membrane and an additional contribution in the chemical potential of the membrane, depending on the presence of M. In the so coupled system, the emergence of traveling waves can be observed above a finite threshold of coupling strength.

DY 39.8 Thu 12:00 H19

Robustness of *in vivo* Min patterns underlines complex protein interaction motives — •Henrik Weyer, Laeschkir Würthner, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany

The Min protein system organizes the symmetric cell division of E. coli bacteria: Two proteins, MinD and MinE, undergo pole-to-pole oscillations via a reaction–diffusion mechanism, and guide the cell-division machinery towards midcell. In elongated, filamentous cells the pole-to-pole oscillations transition into a standing-wave pattern forming several stripes along the cell. We show that modeling of the latent MinE state, which allows for Min pattern formation over a large range of MinE densities, suppresses standing-wave patterns. This effect is explained to demonstrate a generic mechanism that latent states form a homogeneous reservoir in reaction–diffusion systems. We reason that the MinE–MinD interaction cannot be described as a single hydrolysis

step, and that MinE plays a more complex role in the Min protein network, a finding supported by recent experimental evidence.

DY 40: Brownian Motion and Anomalous Diffusion

Time: Thursday 10:00–12:00 Location: H20

DY 40.1 Thu 10:00 H20

Depinning and structural transitions of confined colloidal dispersions under oscillatory shear — •Marcel Hülsberg and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Strongly confined colloidal dispersions under shear exhibit a variety of dynamical phenomena, including a depinning transition, which is accompanied by lateral structural changes [1].

Here, we investigate the depinning behaviour of these systems under pure oscillatory shearing with shear rate $\dot{\gamma}(t) = \dot{\gamma}_0 \cos(\omega t)$, as it is a common scenario in rheological experiments [2].

The colloids' depinning behaviour is assessed from a microscopic level based on particle trajectories, which are obtained from overdamped Brownian Dynamics simulations. The numerical approach is complemented by an analytic one based on an effective single-particle model in the limits of weak and strong driving.

Investigating a broad spectrum of shear rate amplitudes $\dot{\gamma}_0$ and frequencies ω, we observe complete pinning as well as temporary depinning behaviour. We discover that temporary depinning occurs for shear rate amplitudes above a frequency-dependent critical amplitude $\dot{\gamma}_0^{\mathrm{crit}}(\omega)$, for which we attain an approximate functional expression.

Above $\dot{\gamma}_0^{\mathrm{crit}}(\omega)$, we further observe a variety of dynamical structures, whose stability exhibits an intriguing $(\dot{\gamma}_0, \omega)$ dependency. This might enable new perspectives for potential control schemes.

[1] S. Gerloff and S.H.L. Klapp, *Phys. Rev. E* **94**(6), 062605 (2016)
[2] S.M. Fielding, *J. Rheol.*, **64**(3), 723-738 (2020)

DY 40.2 Thu 10:15 H20

Ballistic Hot Brownian Motion — •Xiaoya Su[1], Frank Cichos[1], and Klaus Kroy[2] — [1]Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany — [2]Institute of Theoretical Physics, University Leipzig, Leipzig, Germany

Brownian motion is the erratic motion of particles in a fluid due to the bombardment of the particle with solvent molecules providing thermal energy and viscous friction. It is fundamental for the dynamics of soft matter and defines the prototype of a fluctuation dissipation relation. While at long timescales the motion is purely stochastic, it is at shorter times influenced by hydrodynamic effects and even ballistic at ultrashort timescales. Yet, the ballistic motion, same as the stochastic motion, is still determined by the temperature of the system. Here we explore the transition to the ballistic regime for a hot Brownian particle, i.e. a microparticle which is heated by a laser in an optical trap. In this case the particle temperature is different from the solvent temperature and so far, only theoretical predictions exist for the relevant temperature determining the particle velocity.

We report the first measurements of the thermal non-equilibrium process in a specially designed optical trap which is able to resolve particle displacements of about 20 pm with a time-resolution of 10ns. We show how the mean squared displacement of the particle from the nanosecond to the second timescale changes as a function of the surface temperature of the particle and discuss the model of a frequency dependent effective temperature of hot Brownian motion.

DY 40.3 Thu 10:30 H20

Stochastic action for tubes: Connecting path probabilities to measurement — •Julian Kappler[1], Jannes Gladrow[2,3], Ulrich F. Keyser[3], and Ronojoy Adhikari[1] — [1]DAMTP, Cambridge University, Cambridge, UK — [2]Microsoft Research, Cambridge, UK — [3]Cavendish Laboratory, University of Cambridge, Cambridge, UK

The trajectories of diffusion processes are continuous but nondifferentiable, and each occurs with vanishing probability. This introduces a gap between theory, where path probabilities are used in many contexts, and experiment, where only events with nonzero probability are measurable. We bridge this gap by considering the probability of diffusive trajectories to remain within a tube of small but finite radius around a smooth path. This probability can be measured in experiment, via the rate at which trajectories exit the tube for the first time, thereby establishing a link between path probabilities and physical observables. In my contribution I will show how this link can be used to both measure ratios of path probabilities [1], and to extend the theoretical stochastic action from individual paths to tubes [2]. I will furthermore relate our results to the usual path-integral formalism.

[1] J. Gladrow, U. F. Keyser, R. Adhikari, and J. Kappler. Experimental measurement of relative path probabilities and stochastic actions. Phys. Rev. X 11, 031022 (2021). 10.1103/PhysRevX.11.031022
[2] J. Kappler and R. Adhikari. Stochastic action for tubes: Connecting path probabilities to measurement. Physical Review Research 2(2), 023407 (2020). 10.1103/PhysRevResearch.2.023407

DY 40.4 Thu 10:45 H20

Size matters for Bayesian chemotaxis — •Julian Rode[1], Maja Novak[1,2], and Benjamin M. Friedrich[1,3] — [1]cfaed, TU Dresden, Germany — [2]Department of Physics, University of Zagreb, Croatia — [3]PoL, TU Dresden, Germany

Navigation by chemical cues, e.g., chemotaxis, is employed by single biological cells and animals. The size and speed of search agents dictate noise levels and thus optimal strategies to find a target.

Here, we address information theory of gradient sensing for an ideal agent and ask for optimal strategies as a baseline for real agents. We extend the seminal work on infotaxis [1], by applying its idea of maximizing information gain to agents of finite size. These agents can now measure gradients both by temporal comparison due to their active motion [1], and by spatial comparison across their diameter, prompting an optimal weighting of both information sources [2].

In the absence of noise, trajectories show stereotypic behavior; the entropy of directional uncertainty collapses onto a master curve parameterized by a signal-to-noise ratio. Unlike [1], we account for rotational diffusion, which is prevalent for microscopic agents: Its competition with information gain due to spatial comparison sets an effective measurement time (given by the inverse geometric mean of a rate constant of information gain and the rotational diffusion coefficient), which is different from the typical bound argued by Howard Berg for bacterial chemotaxis (inverse rotational diffusion coefficient) [3].

[1] M. Vergassola et al, Nature (2007); [2] A. Auconi et al., EPL, in press (arXiv:2111.09630); [3] M. Novak et al., New J Phys (2021).

15 min. break

DY 40.5 Thu 11:15 H20

Superstatistics of protein diffusion dynamics in bacteria — •Yuichi Itto — Aichi Institute of Technology, Aichi, Japan — ICP, Universität Stuttgart, Stuttgart, Germany

In recent years, non-Gaussian normal/anomalous diffusion have experimentally been observed in a wide class of living cells. Superstatistics is a "statistics of statistics" with two largely separated time scales for treating nonequilibrium complex systems. Here, a superstatistical diffusion theory [1] is presented for obtaining a q-Gaussian displacement distribution decaying as a power law found for heterogeneous diffusion phenomenon of DNA-binding proteins in bacteria [2]. This theory takes into account the joint fluctuations of both the diffusion exponent and the (inverse) temperature, which are hierarchically combined with a fractional Brownian motion describing a local stochastic process of the proteins. Correlation between the fluctuations is also discussed and its weakness is shown to be essential. The results obtained are in a good agreement with the experimental data.

[1] Y. Itto and C. Beck, J. R. Soc. Interface 18, 20200927 (2021).
[2] A.A. Sadoon and Y. Wang, Phys. Rev. E 98, 042411 (2018).

DY 40.6 Thu 11:30 H20

Generalised master equation for diffusion and reaction problems in heterogeneous media — Daniela Frömberg[1] and •Felix Höfling[1,2] — [1]Department of Mathematics and Computer Science, Freie Universität Berlin — [2]Zuse Institute Berlin

The kinetics of chemical reactions in a heterogeneous or crowded medium significantly deviates from that in a well-mixed, aqueous environment. One example is the partitioning of cell membranes and intracellular spaces, e.g., into cytoplasm and nucleus. For reaction–diffusion

problems in such compartmentalised spaces, we extend a recently proposed generalised master equation (GME) for non-Markovian jump processes [1]. The GME governs the time evolution of the occupation probability of the spatial domains, its main ingredient are first-passage time densities encoding the transport behaviour in each domain. The domains can differ with respect to their diffusivity, geometry, and dimensionality, but can also refer to transport modes alternating between diffusive, driven, or anomalous motion. We discuss further the inclusion of barriers and the Markovian limit of the GME.

For a cherry-pit geometry with a reactive inner domain, we obtain the first-reaction time density and infer the effective reaction rate constant. This rate constant is timescale dependent and exhibits an enhancement at intermediate times by orders of magnitude and an algebraically slow convergence to the long-time limit. Our stochastic approach does not depend on the existence of a stationary distribution and thus overcomes a limitation of the classical Smoluchowski theory.

[1] D. Frömberg and F. Höfling, J. Phys. A **54**, 215601 (2021).

DY 40.7 Thu 11:45 H20

Molecular dynamics simulations of supercooled water in silica pores — •Markus Haneke, Robin Horstmann, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Being highly relevant in biology as well as in technology and other areas, water is subject to extensive research. Especially its anomalies pose questions. Commonly, it is argued that the anomalies of water originate in the supercooled state, which is therefore regularly subject to exploration. To suppress freezing in experimental studies, confinements can be employed, where silica pores proved to be very useful.

Molecular dynamic simulations are a valuable tool to take a closer look. They allow analyses with high spatial and temporal resolution while making it easy to extract dynamic and static information. [1]

Here, we perform simulations to analyse the diffusion of water in silica pores. We want to find the influence of the pore on dynamics, as well as of the capping if the water outside of the pore freezes.

Results of our analysis are, that the diffusion inside of the pore is anomalous and slowed down. The systems show to be subdiffusive. Capping not only restricts diffusion but also slows down local relaxation and yields a nearly triangular probability density of propagation distance, contradicting free 1D-diffusion.

[1] R. Horstmann, L. Hecht, S. Kloth, and M. Vogel. "Structural and Dynamical Properties of Liquids in Confinements: A Review of Molecular Dynamics Simulation Studies". In: Langmuir 2022 38 (21), 6506-6522

DY 41: Nonequilibrium Quantum Many-Body Systems (joint session TT/DY)

Time: Thursday 15:00–18:15 Location: H22

DY 41.1 Thu 15:00 H22

Investigating the non-equilibrium dynamics of two-level systems at low temperature — •Marcel Haas, Mareike Dinger, Lukas Münch, Jan Blickberndt, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg, Germany

The dielectric loss of amorphous materials along with noise and decoherence is the major limiting factor in many applications like superconducting circuits, Josephson junctions and quantum computing. It is mainly determined by atomic tunneling systems described by quantum mechanical two-level systems (TLS), which are broadly distributed low-energy excitations in the sample. The spontaneous phonon emission of an excited TLS gives rise to a relaxation time T_1 and the interaction between TLSs with their thermally excited surrounding induces a decoherence time T_2. These effects mainly determine the measurable dielectric loss in the observed material, which we ascertain by measuring the quality factor of a bridge type superconducting LC-resonator. The dielectric medium in between the capacitor plates is a sputter deposited a-SiO_2 film. The setup shows a unique property when two off-resonant pump tones are applied symmetrically. In this limit, the resonator is emitting at the intermediate frequency of the driving fields. The underlying mechanism can therefore be explained by a nonlinear interaction of the rf-field with the TLSs and the resonator which is creating additional lines in the frequency spectrum. We present first measurements at a frequency of 1 GHz performed with a micro-fabricated superconducting resonator.

DY 41.2 Thu 15:15 H22

Photoinduced prethermal order parameter dynamics in the two-dimensional large-N Hubbard-Heisenberg model — •Alexander Osterkorn and Stefan Kehrein — University of Göttingen, Göttingen, Germany

A central topic in current research in non-equilibrium physics is the design of pathways to control and induce order in correlated electron materials with time-dependent electromagnetic fields. The theoretical description of such processes, in particular in two spatial dimensions, is very challenging and often relies on phenomenological modelling in terms of free energy landscapes. We discuss a semiclassical time evolution scheme that includes dephasing dynamics beyond mean-field and allows to simulate the light-induced manipulation of prethermal order in a two-dimensional model [1] with competing phases microscopically. We calculate the time evolution of the relevant order parameters subsequent to driving with a short laser pulse [2]. The induced prethermal order does not depend on the amount of absorbed energy alone but also explicitly on the driving frequency and amplitude. While this dependency is pronounced in the low-frequency regime, it is suppressed at high driving frequencies.

[1] Phys. Rev. B 39, 11538 (1989)
[2] arXiv:2205.06620

DY 41.3 Thu 15:30 H22

Nonequilibrium dynamics in pumped Mott insulators — •Satoshi Ejima[1], Florian Lange[2], and Holger Fehske[1,2] — [1]Institut für Physik, Universität Greifswald, Greifswald, Germany — [2]Erlangen National High Performance Computing Center, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

The study of systems under optical excitation receives tremendous attention because of both the recent rapid developments of ultrafast pump lasers and the discovery of striking phenomena not observable in equilibrium. Various numerical techniques have been applied to optically excited systems to study nonequilibrium dynamics, e.g., the time-dependent version of exact-diagonalization technique or dynamical mean-field theory. Results for nonequilibrium dynamics based on tensor-network algorithms are still rare, however.

In this talk, we propose a direct numerical scheme in the matrix-product-states (MPS) representation for the computation of nonequilibrium dynamic response functions, which can be used for general (quasi-)one-dimensional systems. Using time-evolution techniques for (infinite) MPS, we calculate, directly in the thermodynamic limit, the time-dependent photoemission spectra and dynamic structure factors of the half-filled Hubbard chain after pulse irradiation. These quantities exhibit clear signatures of the photoinduced phase transition from insulator to metal that occurs because of the formation of so-called η pairs.

[1] S. Ejima et al., Phys. Rev. Res. **2**, 032008(R) (2020)
[2] Phys. Rev. Res. **4**, L012012 (2022)
[3] arXiv:2204.09085

DY 41.4 Thu 15:45 H22

Nonequilibrium non-Markovian steady states in open quantum many-body systems: Persistent oscillations in Heisenberg quantum spin chains — •Regina Finsterhoelzl[1], Manuel Katzer[2], and Alexander Carmele[2] — [1]Department of Physics, University of Konstanz, Germany — [2]Institute of Theoretical Physics, Technical University Berlin, Germany

We investigate the effect of a non-Markovian, structured reservoir on an open Heisenberg spin chain by applying coherent time-delayed feedback control to it. The structured reservoir couples frequency-dependent to the spin chain and therefore induces a memory, thus the spin chain interacts partially with its own past. We demonstrate that with this new paradigm of a non-Markovian temporal driving scheme, it is possible to generate persistent oscillations within the many-body system and thus induce highly non-trivial states which dynamically store excitation within the chain. These oscillations occur at special

points in the stability landscape and persist for different chain lengths and different initial excitations within the chain. We propose a non-invasive partial characterization of the chain by exploiting the fact that the different trapping conditions which arise each relate to specific steady states within the chain.

DY 41.5 Thu 16:00 H22

Approaching the time-dependent quantum many-body problem with Artificial Neural Networks — •Pit Neitemeier and Dante Kennes — RWTH Aachen Institut für Theorie der statistischen Physik

Numerical solutions to quantum many body problems pose a significant challenge due to the curse of dimensionality. In this work I propose a novel Artificial Neural Network (ANN) ansatz and an unsupervised learning scheme to efficiently and flexibly solve time dependent quantum many-body problems. Contrary to previous work I do not rely on ODE Solvers for the time evolution, but parametrize the full wave function using an ANN. This enables a constant cost evaluation and full differentiablity of the wave function. Furthermore I show that it is possible to learn solution bundles that continuously represent the solution for a range of external parameters. The training of these ANNs is highly parallelizeable and reduces sequential operations significantly in comparison to previous work. I benchmark the ansatz for quantum quenches, ramps and pulses of the magnetic field using 1D Ising and Heisenberg Chains.

DY 41.6 Thu 16:15 H22

Entanglement phase transitions in correlated 1D spin chains — •Monalisa Singh Roy, Jonathan Ruhman, Emanuele G. Dalla Torre, and Efrat Shimshoni — Department of Physics, Bar-Ilan University, Ramat Gan 5290000, Israel

Entanglement phase transitions have attracted immense attention in recent years especially in the context of monitored quantum circuits. In such systems the dynamics due to unitary evolution compete with the localization induced by measurements. The phase transition of quantum systems from a phase where its entanglement entropy exhibits volume law for weak monitoring, to a quantum Zeno like phase with where the entanglement entropy obeys area law is well known in many models with unitary dynamics. Some recently proposals have identified a critical phase with a logarithmic scaling of entanglement in non-Hermitian models. We explore such a critical transition in a monitored quantum spin chain model and identify the entanglement transitions in the system under both unitary and non-unitary evolutions.

DY 41.7 Thu 16:30 H22

Feynman-Vernon influence functional approach to quantum transport in interacting nanojunctions: An analytical hierarchical study — •Luca Magazzu and Milena Grifoni — University of Regensburg

We present a nonperturbative and formally-exact approach to the charge transport in interacting nanojunctions using a real-time path-integral method based on the Feynman-Vernon influence functional. Expansion of the influence functional in terms of the number of tunneling transitions results in an exact generalized master equation for the populations in the occupation-number representation, and in a formally exact expression for the current. We apply our method to the exactly solvable resonant level model (RLM) and to the single-impurity Anderson model (SIAM). For both systems, we demonstrate a hierarchical diagrammatic structure. While the hierarchy closes at the second tier for the RLM, this is not the case for the interacting SIAM. Upon inspection of the current kernel, known results from various perturbative and nonperturbative approximation schemes to quantum transport in the SIAM are recovered. Using a simplified fourth-tier scheme, analytical results for the interacting SIAM are presented both in equilibrium and nonequilibrium and with an applied magnetic field.
[1] L. Magazzù and M. Grifoni, Phys. Rev. B 105, 125417 (2022)

15 min. break

DY 41.8 Thu 17:00 H22

In-Gap Band Formation in a Periodically Driven Charge Density Wave Insulator — •Alexander Osterkorn, Constantin Meyer, and Salvatore Manmana — University of Göttingen, Göttingen, Germany

Periodically driven quantum many-body systems host unconventional behavior not realized at equilibrium. Here we investigate such a setup for strongly interacting spinless fermions on a chain, which at zero temperature and strong interactions form a charge density wave insulator. Using unbiased numerical matrix product state methods for time-dependent spectral functions, we find that driving of the correlated charge-density wave insulator leads not only to a renormalization of the excitation spectrum as predicted by an effective Floquet Hamiltonian [1], but also to a cosine-like in-gap feature [2]. This is not obtained for a charge density wave model without interactions. A mean-field treatment provides a partial explanation in terms of doublon excitations. However, the full picture needs to take into account strong correlation effects. [1] Phys. Rev. Lett. 120, 127601 (2018) [2] arXiv:2205.09557

DY 41.9 Thu 17:15 H22

Non-equilibrium phases of matter in 2D using Projected Entangled Pair States — •Augustine Kshetrimayum[1,2], Dante Kennes[3], and Jens Eisert[1,2] — [1]Freie University Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]RWTH Aachen University, Germany

We explore the highly challenging realm of non-equilibrium physics in two spatial dimensions using infinite Projected Entangled Pair States (iPEPS), a two-dimensional tensor network ansatz directly in the thermodynamic limit. By adding disorder in a translationally invariant setting through the use of auxiliary states, we find evidence of Many-body localization (MBL) and Quantum time crystals in 2D.

In our discrete disorder setting, we show that many levels of disorder is required in order to achieve localization and ultimately time crystalline behavior. We discuss how our setting can be realized in programmable quantum simulators.

DY 41.10 Thu 17:30 H22

Charge transport in hybrid semiconductor-cavity systems: an exact diagonalization study — •Sebastian Stumper and Junichi Okamoto — Institute of Physics, University of Freiburg, Freiburg, Germany

Recent experiments demonstrate that the conductivity of organic semiconductors can be enhanced by hybridization with a plasmonic surface [Nat. Mat. 14, 1123 (2015)]. Motivated by these findings, we study a two-band tight-binding chain resonantly coupled to a photonic mode by an exact diagonalization technique. First, we argue that the exciton density and photon number are suppressed by the band gap, an effect which is neglected by the commonly used rotating wave approximation. Second, we determine the excitation of the semiconductor and its impact on the conductivity beyond the rotating wave approximation, i.e., including the off-resonant terms. Clean and disordered cases are compared. Finally, we discuss the real-time dynamics of electrons and holes under a uniform electric field.

DY 41.11 Thu 17:45 H22

Interplay of disorder and interactions in a periodically driven ultracold atomic system — •Arijit Dutta — Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt am Main, Germany

Periodically driven clean noninteracting systems are known to host several interesting topological phases. Particularly, for high frequency driving, they have been found to host the analogues of equilibrium topological phases, like the Haldane phase. However, upon lowering the driving frequencies these systems have been found to host anomalous phases with robust edge modes despite all Chern numbers being zero. Moreover, theoretical works have shown that adding disorder to such anomalous phases leads to quantized charge pumping through the edge modes even when all bulk states become localised. We investigate the fate of these phases in presence of electron-electron interactions of the Falicov-Kimball type.

DY 41.12 Thu 18:00 H22

Non-equilibrium optical conductivity for striped states: A time-dependent Gutzwiller analysis for the single-band Hubbard model — •Christian Martens and Götz Seibold — BTU Cottbus-Senftenberg, Institute of Physics, 03046 Cottbus, Germany

In recent years pump-probe experiments have turned out as a powerful tool to investigate the dynamics of correlated materials, e.g. transition metals or heavy fermion systems. In these experiments the system is prepared in a non-equilibrium state by a strong laser pulse, where the

relaxation is afterwards examined by standard optical techniques. This method has also been applied to stripe ordered nickelates and cuprate superconductors where it allows to study the coupled order-parameter dynamics of charge- and spin-density waves and superconductivity.

Here we use the time-dependent Gutzwiller approximation for the single-band Hubbard model to analyse the non-equilibrium dynamics for stripe ground states of different symmetry. In particular we are interested in the interplay between spin and charge dynamics which is analysed by quenching the system in the charge or spin sector. This allows us to investigate the coupled relaxation dynamics as a function of the inserted energy. In contrast to the Hartree-Fock + random-phase-approximation the optical conductivity shows high-energy double occupancy fluctuations in addition to the low-energy collective mode. In the out-of equilibrium regime we find a softening of both modes depending on the inserted energy. Moreover the double occupancy exitation broadens into a continuum.

DY 42: Statistical Physics of Biological Systems 2 (joint session BP/DY)

Time: Thursday 15:00–16:30 Location: H16

DY 42.1 Thu 15:00 H16

Sensing and making sense of fluctuating cellular states — •Felix J. Meigel[1], Lina Hellwig[2], Philipp Mergenthaler[2], and Steffen Rulands[1,3] — [1]Max Planck Institute for Physics of Complex Systems, Dresden — [2]Neurology Department, Charité University Medicine Berlin — [3]Center for Systems Biology Dresden

The self-organisation of cells into complex tissue relies on the tight regulation of cellular responses to fluctuating cues. Typically, the regulation of cell decisions is attributed to pathways controlling the concentration of molecular species in response to intrinsic or extrinsic signal. Here, by contrast, we show in the paradigmatic example of cell death that cells manipulate how fluctuations propagate across spatial scales to regulate cellular behavior. Specifically, we find that the feedback between molecular and mesoscopic organelle fluctuations gives rise to a quasi-particle degree of freedom whose intriguing kinetic properties construct a kinetic low-pass filter of time-dependent concentrations of signaling molecules. We show that the collective dynamics of the quasi-particle degree of freedom exhibits different kinetics on different temporal scales. This allows cells to distinguish between fast fluctuations and slow, biologically relevant changes in environmental signals. We demonstrate an order of magnitude effect of this phenomenon on the quality of the cell death decision and validate our predictions experimentally by dynamically perturbing the intrinsic apoptosis pathway. Our work reveals a new mechanism of cell fate decision making.

DY 42.2 Thu 15:15 H16

Guidance and optimization in branching morphogenesis — •Mehmet Can Ucar and Edouard Hannezo — Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria

The development of branched, tree-like biological structures such as lung, kidney, or the neurovascular system has been a pivotal question in biology, physics and mathematics. Recently, many studies based on combinatorial, mechanical, or stochastic models explored local, selforganizing rules leading to branched morphologies in specific systems. However, in addition to local interactions, the growth of branched structures is also regulated globally by external chemical or mechanical guidance cues. In this talk, we present our recent theoretical framework that integrates local and global regulatory mechanisms of branching morphogenesis. Combining analytical theory and numerical simulations, we show that branch orientations follow a generic scaling law that depends on the strength of global guidance. Local interactions such as self-avoidance of branches, on the other hand, lead to denser, efficiently space-filling networks, with a minimal influence on the overall shape and territory. These quantitative predictions of the model are corroborated by experimental data on sensory neurons in the zebrafish caudal fin. Finally, we discuss effects of local interactions on optimal tiling of space in branched distribution networks such as in lymphatic vasculature.

DY 42.3 Thu 15:30 H16

Random force yielding transition in spherical epithelia — Aboutaleb Amiri[1], Charlie Duclut[2], Frank Jülicher[1], and •Marko Popović[1] — [1]Max Planck Institute for Physics of Complex Systems, Dresden — [2]Université Paris Diderot, Paris

Developing biological tissues are often described as active viscoelastic fluids on long time-scales, due to fluidization by cell division and apoptosis. However, on shorter time-scales they can behave as amorphous solids with a finite yield stress [Mongera et al., Nature, 2018]. Under shear stress beyond the yield stress value amorphous solids begin to flow. This yielding transition is a dynamical phase transition characterized by a diverging correlation length and a set of critical exponents. Developing tissues are active matter systems whose constitutive cells can propel themselves by exerting traction forces. Recently, a remarkable correspondence has been proposed between uniformly sheared amorphous solids and dense self-propelled particle systems [Morse et al., PNAS, 2021] based on the identical scaling of non-linear properties of their energy landscapes. Here, we use a vertex model of epithelial tissues to study how randomly oriented traction forces fluidize a spherical epithelial tissue. In particular, we identify a sharp transition between quiescent and randomly flowing states separated by the critical value of the traction force magnitude, analogous to the yield stress. Moreover, we show that this transition is characterized by the same set of exponents as the classical yielding transition, and the corresponding scaling relations provide a non-trivial relation between cell geometry, cell rearrangement dynamics and tissue flow.

DY 42.4 Thu 15:45 H16

Biological tissues as living amorphous solids — •Ali Tahaei and Marko Popović — Max Planck Institute for Physics of Complex Systems, Dresden

Biological tissues are often described as viscoelastic fluids on long time-scales. However, on shorter times-scales, tissues can behave as amorphous solids, such as clay, changing shape only when exposed to a shear stress above the material yield stress Σ_c. Amorphous solids near Σ_c display critical behaviour with a diverging correlation length-scale characterising dynamics of plastic activity. Here, we ask how would this critical behaviour be affected by active processes present in biological tissues, such as cell divisions.

In order to model yielding of biological tissues we employ the mesoscopic elasto-plastic model, commonly used to describe yielding of amorphous solids. Here, we extend the classical elasto-plastic model by introducing cell divisions as an additional source of plastic activity. We find that cell divisions strongly fluidise the solid phase of the system at stresses lower than Σ_c, consistent with literature. Furthermore, we find that critical behaviour is strongly suppressed, leading to localised dynamics of plastic activity nucleated by cell divisions. Finally, in our model we can describe how well is the cell division orientation aligned with local shear stress. We find that low alignment strength leads to less mechanically stable tissues where, consequently, most of the plastic flow arises from cell rearrangements, and vice versa.

DY 42.5 Thu 16:00 H16

Order-disorder transition in epithelial tissues — •Kartik Chhajed, Marko Popović, and Frank Jülicher — Max Planck Institute for Physics of Complex Systems, Dresden

Two dimensional packings of cells in developing epithelial tissues are commonly found to be disordered. However, highly organised packings can emerge during development, such as hexagonal pattern of ommatidia in the eye epithelium of the fruit fly. Here, we observe a disorder to order transition in the packing of the fruit fly pupal wing epithelium. In particular, we find a sudden increase in the hexatic order parameter ψ_6, which suggests a presence of hexatic and crystalline phases in two dimensional systems, as described by the classical KTHNY theory. The melting transition scenario with the intermediate hexatic phase has been reproduced in a model of epithelial tissues [Pashupalak et al. Soft Matter, 2020] where the stochastic active forces generated by the cells play the role of an effective temperature. However, both KTHNY theory and recent literature on packings of epithelial tissues assume uniform properties of particles and cells, respectively. In a proliferating tissue cells grow and divide, which inevitably leads to a heterogeneity of cell sizes. Here, we use the vertex model of epithelial

tissues to study how the disorder to order transition is affected by the heterogeneity of cell sizes. We find that reducing cell heterogeneity as a control parameter drives the system through an ordering transition. We compare our results with the experimental data of the fruit fly wing to identify the role of cell size heterogeneity in the observed disorder to order transition.

DY 42.6 Thu 16:15 H16

The Influence of Contact Maps on RNA Structure Prediction — •Christian Faber[1] and Alexander Schug[1,2] — [1]Jülich Supercomputing Centre, FZ Jülich — [2]Steinbuch Centre for Computing, KIT

The 3d structure of Proteins and non coding RNA are essential for their function, but hard to determine via NMR or x-ray crystallography. Therefore an effective way of simulation with the knowledge of the sequence only would be a huge improvement. Impressive progress has been made in recent years, most notably AlphaFold2 for protein structure prediction using Machine Learning techniques. Such a break through is still missing for RNA.

For RNA, there are folding programs such as SimRNA, that simulate the structure with a physical force field [1]. The outcome can be improved by incorporating evolutionary data from homologous sequences. From the evolutionary data, we can make predictions about possible contacts in the form of contact maps [2].

We investigate how contact maps can influence prediction quality and what are particularly valuable contacts. From these insights we develop new measures for machine learning algorithms.

[1] Boniecki, M. J. et al. *SimRNA: a coarse-grained method for RNA folding simulations and 3D structure prediction.* Nucleic Acids Research 44, e63 (2016).

[2] Weigt, M., White, R. A., Szurmant, H., Hoch, J. A., Hwa, T. *Identification of direct residue contacts in protein-protein interaction by message passing.* PNAS 106, 67-72 (2009).

DY 43: Poster Session: Quantum Chaos and Many-Body Dynamics

Time: Thursday 15:00–18:00 Location: P2

DY 43.1 Thu 15:00 P2

Localization persisting under aperiodic driving — •Hongzheng Zhao[1,2], Florian Mintert[2], Johannes Knolle[2,3,4], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Imperial College London, London, United Kingdom — [3]Technical University of Munich, Munich, Germany — [4]Munich Center for Quantum Science and Technology, Munich, Germany

Localization may survive in periodically driven (Floquet) quantum systems, but is generally unstable for aperiodic drives. In this work, we identify a hidden conservation law originating from a chiral symmetry in a disordered spin-1/2 XX chain. This protects indefinitely long-lived localization for general–even aperiodic–drives. Therefore, rather counter-intuitively, adding further potential disorder which spoils the conservation law delocalizes the system, via a controllable parametrically long-lived prethermal regime. This provides a first example of persistent single-particle 'localization without eigenstates'. Reference: arXiv:2111.13558

DY 43.2 Thu 15:00 P2

Prethermalization in confined spin chains — •Stefan Birnkammer, Alvise Bastianello, and Michael Knap — Technical University Munich, Germany

Unconventional nonequilibrium phases with restricted correlation spreading and slow entanglement growth have been proposed to emerge in systems with confined excitations, calling their thermalization dynamics into question. Here, we investigate the many-body dynamics of a confined Ising spin chain, in which domain walls in the ordered phase form bound states reminiscent of mesons. We show that the thermalization dynamics after a quantum quench exhibits multiple stages with well separated time scales. The system first relaxes towards a prethermal state, described by a Gibbs ensemble with conserved meson number. The prethermal state arises from rare events in which mesons are created in close vicinity, leading to an avalanche of scattering events. Only at much later times a true thermal equilibrium is achieved in which the meson number conservation is violated by a mechanism akin to the Schwinger effect.

DY 43.3 Thu 15:00 P2

Enhanced state transfer by complex instability in coupled tops — •Maximilian Friedrich Irenäus Kieler and Arnd Bäcker — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

By considering coupled tops we provide a mechanism for a fast transfer between two specific states representing bits. This crucially relies on that fact that the semiclassical limit corresponds to a higher-dimensional system which allows for more types of stability of fixed points than the two-dimensional case. Tuning the parameters, the coupled tops have fixed points with complex instability. Quantum mechanically this allows for a rapid transfer between coherent states located at these points, which is much faster than the coexisting dynamical tunneling.

DY 43.4 Thu 15:00 P2

Quantum signatures of partial barriers in 4D symplectic maps — •Jonas Stöber, Arnd Bäcker, and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

Partial transport barriers in the chaotic sea of Hamiltonian systems restrict classical transport, as they only allow for a small flux between phase-space regions. Quantum mechanically for 2D symplectic maps one has a universal quantum localizing transition: quantum transport is suppressed if the Planck cell of size h is much greater than the flux Φ, while mimicking classical transport if h is much smaller. The scaling parameter is Φ/h.

In a higher-dimensional 4D map one would naively expect that the relevant scaling parameter is Φ/h^2. However, we show that due to dynamical localization along resonance channels the localization length modifies the scaling parameter. This is demonstrated for coupled kicked rotors for a partial barrier that generalizes a cantorus to higher dimensions.

DY 43.5 Thu 15:00 P2

Metallicity in the Dissipative Hubbard-Holstein Model: Markovian and Non-Markovian Tensor-Network Methods for Open Quantum Many-Body Systems — •Mattia Moroder[1], Martin Grundner[1], François Damanet[2], Ulrich Schollwöck[1], Sam Mardazad[1], Thomas Köhler[3], Sebastian Paeckel[1], and Stuart Flannigan[4] — [1]Department of Physics, Ludwig-Maximilians-Universität München, München, Germany — [2]Institut de Physique Nucléaire, Atomique et de Spectroscopie, CESAM, University of Liège, B-4000 Liège, Belgium — [3]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [4]Department of Physics & SUPA, University of Strathclyde, Glasgow G4 0NG, United Kingdom

We investigate the impact of dissipation on polarons and bipolarons in the paradigmatic Hubbard-Holstein model. We do so by combining the non-Markovian hierarchy of pure states (HOPS) method and the Markovian Quantum Jump (QJ) method with the newly-developed projected-purification (PP) method for matrix-product states (MPS).

By studying the system's dynamics after global quenches from different ground states, we show that dissipation reduces the polaron's mobility and the electron pairing.

We also find that PP gives a significant speedup (proportional to the phononic local Hilbert space dimension) and allows to systematically converge all observables to very high accuracy in an automated fashion.

DY 43.6 Thu 15:00 P2

Time evolution in the one-magnon subspace of the sawtooth chain at the quantum-critical point. — •Jannis Eckseler and Jürgen Schnack — Fakultät für Physik, Universität Bielefeld, Postfach 100131, D-33501 Bielefeld, Germany

It is known for the sawtooth chain to develop a flat band at the quantum-critical point of $J_1 = 2J_2$ [1]. We are looking at the time evolution of several observables in the one-magnon subspace of the

sawtooth chain, especially near that point.

[1] J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. 88 (2002) 167207

DY 43.7 Thu 15:00 P2

Nonequilibrium dynamics in quantum spin systems with neural quantum states — •Damian Hofmann[1], Giammarco Fabiani[2], Johan Mentink[2], Giuseppe Carleo[3], Martin Claassen[4], and Michael Sentef[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free-Electron Laser Science (CFEL), Luruper Chaussee 149, 22761 Hamburg, Gemany — [2]Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [3]Institute of Physics, École polytechnique fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland — [4]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA

Neural quantum states (NQS) are a variational ansatz in which a neural network is used to parametrize the quantum state of a many-body system. NQS-based methods can be applied to learning both ground states and dynamics of quantum many-body systems by optimizing the network weights as variational parameters. In this poster, we present our current efforts in applying NQS methods to simulating strongly correlated quantum systems in and out of equilibrium. In particular, we highlight our recent work on understanding the stability properties of time-evolution algorithms for NQS based on the time-dependent variational Monte Carlo method (Hofmann et al., SciPost Phys. 12, 2022). Furthermore, we will present our ongoing research into the application of NQS to learning states in quantum spin liquid systems.

DY 43.8 Thu 15:00 P2

Source-driven optical microcavities — •Lukas Seemann and Martina Hentschel — TU Chemnitz

Optical microcavities – open billiards for light – are known to possess far field emission patterns that sensitively depend on their geometric shape: the geometry determines the light's nonlinear dynamics and, via the associated unstable manifold and invariant measure, the emission characteristics. However, this behavior might change, and new features can be added, when the microcavity is driven by a local internal light source [1]. Here, we investigate the properties of optical microcavities with sources both with ray and with wave methods. To this end we extend the ray picture by the phase information and collect the wavelength-dependent phase information along the ray trajectories. We use phase-space methods to analyze the source-induced time-dependent dynamics and compare the Poincaré surface of section for rays with phase to the Husimi function dynamics of wave solutions, thereby exploring chances and limitations of ray-wave correspondence.

[1] J.-K. Schrepfer, S. Chen, M.-H. Liu, K. Richter, and M. Hentschel, Phys. Rev. B 104, 155436 (2021)

DY 44: Poster Session: Statistical Physics and Critical Phenomena

Time: Thursday 15:00–18:00 Location: P2

DY 44.1 Thu 15:00 P2

How to distinguish between indistinguishable particles — •Michael te Vrugt — Institut für Theoretische Physik, Center for Soft Nanoscience, Philosophisches Seminar, 48149 Münster, Germany

Does exchanging two indistinguishable particles lead to a new physical state? While the answer appears to be clear in quantum mechanics (no), the situation in *classical* statistical mechanics is up to considerable debate. In this work [1], we show that order-preserving dynamics, a recently developed formalism that allows for an accurate treatment of single-file diffusion within dynamical density functional theory, provides a strong argument for haecceitism (the view that such an exchange does make a difference) since it requires treating observationally indistinguishable particle configurations as being different. This result turns out to have interesting consequences for the concept of thermodynamic equilibrium.

[1] M. te Vrugt, Br. J. Phil. Sci. (forthcoming), doi: 10.1086/718495

DY 44.2 Thu 15:00 P2

Operationally Accessible Uncertainty Relations for Thermodynamically Consistent Semi-Markov Processes — •Benjamin Ertel, Jann van der Meer, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Semi-Markov processes generalize Markov processes by adding temporal memory effects as expressed by a semi-Markov kernel. We recall the path weight for a semi-Markov trajectory and the fact that thermodynamic consistency in equilibrium imposes a crucial condition called direction-time independence for which we present an alternative derivation. We prove a thermodynamic uncertainty relation that formally resembles the one for a discrete-time Markov process. The result relates the entropy production of the semi-Markov process to mean and variance of steady-state currents. We prove a further thermodynamic uncertainty relation valid for semi-Markov descriptions of coarse-grained Markov processes that emerge by grouping states together. A violation of this inequality can be used as an inference tool to conclude that a given semi-Markov process cannot result from coarse-graining an underlying Markov one. We illustrate these results with representative examples [1].

[1] Benjamin Ertel, Jann van der Meer and Udo Seifert, Phys. Rev. E 105, 044113 (2022)

DY 44.3 Thu 15:00 P2

Lane formation of gravitationally driven model colloids in two-dimensional linear channels — •Marc Isele, Kay Hofmann, and Peter Nielaba — Physics Department, University of Konstanz, Konstanz, Germany

We conducted Brownian dynamics simulations to investigate the segregation phenomena of driven model colloids in two-dimensional linear channels. Two kinds of spherical particles of different sizes were driven in the same direction by a gravitational force. The difference in driving force acting on these particles creates a segregation similar to the lane formation of oppositely driven colloids. We had a closer look at parameter values facilitating lane formation and the resulting lanes were examined more closely. This approach creates a system which is easier to reproduce in experiments than the conventional oppositely driven setups by tilting a linear channel with two particle kinds of different size.

DY 44.4 Thu 15:00 P2

Geometric Brownian Information Engine : Essentials of optimal work and performance. — •Rafna Rafeek, Syed Yunus Ali, and Debasish Mondal — Department of Chemistry and Center for Molecular and Optical Sciences & Technologies, Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh, India

We investigate a Geometric Brownian Information Engine (GBIE) in the presence of an error-free feedback controller that transforms the information gathered on the state of particles entrapped in mono-lobal geometric detention into extractable work. We determine the benchmarks for utilizing the available information in an output work and the optimum operating requisites for best performance. Apart from a reference measurement distance xm and feedback site xf , upshots of the information engine also depend on the transverse constant bias force(G). G tunes the entropic contribution in the effective potential and the standard deviation (σ) of the equilibrium marginal probability distribution.

We find that the upper bound of the achievable work shows a crossover from (5/3-2ln2)kBT to 1/2kBT when the system changes from entropy to an energy-dominated one.The higher loss of information during the relaxation process, accredits the lower value of work in entropic instances of GBIE. We recognize that the work extraction reaches a global maximum when xf=2xm with xm=0.6σ, irrespective of the extent of the entropic limitation. Also we explore the effect of entropic control on the unidirectional passage of the particle and efficacy of the GBIE.

DY 44.5 Thu 15:00 P2

Shear flow induced instability of a trapped colloidal particle in a complex medium — •Lea Fernandez and Sabine H.L. Klapp — Institute for Theoretical Physics, TU Berlin

The motion of a colloidal particle in a complex medium, bound by an optical trap and subjected to a shear flow can be modelled by the Lanvegin equations for an over-damped harmonic oscillator in n

dimensions. Here we treat n_{obs} observed, physical variables, with $n = n_{obs} + n_{int}$, and n_{int} internal, auxiliary variables modelling a complex medium. Analytical and numerical results are presented for $n_{obs} = 2$ and $n_{int} = 1$, where the coupling between the observed variables is given by a plane Couette flow. We analyse the dynamics of averages, probability densities, and trajectories using Brownian dynamics and the Smoluchowski equation. Of special interest is the effect of the coupling with the auxiliary variable. The focus is on coupling parameters where the steady shear flow causes a transition from a stationary state to an in-stationary state, corresponding to a delocalisation of the particle, when the shear rate exceeded a critical value.

DY 44.6 Thu 15:00 P2

Quantifying the potential energy landscape within nanoconfinements by MD simulations — •Simon Hefner, Robin Horstmann, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Nanoconfinements find applications in various fields from catalysis to electronics, [1] although the properties of confined systems are still not fully understood. For instance, the effects of different kinds of confinements on the dynamical and structural properties of confined liquids are still elusive. To obtain a better understanding of those effects MD simulations are well suited [2]. Here, we performed simulations for TIP4P/2005 water. Neutral pores of water were prepared. From the time-averaged static density profile in the pore the potential energy landscape was reconstructed and the energy barrier against water motion at the wall and in bulk were calculated and compared. We calculated the temperature and radial dependence of the energy barrier. The translational dynamics of water can be derived form the obtained energy landscape using the Arrhenius law. We further applied these methods to other kinds of pore systems and liquids and compared the results.

[1] Clancy,Adam J. et al. Chem. Rev., **2018**, *118* (16), 7363-7408
[2] Horstmann, R. et al, Langmuir, https://doi.org/10.1021/acs.langmuir.2c00521

DY 44.7 Thu 15:00 P2

Fluctuations of work and heat in a driven entropic potential — •Syed Yunus Ali, Prashanta Bauri, and Debasish Mondal — Department of Chemistry and Center for Molecular and Optical Sciences & Technologies, Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh, India

We consider the motion of an over-damped Brownian particle in two-dimensional bilobal confinement driven by a periodic field in the presence of a transverse bias force. The confinement results in an entropic bistable potential in a reduced dimension. We calculate the work done and absorbed heat over a period and their mean and relative variance fluctuations in entropy and energy-dominated regimes. The average work done and absorbed heat over a period show turnover behavior as a function of noise strength and frequency input. Therefore, these observables can be considered potential quantifiers of the entropic stochastic resonance phenomena. We find that the heat fluctuations over a single period are always greater than the work fluctuations. We also discuss the applicability of steady-state fluctuation theorems in this system.

DY 44.8 Thu 15:00 P2

Exploiting Brownian motion and correlations for computing — •Alessandro Pignedoli[1] and Karin Everschor-Sitte[2] — [1]Twist Group, Faculty of Physics, University of Duisburg-Essen — [2]Twist Group, Faculty of Physics, University of Duisburg-Essen

Brownian motion is a natural phenomenon that can be exploited for computing [1]. Particle swarm optimization [2] based on the ideas of swarm intelligence is an example of this sort of computation. While the random motion of particles allows the exploration of the entire phase space of the system, interactions and driving forces break ergodicity. This allows for an efficient solution to an optimization problem, which can be identified by looking at the system's correlations and statistical observables. To accomplish Brownian computation, we employ a Langevin model to describe magnetic skyrmions [3], which are topologically stable magnetic whirls that have been shown to behave like interacting Brownian particles [4].

[1] C.H. Bennett, Int. J. Theor. Phys. 21, 905 (1982). [2] J. Kennedy and R. Eberhart, Proc. of ICNN'95 * Int. Conf. on Neural Networks, 4, 1942 (1995) [3] K. Everschor-Sitte, J. Masell, R. M. Reeve and M. Kläui, J. Appl. Phys. 124, 240901 (2018) [4] J. Zázvorka, et al. Nat. Nanotechnol. 14, 658 (2019)

DY 44.9 Thu 15:00 P2

Overload wave-memory induces amnesia of a self-propelled particle — •Maxime Hubert[1], Stéphane Perrard[2], Nicolas Vandewalle[3], and Matthieu Labousse[4] — [1]PULS group, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]PMMH, ESPCI Paris and PSL University, Paris, France — [3]GRASP, University of Liège, Liège, Belgium — [4]Guliver, ESPCI Paris and PSL University, Paris, France

"Walking droplets" constitute a model system to investigate active transport dynamics driven by complex memory kernels. The droplet stores positional information in a wavefield at an oil interface that in return serves as a propulsive mechanism. The complexity of the wavefield and the amount of positional information are remotely controlled through a single scalar value, the memory of the system, which corresponds to the persistence time of the waves. In this study, we investigate the high-memory limit of both the droplet and the wavefield dynamics. We show that an overload of memory brings the droplet to a diffusive dynamics which cannot be distinguished from a active markovian dynamics. The wavefield however contains all the correlations of the dynamics and exhibits an energy-minimization principle and equipartition of energy in the eigenmodes of the wavefield.

DY 44.10 Thu 15:00 P2

Coarse-graining of systems with discrete Markovian dynamics — Stefan Klumpp and •Miguel Rodríguez Martín — Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen.

There exists a wide range of physical systems that can be described by discrete Markovian dynamics. In many cases it is desirable to reduce the number of states in order to lower the computational cost or obtain an effective description that captures the most relevant effects at a given scale. A steady state-conserving method of coarse graining based on merging adjacent states and obtaining new transition rates from the optimization of the Kullback-Leibler divergence is generalized by minimizing the Rényi divergence instead. The resulting transition rates depend on the quotients between the steady state probabilities of the merged states in the original system, so a method is developed to compute these transition rates without the need of finding the steady state probabilities. Making use of the similarities between the master equation and Schrödinger's equation, a formulation for classical discrete Markov processes analogous to quantum mechanics is developed, both in the frame of Schrödinger's formulation and second quantization. These are used to study coarse graining under the constraint that the steady state must be conserved.

DY 44.11 Thu 15:00 P2

Molecular dynamics simulations of binary mixtures in nanostructured pores — Niels Müller, Michael Vogel, and •Markus Haneke — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Water and its mixtures are fairly common in nature and technology.

Here, we seek to understand the influence of solid surfaces with nanostructured porous confinements on binary aqueous mixtures. For this purpose, we exploit that MDS allow us to determine structural and dynamical properties in a spatially resolved manner. The inner surfaces and the aqueous mixtures of the simulated systems are made of differently polarized molecules. The composition and temperature are varied, approaching the regime of spinodal decomposition.

We find that the nanostructured surfaces impose a corresponding nanoscopic phase separation onto the confined mixtures. Explicitly, the concentration of the mixture components varies along the pore axis in phase with the surface patterning, where the effect is stronger near the pore walls. Moreover, the particle mobility differs between the components and depends on the position within the porous confinement. In particular, the imposed concentration fluctuations cause diffusion barriers.

DY 44.12 Thu 15:00 P2

Microcanonical analysis of model polymers interacting via many-body dispersion — •Benedikt Ames, Mario Galante, Matteo Gori, and Alexandre Tkatchenko — Department of Physics and Materials Science, Université du Luxembourg

Non-covalent interactions play a crucial role in the energetics and structure formation of many systems of interest for physics, chemistry and biology.

Among computational methods which include van der Waals (vdW) interactions, the many-body dispersion framework (MBD) attains an excellent accuracy by accounting for all orders of the coupling. Its application has shown the importance of going beyond the pairwise (PW) approximation, for example to obtain the correct energy ordering of molecular crystals and for the adhesion of 2D structures. Nevertheless, the phenomena of MBD-driven dynamics remain largely unexplored.

Here, as a means to probe these dynamics, we study the phase transitions of a simplified model polymer via microcanonical inflection point analysis [1], a recent generalization of the notion of phase transitions from the thermodynamic limit to finite-size systems. By contrasting simulations using MBD and PW methods, we explore whether the different characteristics of each vdW model manifest themselves in distinct properties of the polymer's clustering transition.

[1] Koci, Qi and Bachmann, J. Phys.: Conf. Ser. 759, 012013 (2016).

DY 44.13 Thu 15:00 P2

Arcsine laws in non-equilibrium regime — •Avijit Kundu[1,2], Raunak Dey[2], Biswajit Das[2], and Ayan Banerjee[2] — [1]University of Bayreuth, Universitystrasse 30, 95447, Bayreuth, Germany — [2]Indian Institute of Science Education and Research Kolkata, Mohanpur, Kalyani, 741246, India

Most of the processes in the mesoscopic world especially inside living cell are far from thermal equilibrium. The time evolution of such processes is important to study to characterize the processes. Remarkably, Paul Lévy defined arcsine laws for three variables related to the stochastic Wiener process. Here we have studied stochastically driven colloidal particle in a viscous fluid and observed the entropic current, work done on the system or dissipated by it, follow the Lévy arcsine laws in the large time limit. The significant lead of this work is to show the convergence of cumulative distribution to the arcsine law is faster for the case of near equilibrium system where the entropy production rate is smaller. We also have tested the convergence rates of cumulative distributions for different non-equilibrium systems by driving the optically trapped colloidal probe with external noise parameters and changing the flow field by introducing a microbubble in its vicinity.

DY 44.14 Thu 15:00 P2

Phase transition in clustering algorithms — •Julian Zitterich and Alexander K. Hartmann — Institute of Physics, University of Oldenburg, Germany

A well known problem in data analysis and machine learning is the clustering problem. It consists of grouping a set of data vectors into subsets, such that *similar* vectors end up in the same subset. How to define similarity and how to find these subgroups depend much on the investigated problem, thus many algorithms and metrics exists. Also it may that an algorithm is not able to successfully detect structure in the given data. Thus, we study here ensembles of artificially generated data controlled by parameters such that for some parameter values the clustering is *easy* or at least *possible* while for other values it is *hard* or *impossible*. Thus, from a statistical physics viewpoint we are interested in phase transitions of the clustering problem between such phases. Previously, the existence of such phase transitions was observed for a single ensemble in high-dimensional space by using the AMP algorithm [1]. Here, we investigate numerically [2] four different state-of-the-art cluster algorithms and analyse their behaviour for increasingly complex ensembles. Low complexity ensembles are realized by direct sampling of data vectors, while high complexity ensembles are implemented by short simulations of simple models of interacting particles.

[1] T. Lesieur et al., 54th Annual Allerton Conference on Communication, Control, and Computing (Allerton), arXiv:1610.02918 (2016)
[2] A.K. Hartmann, *Big Practical Guide to Computer Simulations*, World Scientific (2015)

DY 44.15 Thu 15:00 P2

Chemfiles: reading and writing atomistic modeling files — •Guillaume Fraux — Institute of Materials, EPFL, Lausanne, Switzerland

Running atomistic simulations produces enormous amounts of data, which has to be post-processed in order to extract scientifically relevant information. Unfortunately, this task is made much harder by the vast menagerie of existing file formats, all containing similar data in a different formatting.

Chemfiles is a software library providing a unified interface to these formats, allowing researchers to spend their time analyzing their data instead of writing file parsers over and over. Chemfiles is implemented in C++, and provides programming interfaces to most of the scientific languages: Python, Fortran, C, Rust and Julia. 21 different formats are currently supported, including both text and binary (i.e. XTC, TNG, DCD, ...) formats. All text formats can be read and written with multiple compression standards (gzip, xz, bzip2). Chemfiles also offers a comprehensive atom selection language, including the unique feature of simultaneous selection of multiple atoms (e.g. `pairs: name(#1) == H and name(#2) == O and distance(#1, #2) < 3.0`).

Overall, chemfiles one of the fastest libraries for reading files used in atomistic simulation, being between 20% and 10 times faster than other commonly used libraries; while offering a simpler and easy to use programming interface; freeing up time for scientists working with these file formats.

DY 44.16 Thu 15:00 P2

Phase transitions for two-stage stochastic minimum spanning tree optimisation problem — •Robert Strassen and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

Phase transitions in classical optimization problems have been studied extensively in statistical physics [1]. Here, we consider two-stage stochastic optimization problems, where the optimization is performed in two different stages, such that in the first stage not all information is available. In particular, we consider the two-stage stochastic minimum spanning tree (MST) problem for undirected graphs with given initial edge costs. In the second stage, one of a set of random scenarios is realized, involving different edge costs. In each stage, edges can be selected such that a spanning tree is finally formed, aiming at a minimum expected total costs. Unlike the conventional MST problem, the two-stage version is generally worts-case "hard" to solve, even though there are problem instances that are "easy". We investigate numerically [2] the problem by the calculation of bounds and applying several approximation algorithms, including one of Dhamdere et al. [3] on various random ensembles of graphs. Our aim is to find out whether there are phase transitions between typical easy and hard problem phases.

[1] A.K. Hartmann and M. Weigt, *Phase Transitions in Optimization Problems*, Wiley-VCH, Berlin 2005
[2] A.K. Hartmann, *Big Practical Guide to Computer Simulations*, World-Scientific, Singapore, 2015
[3] K. Dhamdhere, R. Ravi, M. Singh, IPCO 2005, LNCS **3509**, pp. 321-334, (2005)

DY 44.17 Thu 15:00 P2

Critical Casimir effect in the square-lattice Ising model with quenched surface disorder — •Luca Cervellera and Alfred Hucht — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

For the 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 random boundary conditions at one boundary, we determine the full density of thermodynamic states $\omega(\delta F, m_B)$, with residual free energy δF and boundary magnetization m_B at criticality. From this quantity we can derive the disorder averaged Casimir potential for different aspect ratios and disorder ensembles.

DY 44.18 Thu 15:00 P2

Anomalous collective dynamics of auto-chemotactic populations — Jasper van der Kolk[1], Florian Rasshofer[1], •Richard Swiderski[1], Astik Haldar[2], Abhik Basu[2], and Erwin Frey[1,3] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Munich, Germany — [2]Theory Division, Saha Institute of Nuclear Physics, HBNI, 1/AF Bidhannagar, Calcutta 700 064, West Bengal, India — [3]Max Planck School Matter to Life, Hofgartenstraße 8, 80539 Munich, Germany

While the role of local interactions in nonequilibrium phase transitions is well studied, a fun- damental understanding of the effects of long-range interactions is lacking. We study the critical dynamics of reproducing agents subject to auto-chemotactic interactions and limited resources. A renormalization group analysis reveals distinct scaling regimes for fast (attractive or repulsive) interactions; for slow signal transduction the dynamics is dominated by a diffusive fixed point. Further, we present a novel nonlinear mechanism that stabilizes the continuous transition against the emergence of a characteristic length scale due to a chemotactic collapse.

DY 44.19 Thu 15:00 P2

Multifractality at the integer quantum Hall transition — •Martin Puschmann[1], Daniel Hernangómez-Pérez[2], Bruno Lang[3], Soumya Bera[4], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93053 Regensburg, Germany — [2]Department of Molecular Chemistry and Material Science, Weizmann Institute of Science, Rehovot 7610001, Israel — [3]IMACM and Institute of Applied Computer Science, Bergische Universität Wuppertal, D-42119 Wuppertal, Germany — [4]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

The quantum Hall transitions are still one of the bigger mysteries of condensed matter theory. In the past twenty years several conjectures have been made as to what the field theory of the critical fixed point of the integer (class A) quantum Hall transition could be. The multifractal spectrum provides a characteristic fingerprint of the phase transition. Here, recent analytical work predicts a parabolic dependency of the anomalous dimension $\Delta_q = q(1-q)/4$, where the exponents $\tau_q = 2(q-1) + \Delta_q$ describe the system-size scaling of wavefunction moments $|\Psi|^{2q}$ [1]. In great analogy to our previous analysis on the spin (class C) quantum Hall transition [2], we investigate the multifractal spectrum of the class A transition and similarly demonstrate the presence of quartic terms in Δ_q. Our findings are thus clearly inconsistent with the strict parabolicity predicted for "traditional" conformal field theories. [1] M. R. Zirnbauer, Nucl. Phys. B 941, 458 (2019) [2] M. Puschmann et al., Phys. Rev. B 103, 235167 (2021)

DY 44.20 Thu 15:00 P2

Detection of defects in soft quasicrystals with neural networks — •Ali Doener and Michael Schmiedeberg — Theoretische Physik I, Erlangen, DE

The aim of this work is to construct and employ a neural network for the detection of topological defects in dodecagonal quasicystalline patterns. Even though quasircrystals are aperiodic, they exhibit a longe-range order. Furthermore, in principle any discrete rotational symmetry can occur.

In this work, dodecagonal quasicrystalline patterns in two-dimensions with a built-in dislocation are generated and employed as input images of the neural network. The network then should figure out not only the position but also the type of the Burgers vector of the defect.

Our trained neural network is able to recognize the type of the Burgers vector very good. The position of the dislocation is recognized up to a mean deviation from the real position that is much smaller that the small length scale in the quasicrystals. In future, we want to train the network with patterns that contain multiple dislocations as well as phasonic excitations.

DY 45: Poster Session: Nonlinear Dynamics, Pattern Formation, Data Analytics and Machine Learning

Time: Thursday 15:00–18:00 Location: P2

DY 45.1 Thu 15:00 P2

Influence of protective measures on rare-event behavior of the dynamics of the SIR model. — •Timo Marks, Yannick Feld, and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

Since the outbreak of the SARS-CoV-2 pandemic in early 2020, there has been a surge of interest in modeling disease spreading. The basis of many more complex models is the SIR model [1], in which the population is divided into a group of *Susceptible*, *Infected* and *Recovered* individuals.

Here, the SIR model is applied to a small-world ensemble that can model social interactions of a real population [2]. Using large-deviation methods and in particular the Wang-Landau algorithm, the distributions of quantities of interest can be calculated over basically the full support [3]. To include protective measures, once a predefined threshold of simultaneously infected nodes is reached, the transmission parameter is decreased. We compare the impact of these measures with unrestrained disease spreading on the level of the full probability distributions, which were obtained down to probabilities such as 10^{-50}. We thereby observe significant changes in the shape of the distributions.

[1] W. O. Kermack and A. G. McKendrick, Proc. R. Soc. Lond. A **115**, 700*721 (1927)
[2] S. Milgram, Psychology Today **1**, 60*67 (1967)
[3] Y. Feld, A. K. Hartmann, PhysRevE.105.034313 (2022)

DY 45.2 Thu 15:00 P2

Pattern Formation in non-ideal systems: From Turing patterns to active droplets — •Lucas Menou and David Zwicker — Max Planck Institute für dynamik und selbstorganisation, Göttingen, Germany

Turing's seminal reaction-diffusion model explains how patterns form in non-equilibrium systems. Typical Turing models assume ideal diffusion, which implies dilute or ideal systems. In contrast, active droplets use chemical reactions to control phase separation emerging in strongly interacting systems. We unite both theories by combining the classical Cahn-Hilliard model, which describes non-ideal solutions, with the typical non-linear reactions responsible for Turing patterns. We find that interactions can promote or suppress the emergence of periodic patterns. Interestingly, patterns can form even when all species have equal diffusivity, which is impossible in traditional Turing models. Taken together, our theory shows a rich behavior that interpolates between the traditional Turing patterns and active droplets.

DY 45.3 Thu 15:00 P2

Chaotic Diffusion in Delay Systems: Giant Enhancement by Time Lag Modulation — •Tony Albers, David Müller-Bender, Lukas Hille, and Günter Radons — Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

We consider a typical class of systems with delayed nonlinearity, which we show to exhibit chaotic diffusion. It is demonstrated that a periodic modulation of the time-lag can lead to an enhancement of the diffusion constant by several orders of magnitude. This effect is the largest if the circle map defined by the modulation shows mode locking and more specifically, fulfills the conditions for laminar chaos. Thus we establish for the first time a connection between Arnold tongue structures in parameter space and diffusive properties of a delay system. Counterintuitively, the enhancement of diffusion is accompanied by a strong reduction of the effective dimensionality of the system.

Details can be found in: T. Albers, D. Müller-Bender, L. Hille, and G. Radons, Phys. Rev. Lett. **128**, 074101 (2022)

DY 45.4 Thu 15:00 P2

Bistable vortices formed by active particles with retarded interactions — Xiangzun Wang[1], •Pin-Chuan Chen[2], Klaus Kroy[2], Viktor Holubec[3], and Frank Cichos[1] — [1]Peter Debye Institute for Soft Matter Physics, Leipzig Univeristy, Leipzig, Germany — [2]Institute for Theoretical Physics, Leipzig University, Leipzig, Germany — [3]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

In recent experiments done in the Molecular Nanophotonics Group in the Peter Debye Institute, thermophoretic microswimmers are observed to self-assemble into bi-stable rotational modes due to retarded attractive interactions.

For the particular case where a single swimmer is attracted to an immobilized target, we show how we can analytically understand such non-linear stochastic time-delayed system. This could be achieved by Taylor expanding the equation for small time delay. The system can then be described by an overdamped Langevin equation with a potential determined by time delay, and the transition in between the two stable modes is well predicted by Kramers' escape rate. However, expanding the delayed term in Taylor series is actually not as trivial as it seems to be, as instability would occur if we keep derivatives up to arbitrarily high orders.

For the case where multiple swimmers are present, the swimmers form a cluster with co-rotating and counter-rotating shells. We further discuss the competition between the time-delay and hydrodynamic effects, which result in this phenomenon.

DY 45.5 Thu 15:00 P2

Synchronizing Cells Based on Local Interactions — •Stephan

Kremser, Mareike Bojer, and Ulrich Gerland — Physics Department, Technical University of Munich

Tissue-wide temporal synchronization of cellular processes is a desirable property for many systems in synthetic and developmental biology. Here, we look at a setting were cells have only limited information about the behavior of neighboring cells, receiving new information only after these neighbors change their internal state. Under these assumptions, we ask if global synchronization can be reached based on local (e.g. direct contact) interactions. We develop a conceptual model of the synchronization process and explore it computationally for different dimensions and interaction network topologies of the tissue. We show that temporal corrections to cellular processes based on magnitude ('proportional feedback control') or sign ('on-off feedback control') of local time differences are enough to conserve local synchronization and bound global asynchrony by a constant independent of time for a long period of time. This allows us to establish a link to the physics of growing surfaces and to investigate the interplay of patterning and synchronization dynamics.

DY 45.6 Thu 15:00 P2

Network complexity versus network synchronicity: A case study of the Kuramoto model on complex networks — Archan Mukhopadhyay and •Jens Christian Claussen — University of Birmingham, UK

During the last two decades, complexity measures for graphs and networks have gained significant attention (see [1] for a comparison), especially in the aim to distinguish "complex" topologies from regular lattices as well as random structures. However, what is the influence of topology on dynamics? Here we specifically analyze synchronization in a network of Kuramoto oscillators where the topology (between a high-complexity graph and a random graph) is parameterized by a complexity measure, as Offdiagonal Complexity [2] or one of the other graph complexity measures. This approach may provide a new light on both the influence of complexity on synchronization, as well as the complexity measures and which aspects of dynamical complexity these may predict.

[1] J. Kim, T. Wilhelm, Physica A 387, 2637 (2008)
[2] Jens Christian Claussen, Physica A 375, 365 (2007)

DY 45.7 Thu 15:00 P2

Quantum synchronization in a network of dissipatively coupled oscillators — •Juan Nicolas Moreno, Christopher w. Wächtler, and Alexander Eisfeld — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Synchronization in classical systems has a long history and by now is a very well understood phenomenon. However, the question whether the classical notions of synchronization can be extended to the quantum regime has only recently been addressed in investigations of classically inspired models like quantum Van der Pol oscillators as well as models without classical analog. Inspired by the theoretical prediction that two-level atoms are able to synchronize even without interacting directly [1], we investigate a network of dissipatively coupled quantum harmonic oscillators. Within a mean-field approximation we find that the network is able to synchronize. For the fully quantum system described in terms of a Lindblad master equation we analyze various measures that have been proposed in the literature. Additionally, we investigate the Liouvillian spectrum in order to draw connections between the spectrum and the synchronization measures.

[1] PRA 101, 042121 (2020)

DY 45.8 Thu 15:00 P2

Neural Network-Based Approaches for Multiscale Modelling of Topological Defects — •Kyra Klos[1], Karin Everschor-Sitte[2], and Friederike Schmid[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]University of Duisburg-Essen, Duisburg, Germany

Topological defects and their dynamics are a heavily researched topic in a wide range of physics fields [1].

Due to the multiscale character of those defect structures, numerically simulating a large number of them in full microscopic detail gets highly computationally expensive, as the large size of associated deformation fields around each core leads to a complex interaction pattern.

To give a possible insight into the connection between the macroscopic (particle) description of a model with topological defects and the underlying microscopic structure, we propose the use of neural networks. With a spin-dynamic simulated microscopic model as training data, we use a conditional generative adversarial network system [2] with Wasserstein-loss [3] to generate reasonable spin-configurations from given defect configuration inputs. To guarantee the generation of realistic spin configuration, we also include additional physical constraints into our generator.

[1] Mermin N. D., Rev. Mod. Phys. 51, 591, (1979)
[2] Mirza M. ; Osindero S., arXiv:1411.1784v1, (2014)
[3] Arjovsky M. et al., ICML, PMLR 70, 214, (2017)
[4] Goodfellow I. et al., NeurIPS, (2014)

DY 45.9 Thu 15:00 P2

Characterizing quasicrysalline patterns with neural networks — •Jonas Buba and Michael Schmiedeberg — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

There exist multiple ways to generate two dimensional quasicrystal patterns such as superpositions of plane waves [1-3] or projection methods [4], each using different parametrisations. A deep convolutional Autoencoder is utilized to determine whether an artifical neural network is capable of finding sufficient parametrisations for these patterns.

Furthermore another neural network was used to classify them by symmetry. Finally, deep dream methods [5] are employed to analyze which features the artificial intelligence bases its symmetry classification on. Currently we are trying to find out how the deep dream approach can be applied to modify existing patterns by enhancing features corresponding to specific symmetries.

[1] D.S. Rokhsar, N.D. Mermin, and D.C. Wright, Acta cryst. A44, 197 (1988). [2] S.P. Gorkhali, J. Qi, and G.P. Crawford, J. Opt. Soc. Am. B 23, 149 (2005). [3] M. Schmiedeberg and H. Stark, J. of Phys.: Cond. Matter 24(28), 284101 (2012). [4] M. Duneau and A. Katz, Phys. Rev. Lett. 54, 2688 (1985). [5] A. Mordvintsev, C. Olah, and M. Tyka, "Inceptionism: Going Deeper into Neural Networks", Google AI Blog (2015).

DY 45.10 Thu 15:00 P2

Influence of delay-times on photonics reservoir computing performance — •Lina Jaurigue and Kathy Lüdge — Institut f. Physik, Technische Universität Ilmenau, Weimarer Str. 25, 98684 Ilmenau, Germany

Reservoir computing is a machine learning approach that utilises the non-linear responses of dynamical systems to perform computational tasks. Due to the relative simplicity of this approach the implementation in hardware is practicable, particularly the delay-based reservoir computing paradigm. Delay-based reservoirs use a single non-linear node subject to self-feedback. The high-dimensional dynamics that arise due to the feedback are utilised by driving the reservoir with time-multiplexed inputs. There have been a number of successful implementations of delay-based reservoirs in electronic, opto-electronic and photonic systems, among others. However, a challenge that remains is the efficient optimisation of a reservoir for performance on a variety of tasks. To this end we explore the influence of the delay-time on the performance of time-series prediction tasks and compare the computational performance of different methods of including task specific delay-timescales in a photonic reservoir setup.

DY 45.11 Thu 15:00 P2

Reservoir computing with memory cells: Impact of perturbations and phase effects — •Noah Jaitner[1], Elizabeth Robertson[3], Lina Jaurigue[2], Janik Wolters[3], and Kathy Lüdge[2] — [1]Institute of Theoretical Physics, Technische Universität-Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut f. Physik, Technische Universität Ilmenau, Weimarer Str. 25, 98684 Ilmenau, Germany — [3]Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Insitut für Optische Sensorsysteme, Rutherfordstr. 2, 12489 Berlin, Germany

Reservoir computing is a versatile, fast-trainable approach for machine learning that utilities the capabilities of dynamical systems. The common approach is to use a nonlinear element and a delay line to construct a virtual network. These virtual networks have limited topology. By utilizing cesium cells as coherent optical memory cells to create a hybrid architecture [1] the limitations of topology can be overcome and a more dynamically versatile virtual network can be created. The optical memory used in the corresponding experiment performs well in memory bandwidth but experiences high noise levels. [2] The dynamics and noise resistance of this approach is examined to find an optimal approach for different time series prediction tasks.

[1] L. C. Jaurigue, E. Robertson, J. Wolters and K. Lüdge Entropy **23**, 1099-4300 (2021).
[2] L. Esguerra, L. Meßner, E. Robertson, N. V. Ewald, M. Gündoan and J. Wolters arXiv:2203.06151.

DY 45.12 Thu 15:00 P2

Reconstructing spatiotemporal chaos in three-dimensional excitable media based on surface data — •Inga Kottlarz[1,2], Sebastian Herzog[1,3], Roland Stenger[1,2], Baltasar Rüchardt[1,4], Stefan Luther[1,4,5], and Ulrich Parlitz[1,2,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Dynamics of Complex Systems, Georg-August-Universität Göttingen, Göttingen, Germany — [3]Department for Computational Neuroscience, Third Institute of Physics - Biophysics, University of Göttingen, Göttingen, Germany — [4]German Center for Cardiovascular Research (DZHK), partner site Göttingen, Robert-Koch-Str. 42a, 37075 Göttingen, Germany — [5]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Robert-Koch-Str. 40, 37075, Göttingen, Germany

The cardiac muscle is an excitable medium that can exhibit complex dynamics, including spatiotemporal chaos associated with (fatal) cardiac arrhythmias. While mechanical motion within the myocardium can be observed with ultrasound, there are no noninvasive techniques (to date) to measure the electrical state within the tissue. To overcome this limitation of observable quantities, we address the task of predicting the electrical state inside the heart from surface data using data-driven reconstruction by means of artificial neural networks. We study the feasibility of this approach in a homogenous and isotropic excitable medium with spatiotemporal dynamics in three spatial dimensions, applying and comparing different deep learning methods (i.e. LSTM, Convolutional Autoencoder, ...).

DY 45.13 Thu 15:00 P2

Ordinal Patterns as Robust Biomarkers in Multichannel EEG Time Series — •Inga Kottlarz[1,2], Sebastian Berg[1], Diana Toscano-Tejeida[3], Iris Steinmann[3], Mathias Bähr[4], Stefan Luther[1,5,6], Melanie Wilke[3,7], Ulrich Parlitz[1,2,6], and Alexander Schlemmer[1,6] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Dynamics of Complex Systems, Georg-August-Universität Göttingen, Göttingen, Germany — [3]Department of Cognitive Neurology, University Medical Center Göttingen, Göttingen, Germany — [4]Department of Neurology, University Medical Center Göttingen, Göttingen, Germany — [5]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Göttingen, Germany — [6]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen, Göttingen, Germany — [7]German Primate Center, Leibniz Institute for Primate Research, Göttingen, Germany

Neurobiological changes in healthy and pathological aging and their electrophysiological correlates (EEG) are still an important topic in the neuroscience community. We extract ordinal patterns and frequency-domain based features from multichannel EEG time series to differentiate between two age groups and also between individuals, using functional connectivity and single channel features. We analyse the separation of EEG features from different age groups and individuals and demonstrate that ordinal pattern-based measures yield results comparable to frequency-based measures applied to preprocessed data, and outperform them if applied to raw data.

DY 46: Poster Session: Complex Fluids, Soft Matter, Active Matter, Glasses and Granular Materials

Time: Thursday 15:00–18:00 Location: P2

DY 46.1 Thu 15:00 P2

Analysis of liquid distribution in microchannel systems using the electro-hydraulic analogy — •Marius Pätzold[1], Felix Senf[1], Carl E. Krill III[2], and Othmar Marti[1] — [1]Institut für experimentelle Physik, Universität Ulm — [2]Institut für funktionelle Nanosystem, Universität Ulm

The research program investigates the calculation of leakages in hydraulic systems by modelling the latter using electric resistor networks as an alternative to simulations employing computational fluid dynamics.

Based on a rigid geometry that describes a network of channels having rectangular cross sections of constant height, the hydraulic properties of the network are examined. The system is then modelled using an electric resistor network that incorporates these hydraulic properties. For a given pressure drop between the inlet and outlets, the model can be solved and leakages can be calculated using a modified nodal analysis.

The results show that modelling the geometry in this manner can be an efficient alternative to simulations using computational fluid dynamics within the requirements set by the electric-hydraulic analogy. Modelling hydraulic networks that are not within these requirements, like those with very short channels or highly complex channel networks, leads to the propagation of errors through the network, resulting in significant differences between the modelling and simulation approach.

DY 46.2 Thu 15:00 P2

Topological fine structure of smectic grain boundaries and tetratic disclination lines within three dimensional smectic liquid crystals* — Paul A. Monderkamp[1], René Wittmann[1], •Michael te Vrugt[2], Axel Voigt[3], Raphael Wittkowski[2], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany — [2]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [3]Institut für Wissenschaftliches Rechnen, Technische Universität Dresden, 01062 Dresden, Germany

Based on recent insights into the orientational topology of smectic grain boundaries in two dimensions, we analyse boundaries in three-dimensional confined smectics from the perspective of tetratic symmetry. Monte-Carlo simulations show the emergence of orientational grain boundaries. Using a 3d tetratic order parameter constructed from the Nelson-Steinhardt invariants, we show that the orientational topological fine structure of the planar smectic grain boundaries can be interpreted as a pair of tetratic disclination lines that are located on the edges of the nematic domain boundary [1]. Thereby, we shed light on the fine structure of the orientational topology of grain boundaries in three-dimensional confined smectics.

[1] P. A. Monderkamp et al., Phys. Chem. Chem. Phys. (2022), https://doi.org/10.1039/D2CP00060A

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DY 46.3 Thu 15:00 P2

From a microscopic inertial active matter model to the Schrödinger equation* — •Michael te Vrugt[1,2], Tobias Frohoff-Hülsmann[1], Eyal Heifetz[3], Uwe Thiele[1], and Raphael Wittkowski[1,2] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [3]Porter School of the Environment and Earth Sciences, Tel Aviv University, 69978 Tel Aviv, Israel

Field theories for the one-body density of an active fluid, such as the paradigmatic active model B+, are simple yet very powerful tools for describing phenomena such as motility-induced phase separation. No comparable theory has been derived yet for the underdamped case. In our work [1], we introduce active model I+, an extension of active model B+ to particles with inertia. The governing equations of active model I+ are systematically derived from the microscopic Langevin equations. We show that, for underdamped active particles, thermodynamic and mechanical definitions of the velocity field no longer coincide and that the density-dependent swimming speed plays the role of an effective viscosity. Moreover, active model I+ contains the Schrödinger equation in Madelung form as a limiting case, allowing to find analoga of the quantum-mechanical tunnel effect and of fuzzy dark matter in the active fluid. We investigate the active tunnel effect analytically and via numerical continuation. [1] M. te Vrugt et al., arXiv:2204.03018

**Funded by the Deutsche Forschungsgemeinschaft (DFG) – grant 283183152.*

DY 46.4 Thu 15:00 P2

Inertial Active Particles in Unbiased ac Fields Sediment at the Top Wall — •José Carlos Ureña Marcos and Benno Liebchen — Institut für Physik Kondensierter Materie, Technische Universität Darmstadt, Darmstadt, Germany

A detailed understanding of the controllability of the swimming direction of active particles through external fields is crucial for many of their proposed future applications, from nanomedicine to bioapplications.

While such steering is often achieved with dc fields with a net gradient, we show in this work that the use of rapidly oscillating ac fields allows the steering of inertial active particles even in the absence of a net gradient. To demonstrate this, we develop an analytical framework which shows that fast ac fields can stabilise fixed points in the dynamics of active particles which would otherwise be unstable.

To exemplify the applicability of this scheme, we explore inertial active particles in a gravitational field and observe that, in the presence of a rapidly oscillating ac field, a substantial fraction of them persistently travel in the upward direction and sediment at the top wall of the simulation box.

DY 46.5 Thu 15:00 P2

Rheological properties of Stcokmayer supracolloidal magnetic polymers under shear flow — •Vladimir Zverev[1], Ekaterina Novak[1], and Ivan Novikau[2] — [1]UNIVIE, Vienna, Austria — [2]Ekaterinburg, Russia

Supracolloidal magnetic polymers (SPMs) are polymer-like structures in which magnetic nanoparticles Construction SPMs has recently been made possible. Their advantage is that they keep their structure independently from the temperature. SPMs can be potentially used as an alternative to nanoparticles in magnetic fluids to obtain a desired and easily controlled magnetic or rheological response.

We assume SMPs formed by monodisperse magnetic colloids, modeled as identical spherical beads. We consider SMPs of four different topologies: chain-, Y-, X- and ring-like ones. Using Langevin dynamics simulations, we pay our attention to solutions of filaments, the magnetic nanoparticles in which are not only interacting via dipole-dipole potential but also via short-range attractive forces (Van der Waals force). Such filaments tend to aggregate in dense spherical droplet-like clusters. The resulting composite soft colloid is placed in the microchannel, where its behavior in the shear flow under influence of an external field is investigated, varying a wide range of system parameters. It was found that clusters can demonstrate oscillating in time magnetic response and complex mutual infulence of the flow and the magnetic field.

The work was supported by RSF 19-72-10033.

DY 46.6 Thu 15:00 P2

Experimental study of statistical structures and forces in granular matter — Amelie Mayländer[1], Clara C. Wanjura[2], Lukas Reiter[1], Raphael Blumenfeld[3,2], and •Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, D-89069 Ulm — [2]Cavendish Laboratory, University of Cambridge, Cambridge, CB3 0HE, UK — [3]Gonville & Caius College, University of Cambridge, Trinity Street, Cambridge CB2 1TA, United Kingdom

We investigated the structure-forces coevolution in rotational shear of a planar assembly of photo-elastic polyurethane-discs of four different sizes under constant confining stress. Disc positions and contacts were determined using unpolarized red light. A dark-field polariscope, using circularly polarized blue light, detected mechanical deformations and the force network. The experiment ran through: a de-correlation step, initial state preparation, steady-state dynamics.

Repeated measurements of the structure and cell order distribution of the geometric contact network were carried out, validating theoretical predictions of detailed balance[1] and maximum entropy[2]. Simultaneously detected force chain networks had more cells of higher orders than the geometric network, providing less than maximum entropy. This is attributed to the sensitivity of force detection to low-force contacts. Characteristic differences also existed in the shapes of small cells.

[1] C. C. Wanjura et al., Granular Matter 22, 91 (2020).
[2] X. Sun et al., Phys. Rev. Lett. 125, 268005 (2020)

DY 46.7 Thu 15:00 P2

Ising-like critical behavior of vortex lattices in an active fluid — •Henning Reinken[1], Sebastian Heidenreich[2], Markus Bär[2], and Sabine H. L. Klapp[1] — [1]Technische Universität Berlin — [2]Physikalisch-Technische Bundesanstalt Berlin

Turbulent vortex structures emerging in bacterial active fluids can be organized into regular vortex lattices by weak geometrical constraints such as obstacles [1,2]. Here we show, using a continuum-theoretical approach [3], that the formation and destruction of these patterns exhibit features of a continuous second-order equilibrium phase transition, including long-range correlations, divergent susceptibility, and critical slowing down. The emerging vorticity field can be mapped onto a two-dimensional (2D) Ising model with antiferromagnetic nearest-neighbor interactions by coarse-graining. The resulting effective temperature is found to be proportional to the strength of the nonlinear advection in the continuum model [4].

[1] D. Nishiguchi, I. S. Aranson, A. Snezhko, and A. Sokolov, Nat. Commun. **9**, 4486 (2018)
[2] H. Reinken, D. Nishiguchi, S. Heidenreich, A. Sokolov, M. Bär, S. H. L. Klapp, and I. S. Aranson, Commun. Phys. **3**, 76 (2020)
[3] H. Reinken, S. H. L. Klapp, M. Bär, and S. Heidenreich, Phys. Rev. E **97**, 022613 (2018)
[4] H. Reinken, S. Heidenreich, M. Bär, and S. H. L. Klapp, Phys. Rev. Lett. **128**, 048004 (2022)

DY 46.8 Thu 15:00 P2

Cohesive rotation of particles with misaligned perception-dependent motility — •Rodrigo Saavedra, Gerhard Gompper, and Marisol Ripoll — Institute of Biological Information and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

Systems of agents with discontinuous motility that activate according to visual perception rules have been found to aggregate into cohesive groups. Here we study the formation of rotating cohesive clusters by considering the particles' vision cone to have a fixed misalignment with respect to the self-propulsion direction. Together with the motility rule, we find this mechanism to facilitate both cohesion and rotation of the cluster. The presence of steric interactions translates into a compact cluster which might eventually be driven by particles in its outer layer. We systematically explore the effect of misalignment and perception on the cluster morphology by means of particle-based numerical simulations. We find good agreement of the results with a proposed coarse-grained model.

DY 46.9 Thu 15:00 P2

Diffusion in a sulfonated co-polynaphthoyleneimide proton exchange membrane studied by NMR — •Celine Wolter, Alexei Privalov, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Darmstadt, Germany

Nowadays, most fuel cells are based on proton-exchange membranes such as Nafion, which contain fluorine and therefore have some disadvantages for disposal. One alternative are flourine-free hydrocarbon-based polymers. Their respective characteristics for use in fuel cells are similar to Nafion membranes, but they are easier and cheaper to produce and recycle. An important parameter for these systems is the proton diffusion coefficient, since it is related to charge transfer across the membrane and removal of the resulting water. We investigated self-diffusion in a sulfonated co-polynaphthoylenimide proton exchange membrane using ^{1}H static field gradient (SFG) nuclear magnetic resonance (NMR). The polymer under study has a ratio of hydrophilic to hydrophobic groups of 60:40, and the saturation humidity of the samples varies from 31% to 100%. For this polymer, the magnetization transfer effects between protons in the membrane framework and water protons must be taken into account. To do this, we applied a model that accounts for such exchange phenomena and were able to determine the diffusion coefficients within a few percent uncertainty in the temperature range from 190 K to 365 K. We found a significant decrease in diffusion at low water concentrations and an increase in activation energy below 250 K, indicating a change in the diffusion mechanism.

DY 46.10 Thu 15:00 P2

Non-mechanical Electrowetting Pump On a Chip — •Sebastian Bohm[1,2], Hai Binh Phi[2], Lars Dittrich[2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Theoretische Physik 1, Weimarer Str. 25, 98693 Ilmenau — [2]5microns GmbH, Ehrenbergstr. 11, 98693 Ilmenau

Numerical simulations suggests that by using the EWOD (electrowetting-on-dielectric) effect a micropump can be manufactured, that works completely without any moving components [1,2]. The volume stroke is generated by the periodic movement of liquid-

vapor interfaces in a large number ($\approx 10^6$) of microcavities ($\Delta V \approx 1$ pl per cavity). Passive Tesla-Diodes are used to rectify the resulting volume stroke to completely forgo any moving parts. Even though our simulation suggests a high efficiency comparable to that of conventional designs in particular for small pumps, the actual realization poses multiple challenges. In this work, first experimental results of the characterization of the micropump are presented. The manufacturing process is described, which is based on an smart combination of processes commonly used in microsystems technology. This enables a cost-effective manufacturing that can be carried out entirely on wafer level. In addition, the direct integration of the pump into wafer-based microfluidic or lab-on-a-chip applications is facilitated. Possible use cases are presented and discussed.

[1] Bohm, S., Dittrich, L., Runge, E.; COMSOL Conference 2020 Europe, 14-15. Oct. 2020 online
[2] Hoffmann et al.; patent DE 11 2011 104 467 (2012)

DY 46.11 Thu 15:00 P2

Collective Behaviour of Active Assemblies Induced by Internal Feedback — •Lisa Rohde and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, Linnéstr. 5, 04103 Leipzig, Germany

Collective phenomena and self-organising processes in nature such as structure formation of cells or flocking of birds are generated by physical interactions between autonomous objects ruled by feedback, information processing or sensing. Recently there has been an increasing interest in studying the collective behaviour of artificial active particles that provide the basic functionality of self-propulsion on the microscale. Here, we introduce physical interactions between artificial microswimmers in a crowded environment by implementing feedback rules to mimic the self-organisation of their living counterparts. We use differently shaped Janus particles capped with a thin gold layer. They are driven by self-thermophoresis, which we control by heating the gold layer with a laser. Depending on the shape of the Janus particle we observe different clustering behaviour as a result of a positive feedback mechanism by which Janus particles are attracted due to a temperature increase of a growing cluster. Our system reacts on hydrodynamic flow fields that are internally induced by other components by showing for example, a polarised motion of particles when being subjected to the feedback loop. We investigate and quantify the role of shape dependent hydrodynamic flow fields on the feedback mechanism by dedicated experiments on the clustering of active assemblies.

DY 46.12 Thu 15:00 P2

Bacterial swimmers' motility under external and light-induced flows — •Valeriia Muraveva[1,2], Robert Grossmann[1], Marek Bekir[2], Svetlana Santer[2], and Carsten Beta[1] — [1]Biological Physics, University of Potsdam, Potsdam, Germany — [2]Smart Soft Matter, University of Potsdam, Potsdam, Germany

We report on changes in the swimming strategy of rod-shaped bacteria under flow conditions.

To swim bacteria utilise lash-like organelles on the cell body, flagella. The model organism for this study is the soil bacterium Pseudomonas putida, which has a rod-shaped body and multiple flagella located at one pole of the cell, so they can act in concert to drive the bacterium in a single direction. The strategy of switching between different swimming modes in bulk was well described. Here, we study the cells' locomotion strategy under flow to better understand the processes of infection spreading and biofilm formation in a natural environment.

To create shear stress conditions hydrodynamic flows are used. For varying the geometry of flow patterns on the micron-scale we also use light-induced flow technics (in particular thermo-osmosis on a gold surface) to create flow locally and to advect or trap swimming bacteria.

To analyse the well-known "run-and-turn" strategy, we concentrate on characteristic features of the swimming pattern: changes in the run-time and turn angle distributions. We also study mutant cell lines under flow (cells with partial or total deficiency in motor function) to elucidate the role of the different components of the motility apparatus in this process.

DY 46.13 Thu 15:00 P2

Phase behaviour of mixtures of attractive rods and spheres — Anja Kuhnhold and •Eleonora Foschino — nstitute of Physics, Albert-Ludwigs-University Freiburg, Germany

The aim of this project is to study a mixture of anisotropic rod-shaped particles and spherical particles in a bulk by means of Monte Carlo simulations. The goal is to find regions in the parameter space that show stable de-mixed phases in three-dimensional systems and stable mixed phases in two-dimensional systems. This would be preliminary to the study of thickness-dependent de-mixing during film growth, which was observed and studied in experiments with blends of organic molecular semiconductors (JR. Banerjee et Al., "Evidence for Kinecally Limited Thickness Dependent Phase Separaon in Organic Thin Film Blends", 2013).

The simulation is based on an implementation of the Metropolis algorithm in a box with periodic boundary conditions. Rod-shaped particles are modelled as hard spherocylinders and spherical particles as hard spheres, and the spheres/rods composition is kept constant, as well as the volume of the simulation box. All particles interact through hard-body repulsion and an additional pair potential, to mimic van der Waals interactions between molecules in the mixture. The parameter space includes the rod-shaped particles' dimensions (the spherocylinders' diameter with respect to the spheres' diameter and the aspect ratio), as well as the strengths and ranges of the attractive interaction.

DY 46.14 Thu 15:00 P2

Electrophoretic mobility of liquid droplets — •Alexander Reinauer and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

Electrophoresis of liquid droplets displays many complex phenomena with applications for phase separation and transport in biological systems. It is significantly more complex than particle electrophoresis due to the mobility of the surface charges as well as the non-rigid nature of the fluid-fluid interface. To investigate the different contributions we conduct a lattice Boltzmann (LB) simulation study of freely suspended liquid droplets under application of an external electric field. We use the Color-Gradient multicomponent LB extension which is coupled to a lattice electrokinetics model for dissolved charged chemical species. Our ongoing study intends to quantify the influence of the viscosity ratio, the salt concentration as well as the charge of the droplet on the measured electrophoretic mobility.

DY 46.15 Thu 15:00 P2

Capacitive Density Functional Theory – C++ support for classical Density Functional Theory implementations — •Moritz Bültmann, Philipp Pelagejcev, and Andreas Härtel — Institute of Physics, University of Freiburg, Germany

CapDFT is a C++ library and provides functional implementations and methods to implement classical Density Functional Theory (DFT) calculations. It is currently developed in our Statistical Physics of Soft Matter and Complex Systems group at the University of Freiburg and we would be happy to discuss ideas and concepts at our poster.

DY 46.16 Thu 15:00 P2

The Scallop Theorem and Swimming at the Mesoscale — •Maxime Hubert[1], Oleg Trosman[1], Ylona Collard[2], Alexander Sukhov[3], Jens Harting[3], Nicolas Vandewalle[2], and Ana-Sunčana Smith[1,4] — [1]PULS group, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]GRASP, University of Liège, Liège, Belgium — [3]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Forschungszentrum Jülich, Nürnberg, Germany — [4]Group for Computational Life Sciences, Ruđer Bošković Institute, Zagreb, Croatia

By comparing theoretical modeling, simulations and experiments, we show that there exists a swimming regime at low-Reynolds number solely driven by the inertia of the swimmer itself. This is demonstrated by considering a dumbbell with an asymmetry in coasting time in its two spheres. Despite deforming in a reciprocal fashion, the dumbbell swims by generating a non-reciprocal Stokesian flow, which arises from the asymmetry in coasting times. This asymmetry acts as a second degree of freedom, which allows for recasting the scallop theorem at the mesoscopic scale at the lowest level of theory.

DY 46.17 Thu 15:00 P2

Fisher-Widom line for systems with competing repulsive and attractive interaction — •Matthias Gimperlein and Michael Schmiedeberg — FAU Erlangen-Nuremberg, Germany

We study colloid-polymer mixtures interacting via a Double-Square-Well potential (DSW-potential) consisting of hard core repulsion, short range attraction and longer range repulsive interaction. The Fisher-Widom line (FW-line) can be used as an indicator for the interplay between repulsion and attraction in the system. It seperates regimes of monotonically (attraction dominates) or oscillatory (repulsion dom-

inates) decaying pair correlation function in the phase diagram.

Solving the Ornstein-Zernike equation we find that the regime of monotonically decaying pair correlation function decreases. On the high density side of the phase diagram repulsion dominates (hard core interaction), but the introduction of the longer range repulsive step leads to a dominance of repulsion also on the low density side of the phase diagram. Only for intermediate densities and temperatures close to the critical temperature attraction dominates the system.

Further research includes a detailed check and analysis of the theoretical results by Brownian Dynamics simualtions. The intersection of the binodal and the FW-line could be interesting for the structure of systems below the binodal line and eventually for gel network formation.

DY 46.18 Thu 15:00 P2

Self-propelled Ellipsoidal Swimmers — •Gordei Anchutkin[1], Viktor Holubec[2], Artem Ryabov[3], and Gordei Anchutkin[1] — [1]Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Institute for Theoretical Physics, Leipzig University, 04103 Leipzig, Germany — [3]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, CZ-180 00 Praha, Czech Republic

The active motion of microswimmers has attracted broad interest for the last decades. A variety of active particles with different shapes and designs have been demonstrating various applications from biosensing to synergistic drug delivery most of them, though, with spherical particles involving a single orientational relaxation time. To generalize the complexity of active microswimmers* behavior, we investigate the fundamentals of active motion for microswimmers with multiple timescales of rotational diffusion. We investigate Janus ellipsoids thermophoretically propelled along the short axis of the ellipsoid. We report three different motion regimes of Janus ellipsoids: the active ballistic motion, run and tumble, and the diffusive regime. Using mean squared displacement analysis, we describe each regime and the corresponding time scales and show the coupling between translational and orientational motions. Our experimental results are compared to a theoretical model of an active ellipsoid motion. The different modes of active motion on different timescales deliver interesting perspectives to explore the interaction with obstacles and other particles at different densities.

DY 46.19 Thu 15:00 P2

Hyperspace-simulations of quasicrystalline structures on periodic substrates — •Johannes Schöttner and Michael Schmiedeberg — FAU, Erlangen, Deutschland

We perform Monte Carlo simulations a toy model where particles move on a hyperlattice. Therefore, jumps in hyperspace corresponding to phasonic flips are considered while phononic noise is not taken into account. Note that the interaction energy is determined after the particles have been projected onto the physical space. This approach can be used to learn about the stability and other physical properties of quasicrystals. Our work here is motivated by experiments [1] where quasi-crystalline structures grows self-organized on a crystalline surface. Therefore, we consider an external periodic potential that acts in our toy model. Our goal is to investigate how phasonic modes are influenced by the external periodic potential. A major advantage of our approach is that by construction we know all hyperspace positions of all particles. Furthermore, phasonic excitations due to the external potential can be determined without ambiguity. [1] Förster et al., Nature, 502:215*218, 10 (2013)

DY 46.20 Thu 15:00 P2

Theory of scanning gate Microscopy in graphene — •Xianzhang Chen[1,2], Guillaume Weick[2], Dietmar Weinmann[2], and Rodolfo Jalabert[2] — [1]Lanzhou Center for Theoretical Physics, and Key Laboratory for Magnetism and Magnetic Materials of MOE, Lanzhou University, Lanzhou, Gansu 730000, China — [2]Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, F-67000 Strasbourg, France

The conductance of graphene nanoribbons and quantum point contacts under scanning gate microscopy tip has been systematically studied. The first- and second-order conductance corrections caused by the tip potential disturbance in armchair graphene are expressed in terms of the scattering states of the unperturbed structure using a scattering approach for a noninvasive probe. The second-order term prevails in the conductance plateaus for armchair graphene strips, but the first-order corrections dominate everywhere at the conductance steps for graphene shaped in quantum point contact. For the stronger tip, where the perturbation approach breaks down, we discovered that conductance corrections exhibit resonance effects at specific values of the tip potential width and strength, which can be regarded as carriers trapped below the tip. Additionally, the numerical results for zigzag graphene also follow the weak probe theory.

DY 46.21 Thu 15:00 P2

Characterization and control of traffic-jam transition for self-propelled particles with q-fold discrete symmetry: The restricted Active Potts Model — •Swarnajit Chatterjee[1], Mintu Karmakar[2], Matthieu Mangeat[1], Heiko Rieger[1], and Raja Paul[2] — [1]Saarland University, Saarbrücken, Germany — [2]Indian Association for the Cultivation of Science, Kolkata, India

We undertake comprehensive numerical simulations of the q-state active Potts model (APM) [EPL **130**, 66001 (2020); Phys. Rev. E **102**, 042601 (2020)] applying distinct volume exclusions to the self-propulsion of the active particles in the quest to explore the characteristics of the emerging phases, kinetic arrest, and jamming transitions. We broadly explore two scenarios where (a) the population of a lattice site is prearranged (hard-core restriction) and (b) particle movements are governed by a local repulsive field (soft-core restriction) and show that such effects lead to a surprisingly rich variety of self-organized spatial patterns. While bands and lanes of moving particles commonly occur without or under weak volume exclusion, strong volume exclusion along with low temperature, high activity, and large particle density facilitates traffic jams. Through a number of phase diagrams, we identify the phase boundaries separating the jammed and free-flowing phases and study the transition between these phases which provide us with both qualitative and quantitative predictions of how jamming might be delayed or dissolved. We further validate our numerical findings with a hydrodynamic model description.

DY 46.22 Thu 15:00 P2

Polar flocks with discretized directions: the active clock model approaching the Vicsek model — •Matthieu Mangeat, Swarnajit Chatterjee, and Heiko Rieger — Universität des Saarlandes, Saarbrücken, Germany

We study the off-lattice two-dimensional q-state active clock model (ACM) as a natural discretization of the Vicsek model (VM) [Phys. Rev. Lett. **75**, 1226 (1995)] describing flocking. The ACM consists of particles able to move in the plane in a discrete set of q equidistant angular directions, as in the active Potts model (APM) [EPL **130**, 66001 (2020); Phys. Rev. E **102**, 042601 (2020)], with a local alignment interaction inspired by the ferromagnetic equilibrium clock model. A collective motion emerges at high densities and low noise. We compute phase diagrams of the ACM and explore the flocking dynamics in the region, in which the high-density (polar liquid) phase coexists with the low-density (gas) phase. We find that for a small number of directions, the flocking transition of the ACM has the same phenomenology as the APM, including macrophase separation and reorientation transition from transversal to longitudinal band motion as a function of the particle self-propulsion velocity. For a larger number of directions, the flocking transition in the ACM becomes equivalent to the one of the VM and displays microphase separation and only transverse bands, i.e. no reorientation transition. Concomitantly also the transition of the $q \to \infty$ limit of the ACM, the active XY model (AXYM), is in the same universality class as the VM. We also construct a coarse-grained hydrodynamic description for the ACM and AXYM akin to the VM.

DY 47: Members' Assembly

Time: Thursday 18:30–19:15 Location: H19

All members of the Dynamics and Statistical Physics Division are invited to participate.

DY 48: Invited Talk Kathy Lüdge (joint session DY/SOE)

Time: Friday 9:30–10:00 Location: H19

Invited Talk DY 48.1 Fri 9:30 H19

Photonic Reservoir Computing: Analytic insights and possibilities for optimization — Lina Jaurigue[1], Felix Köster[2], and •Kathy Lüdge[1] — [1]Institute of Physics, Technische Univ. Ilmenau, Weimarer Str. 25, 98684 Ilmenau — [2]Institute of Theoretical Physics, Technische Univ. Berlin, Hardenbergstr. 36, 10623 Berlin

Reservoir computing has gained a lot of attention because its relatively simple setup that can be easily implemented in hardware, specifically with optical devices. Using one nonlinear node, i.e., a laser with an optical feedback loop and time-multiplexed input, already allows to solve complex time-series prediction tasks after a proper training via linear regression. Nevertheless, the performance depends on properly adjusted timescales and not every physical system is suitable for a given task [1].

We present ways to improve the computing performance of delay-based photonic reservoir computing systems using delay-time tuning, and we discuss to what extent delay-coupled laser-networks with more than one optical element can be beneficial to improve the overall performance. Furthermore, we discuss analytic insights into the information processing capacity of a reservoir computing system and its correlation to the linear system response of the reservoir as well as to the series expansion of a chosen task.

[1] T. Hülser, F. Köster, L. C. Jaurigue, and K. Lüdge, Opt. Mater. Express 12, 1214 (2022).

DY 49: Statistical Physics: General

Time: Friday 9:30–12:15 Location: H20

DY 49.1 Fri 9:30 H20

Large-Deviation Properties of Non-equilibrium RNA Work Processes — •Peter Werner and Alexander K. Hartmann — Institute of Physics, University of Oldenburg, Germany

The Higgs *RNA model* [1] is one of the few cases of a model with quenched disorder and complex free energy landscape, where *exact* partition function calculation and sampling can be done in polynomial time. Building on previous work [2], non-equilibrium properties of this model are investigated further. Here, we are interested in the case where, by applying an external force, RNAs are stretched or refolded, like it is also done in experiments with real RNA. Such processes are realized by first sampling an RNA secondary structure in equilibrium and subsequently performing a non-equilibrium MC Simulation during which the external force parameter is varied. The performed physical work W and secondary structures are measured during the processes.

By utilizing a *large-deviation algorithm* that is based on biasing random numbers [3], we are able to measure the work distributions $P(W)$ over a wide range of the support down to probabilities such as 10^{-40}. We show how work distributions and the corresponding *large-deviation rate function* behave under an appropriate length variations of various nucleotide sequences, specifically, whether the *large-deviation* principle holds.

[1] P. G. Higgs, Phys. Rev. Lett., **76**, 704 (1996)
[2] P. Werner and A. K. Hartmann, Phys. Rev. E **104**, 034407 (2021)
[3] A. K. Hartmann, Phys. Rev. E **89**, 052103 (2014)

DY 49.2 Fri 9:45 H20

Choosing the right event (in non-reversible event-chain Monte Carlo) — •Philipp Höllmer[1], Nicolas Noirault[2], Botao Li[2], A. C. Maggs[3], and Werner Krauth[2] — [1]University of Bonn, Germany — [2]École normale supérieure de Paris, France — [3]ESPCI Paris, France

The general framework of event-chain Monte Carlo (ECMC) constructs non-reversible Markov chains for continuous statistical-physics models ranging from hard-disk systems to long-range interacting molecular systems. Over recent years, several algorithms from the family of ECMC have been proposed, which, in the event-driven formulation of ECMC, only differ in their treatment of events (e.g., of disk collisions in a hard-disk system). Still, we show that different variants can have widely different performances. As a first example, we consider locally stable sparse hard-disk packings. Using a scaling theory confirmed by simulation results, we obtain two classes for the escape from slightly relaxed hard-disk packings parameterized by a relaxation parameter. In one class, the escape time varies algebraically with the relaxation parameter. In the other class, the escape time only scales as the logarithm of the relaxation parameter. As a second example, we consider integrated autocorrelation times in dense systems of flexible extended hard-disk dipoles. Here, the ECMC variants show order-of-magnitude spreads. We expect the performance differences to carry over to long-range interacting molecular systems, where the choice of the optimal ECMC variant is thus highly important.

DY 49.3 Fri 10:00 H20

The GOE ensemble for quasiperiodic tilings without unfolding: r-value statistics — •Rudolf A. Römer[1] and Uwe Grimm[2] — [1]University of Warwick, Coventry, UK — [2]Open University, Milton Keynes, UK

We study the level-spacing statistics for non-interacting Hamiltonians defined on the two-dimensional quasiperiodic Ammann–Beenker (AB) tiling. When applying the numerical procedure of "unfolding", these spectral properties in each irreducible sector are known to be well-described by the universal Gaussian orthogonal random matrix ensemble. However, the validity and numerical stability of the unfolding procedure has occasionally been questioned due to the fractal self-similarity in the density of states for such quasiperiodic systems. Here, using the so-called r-value statistics for random matrices, $P(r)$, for which no unfolding is needed, we show that the Gaussian orthogonal ensemble again emerges as the most convincing level statistics for each irreducible sector [1]. The results are extended to random-AB tilings where random flips of vertex connections lead to the irreducibility.

[1] U. Grimm, R. A. Römer, Phys. Rev. B **104**(6), L060201 (2021)

DY 49.4 Fri 10:15 H20

Classical density functional theory and the primitive model: beyond the standard mean-field approximation — •Moritz Bültmann and Andreas Härtel — Albert-Ludwigs-Universität Freiburg, Physikalisches Institut

To understand the physics of electrolyte solutions one often uses the *primitive model*, where ions are represented by charged hard spheres in a dielectric background. The powerful theory of density functionals, which is widely known from quantum mechanics, can also be applied to such systems in the context of statistical physics. There, the first order of a functional perturbation yields the *mean-field electrostatic functional*, which also contributes at particle separations that are forbidden due to the hard-core interations.

In this talk I summarize our findings from the article [J. Phys.: Condens. Matter **34** 235101], where we modified the mean-field functional such that the occuring pair potential is constant for distances smaller than hard-core contact. The resulting formalism involves weighted densities similar to the ones used in most hard-sphere functionals. Comparing different functionals and result from MD simulations, we analyze density profiles, direct and total correlation functions, and thermodynamic sum rules. Thereby, we found that the modifications improved the predictions compared to the standard mean-field functional significantly. Finally, I report on recent findings of the modified mean-field functional e.g. concerning the decay behavior of total correlation functions.

DY 49.5 Fri 10:30 H20

Recoil experiments determine the eigenmodes of viscoelastic fluids — Karthika Krishna Kumar[1], Félix Ginot[1], •Juliana Caspers[2], Luis Reinalter[1], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Germany — [2]Institute for Theoretical Physics, Georg-August Universität Göttingen, Germany

Probing viscoelastic media using colloidal particles reveals their com-

plex relaxation processes at the microscopic level. Unlike Newtonian fluids, viscoelastic fluids can store and dissipate energy on much longer timescales because of their microstructure, therefore, these materials play a significant role in many technical applications. In this work, we perturb a viscoelastic fluid by driving a colloidal particle through the fluid using an optical tweezer. On deforming the viscoelastic matrix, the fluid tries to relax back by pushing the particle to recoil when the trap is turned off. The trajectory of such a recoiling particle exhibits a bi-exponential behavior indicating two distinct relaxation processes of the fluid. Detailed investigation shows that a microscopic model, with two fictitious bath particles connected to the probe particle via harmonic springs, explains the observed behavior. The analytical solution to the model also reveals two more timescales corresponding to the relaxation of the bath particles when the probe is fixed. The need for two bath particles to explain the results can be justified by considering the fluid as a glassy system, however, further experiments are required to confirm this.

15 min. break

DY 49.6 Fri 11:00 H20

FIPS: A generic framework for many-particle simulations focusing on efficiency and reliability* — •Julian Jeggle and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Numerical calculation of particle trajectories in many-particle systems is an important class of molecular dynamics (MD) simulations that has been implemented in well-known MD packages such as GROMACS, HOOMD-blue, and LAMMPS. Recently, efforts have been made to develop more flexible data models for this task with the help of modern programming techniques. In this talk, we present further advancements into this direction in the form of FIPS, the *flexibly integrating particle simulator*. This tool enables the simulation of many-particle systems and their dynamics described by a domain specific language heavily inspired by GPU shaders. Unlike traditional MD packages, we utilize just-in-time compilation and shared-state concurrency to achieve a high degree of efficiency. To increase resilience towards programming errors, our implementation is tightly coupled to Rust, a novel systems programming language with a focus on reliability, in particular for concurrent applications.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – Project-ID 433682494 - SFB 1459

DY 49.7 Fri 11:15 H20

The reversible heat production during the electric double layer buildup: Analysis with an extension of the primitive model by hydration shells — •Philipp Pelagejcev, Fabian Glatzel, and Andreas Härtel — Albert-Ludwigs-Universität Freiburg

The reversible heat production during the electric double layer (EDL) buildup was measured experimentally [Janssen et al., Phys. Rev. Lett. 119, 166002 (2017)] and in theoretical work [Glatzel et al., J. Chem. Phys. 154, 064901 (2021)], it was found that steric interactions of ions with the flat electrodes, which result in the so-called Stern layer, are sufficient to explain the experimental results. In the latter only symmetric ion sizes in a restricted primitive model were examined.

In this work, I present the impact of ion asymmetry on the reversible heat production for each electrode separately. Additionally, an extension of the primitive model where hydration shells of ions can evade in the vicinity of the electrodes is discussed. With this extended model one can describe situations where one electrode is heated and the other electrode is cooled simultaneously during charging, while both electrodes together behave similarly to the already mentioned experimental results.

Thus, in experiments the heat production should be measured for each electrode separately. By this, the importance of certain ingredients for a primitive model based electrolyte could be evaluated experimentally, finally leading to a deeper understanding of EDLs. (Reference: [Pelagejcev et al., J. Chem. Phys. 156, 034901 (2022)])

DY 49.8 Fri 11:30 H20

Uncovering broken detailed balance hidden by unknown degrees — •Gabriel Knotz, Till moritz Münker, Timo Betz, and Matthias Krüger — Fakultät für Physik, Georg-August-Universität, Göttingen, Germany

The complex nature of non equilibrium systems remains a challenging task in statistical physics, but especially for living matter. A major experimental problem is, that often some relevant degrees cannot be observed (are hidden) which complicates theoretical analysis. We study a non-equilibrium model with two degrees of freedom. If both degrees are observed, the breaking of detailed balance can easily be quantified. However, by treating one of the degrees as hidden, the trajectory of the other is time reversal symmetric. To still detect the breakage of detailed balance we can use a new quantity, the mean backward relaxation (MBR), that measures the relaxation of displacements caused by the fluctuating forces. By deriving rigorous statements for equilibrium in general and calculating the MBR for the non-equilibrium system, we show that the MBR reveals that the system breaks detailed balance even though one degree is hidden. Further we are able to relate the deviation of the MBR compared to an equilibrium system to an effective energy. This analysis adds a new approach to systems that deal with unknown, but relevant non-equilibrium degrees of freedom.[1]

[1] Till M. Muenker, Gabriel Knotz, Matthias Krüger and Timo Betz. *Onsager regression characterizes living systems in passive measurements.* bioRxiv: 2022.05.15.491928

DY 49.9 Fri 11:45 H20

Generalized hydrodynamics description of the classical Toda lattice and high-low pressure domain wall initial conditions — •Christian Mendl and Herbert Spohn — Technische Universität München (TUM)

We review and discuss generalized hydrodynamics applied to the classical Toda lattice, a paradigmatic example for an interacting integrable system. One first identifies the Lax matrix of the system, which is closely related to the microscopic conservation laws. For the Toda lattice, the free energy can be expressed in terms of the eigenvalue spectrum of the Lax matrix. One finally arrives at semi-analytic formulas for dynamical correlation functions in equilibrium, which show good agreement with molecular dynamic simulations.

In the second part, we focus on domain wall initial conditions, for which the left and right half lattice are in thermal equilibrium but with distinct parameters. The particular case of interest is a jump from low to high pressure at uniform temperature and zero mean velocity, whereby the scaling function for the average stretch is forced to change sign. The hydrodynamic equations seem to be singular at zero stretch, but nevertheless the self-similar solution exhibits smooth behavior.

[1] C. B. Mendl, H. Spohn, High-low pressure domain wall for the classical Toda lattice, SciPost Phys. Core 5, 002 (2022)

[2] H. Spohn, Hydrodynamic equations for the Toda lattice, arXiv:2101.06528

[3] H. Spohn, Generalized Gibbs ensembles of the classical Toda chain, J. Stat. Phys. 180, 4 (2020)

DY 49.10 Fri 12:00 H20

The square-lattice Ising model on the rectangle — •Fred Hucht — Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg

For the square-lattice Ising model, the universal critical Casimir potential and force scaling functions can be calculated exactly for many geometries and boundary conditions. We present a recent exact solution of the square lattice Ising model on the $L \times M$ rectangle, with open boundary conditions in both directions [1], in terms of the determinant of a $M/2 \times M/2$ Hankel matrix $\mathbf{H}$. The $M-1$ independent matrix elements of $\mathbf{H}$ are Fourier coefficients of a certain symbol function, which is given by the ratio of two characteristic polynomials. These polynomials are associated to the different directions of the system, encode the respective boundary conditions, and are directly related through the symmetry of the considered Ising model under exchange of the two directions. This representation is a major simplification of earlier results [2,3].

[1] A. Hucht, *J. Phys. A: Math. Theor.* **54**, 375201 (2021). arXiv:2103.10776.
[2] A. Hucht, *J. Phys. A: Math. Theor.* **50**, 065201 (2017). arXiv:1609.01963, erratum [4].
[3] A. Hucht, *J. Phys. A: Math. Theor.* **50**, 265205, (2017). arXiv:1701.08722.
[4] A. Hucht, *J. Phys. A: Math. Theor.* **51**, 319601 (2018).

DY 50: Active Matter 5 (joint session DY/BP/CPP)

Time: Friday 10:00–12:45 Location: H18

DY 50.1 Fri 10:00 H18

Anomalous cooling and overcooling of active colloids — •Fabian Jan Schwarzendahl and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

The phenomenon that a system at a hot temperature cools faster than at a warm temperature, referred to as the Mpemba effect, has been recently realized for trapped colloids. Here, we investigate the cooling and heating process of a self-propelling active colloid using numerical simulations and theoretical calculations with a model that can directly be tested in experiments. Upon cooling activity induces a Mpemba effect and the active particle escapes an effective temperature description. At the end of the cooling process the notion of temperature is recovered and the system can exhibit even smaller temperatures than its final temperature, a surprising phenomenon which we refer to as activity-induced overcooling.

DY 50.2 Fri 10:15 H18

Active Ornstein-Uhlenbeck model for self-propelled particles with inertia — •Gia Huy Philipp Nguyen, René Wittmann, and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany

Self-propelled particles, which convert energy into mechanical motion, exhibit inertia if they have a macroscopic size or move inside a gaseous medium, in contrast to micron-sized overdamped particles immersed in a viscous fluid. We have studied an extension of the active Ornstein-Uhlenbeck model, in which the self-propulsion is described by colored noise, to access these inertial effects affecting their translational motion [1]. In this talk, analytical solutions of the mean displacement, mean-squared displacement and velocity autocorrelation function will be discussed for a free active particle and in more general settings including an active dimer, a time-dependent mass and various external forces.

[1] G. H. P. Nguyen, R. Wittmann, H. Löwen, J. Phys.: Condens. Matter 34, 035101 (2021)

DY 50.3 Fri 10:30 H18

A quantitative scattering theory of active particles — •Thomas Ihle[1], Rüdiger Kürsten[1], and Benjamin Lindner[2] — [1]Institute for Physics, University of Greifswald, Greifswald — [2]Institute for Physics, Humboldt University of Berlin, Berlin

We consider a particular model of self-propelled particles with Kuramoto-type alignment interactions. Starting from the N-particle Fokker-Planck equation we observe that the usual factorization Ansatz of the probability density, often called Molecular Chaos approximation, predicts a relaxation behavior which qualitatively disagrees with agent-based simulations. Therefore, we develop a scattering theory which resolves the time-evolution of the two-particle correlation function, i.e. goes beyond the mean-field approximation. The theory does not require input from agent-based simulations; it is self-consistent and leads to analytical expressions. We show that this theory predicts the relaxation behavior of the system and the transport coefficients with high precision in certain parameter ranges.

DY 50.4 Fri 10:45 H18

Hierarchical self-organization in communicating polar active matter — •Alexander Ziepke[1], Ivan Maryshev[1], Igor S. Aranson[2], and Erwin Frey[1] — [1]Ludwig-Maximilians-Universität München, München, Germany — [2]Pennsylvania State University, University Park PA, USA

Self-organization in active matter plays an important role for various biological and artificial systems. In numerous cases, inter-agent communication is a key mechanism for the formation and localization of critical structures, such as the fruiting body in Dictyostelium discoideum or aggregation clusters in quorum-sensing bacteria. Despite its importance, the specific role of communication and its interplay with self-propulsion remains largely unexplored.

We propose a model for communicating active matter that endows self-propelled polar agents with information processing and signal relaying capabilities. We show that information processing greatly enriches the ability of these systems to form complex structures, allowing them to self-organize through a range of different collective dynamical states at multiple hierarchical levels. This provides insights into the role of self-sustained signal processing for self-organization in biological systems and opens pathways for applications using chemically driven colloids or microrobots.

DY 50.5 Fri 11:00 H18

Collective transport of microparticles by active cells — •Robert Grossmann[1], Kevin Meissner[1], Fernando Peruani[2], and Carsten Beta[1] — [1]University of Potsdam, Potsdam, Germany — [2]CY Cergy Paris Université, Cergy-Pontoise, France

Motivated by the challenge of targeted delivery of micron-sized objects, we investigate a novel type of bio-hybrid active matter, composed of motile cells acting as autonomously moving agents that transport passive cargoes. The transport process is a collective phenomenon: a bead can be lost by one cell and may picked up by another one, or multiple cells transport one bead together, thereby giving rise to an intermittent, stochastic stop-and-go dynamics. Combining experiment and active matter theory, we investigate the emerging transport properties of this system. We first deduce the waiting time distributions of active and passive transport episodes from experiments with the amoeba *Dictyostelium discoideum*: whereas the duration of actual transport phases – determined by the time that cells and cargoes are in contact – are exponentially distributed, the waiting time distribution for passive periods exhibits power-law characteristics which results from the search of cells looking for immobile colloids. We predict displacement distributions and the mean-squared displacement of colloids based on the statistics of waiting times and particularly point out a crossover from normal to subdiffusive scaling. These results provide the basis for the future design of cellular micro-carriers and for extending our findings to more advanced transport tasks in complex, disordered environments, such as tissues.

DY 50.6 Fri 11:15 H18

Odd viscosity and active turbulence of hydrodynamic microrotors — •Joscha Mecke[1], Yongxiang Gao[2], Dirk G.A.L. Aarts[3], Alberto Medina[1], Gerhard Gompper[1], and Marisol Ripoll[1] — [1]Institute of Biological Information Processing, Forschungszentrum Jülich, Germany — [2]Institute for Advanced Study, Shenzhen University, China — [3]Department of Chemistry, University of Oxford, UK

Suspensions of rod-like silica colloids with a ferromagnetic head are considered in a rotating magnetic field applied parallel to a substrate. The magnetic moment is oriented perpendicular to the rod axis which implies a non-equilibrium vertical orientation to the substrate and synchronous spinning in the rotating field. We combine experiments and simulations to study the collective properties of these rotors. The hydrodynamic flows generated by the colloid rotations induce a cascade of translational motions in the neighbouring colloids. Thus, the rotors can be regarded as active matter with transport coefficients varying with local configuration and thus rotor density. The competition between hydrodynamic and steric interactions renders the translational dynamics non-monotonous in rotor density. The ensemble dynamics shows the emergence of eddies of various sizes reminiscent of turbulence. Furthermore, the rotor fluid is a realisation of a chiral active fluid with odd viscosity, that manifests itself in stress forces orthogonal to the direction of shear. In vortex flow, the stress acts like an effective pressure leading to density-vorticity correlations. Our experimental and numerical results are found to be in agreement.

DY 50.7 Fri 11:30 H18

Two-temperature activity drives liquid-crystal and crystalline order in soft repulsive spherocylinders — •Jayeeta Chattopadhyay, Sindhana Pannir-Sivajothi, Kaarthik Varma, Sriram Ramaswamy, Chandan Dasgupta, and Prabal K. Maiti — Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India

We study the scalar activity induced phase separation and liquid crystal ordering in a system of Soft Repulsive Spherocylinders (SRS) of various aspect ratios (L/D). Activity was introduced by increasing the temperature of half of the SRS (labeled 'hot') while maintaining the temperature of the other half constant at a lower value (labeled 'cold'). The difference between the two temperatures scaled by the lower tem-

perature provides a measure of the activity. We find that activity drives the cold particles through a phase transition to a more ordered state and the hot particles to a state of less order compared to the initial equilibrium state. For L/D = 5, the cold components of a homogeneous isotropic (I) structure acquire nematic (N) and, at higher activity, crystalline (K) order. Similarly, the cold zone of a nematic initial state undergoes smectic (Sm) and crystal ordering while the hot component turns isotropic. Interestingly, we observe liquid crystal ordering for the spherocylinders having aspect ratio below Onsager's limit. The hot particles occupy a larger volume and exert an extra kinetic pressure, confining, compressing and provoking an ordering transition of the cold-particle domains.

Ref:Phys. Rev. E104, 054610 (2021).

DY 50.8 Fri 11:45 H18

Spontaneous trail formation in populations of communicating active walkers — Zahra Mokhtari[1], Robert I. A. Patterson[2], and •Felix Höfling[1,3] — [1]Dept. Mathematics and Computer Science, Freie Universität Berlin — [2]WIAS Berlin — [3]Zuse Institute Berlin

How do ants form long stable trails? Despite abundant evidence that trail formation in colonies of insects or bacteria originates in their sensing of and responding to the deposits of chemicals that they produce, there is no consensus on the minimum required ingredients for this phenomenon. To address this issue, here, we develop an agent-based model in terms of active random walkers communicating via pheromones, which can generate trails of agents from an initially homogeneous distribution [1]. Based on extensive off-lattice computer simulations we obtain qualitatively the non-equilibrium state diagram of the model, spanned by the strength of the agent-chemical interaction and the number density of the population. In particular, we demonstrate the spontaneous formation of persistent, macroscopic trails, and highlight some behaviour that is consistent with a dynamic phase transition. We also propose a dynamic model for few macroscopic observables, including the sub-population size of trail-following agents, which captures the early phase of trail formation. At high densities and for strong alignment, we observe that rotating clusters ("ant mills") are more stable than trails and can swallow them up.

[1] Z. Mokhtari, R. I. A. Patterson & F. Höfling, New J. Phys. **24**, 013012 (2022).

15 min. break

DY 50.9 Fri 12:00 H18

Dynamics of microalgae in a porous environment — •Florian von Rüling, Liubov Bakhchova, Dmitry Puzyrev, Ulrike Steinmann, and Alexey Eremin — Otto von Guericke University Magdeburg, Germany

The navigation through complex environments is a task the microalgae *Chlamydomonas reinhardtii* are frequently confronted with in their natural habitats, where they encounter suspended and sedimented particles as well as rough surfaces. To investigate the motion in heterogeneous surroundings, we observe dilute and crowded active colloidal suspensions of *Chlamydomonas* in quasi-two-dimensional microstructured PDMS-channels. Arrays of cylindrical or elongated pillars with varying lattice spacing and obstacle orientation serve as artificial porous environments. The swimmer behaviour is characterised by means of velocity and orientation autocorrelation functions, trajectory straightness, velocity distributions and the reflection/transmission coefficients for the porous segments.

DY 50.10 Fri 12:15 H18

Extending the active Phase Field Crystal model to describe motility-induced condensation and crystallization — •Max Philipp Holl[1] and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, Universität Münster — [2]Center for Nonlinear Science, Universität Münster

The passive conserved Swift-Hohenberg equation (or phase-field-crystal [PFC] model) corresponds to a gradient dynamics for a single order parameter field related to density [1]. It provides a microscopic continuum description of the thermodynamic transition between liquid and crystalline states. A recent extension allows one to investigate both, vapour-liquid and liquid-solid transitions [3]. We first discuss the bifurcation and phase structure of this passive, i.e., thermodynamic model. Our subsequently introduced extension of the standard active PFC model [2] is able to describe passive and active (motility-induced) vapour-liquid and liquid-solid transitions. This is shown through a bifurcation and phase analysis based on path continuation supplemented by time simulations.

[1] H. Emmerich, H. Löwen, R. Wittkowski, T. Gruhn, G. I. Tóth, G. Tegze, and L. Gránásy. Phase-field-crystal models for condensed matter dynamics on atomic length and diffusive time scales: an overview. Adv. Phys., 61:665-743, 2012 [2] A. M. Menzel and H. Löwen. Traveling and resting crystals in active systems. Phys. Rev. Lett., 110:055702, 2013 [3] Z.-L. Wang, Z. Liu, Z.-F. Huang, and W. Duan. Minimal phase-field crystal modeling of vapor-liquid-solid coexistence and transitions. Phys. Rev. Materials, 4:103802, 2020

DY 50.11 Fri 12:30 H18

Engines driven by active fields — •Patrick Pietzonka[1] and Michael E. Cates[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom

On macroscopic scales, where trajectories of individual particles cannot be observed, active matter may appear like matter in thermal equilibrium. We discuss how the non-equilibrium character of active matter can nonetheless be revealed by using it as a working medium of engines delivering mechanical work in an isothermal environment. We focus on scalar active field theories such as the active model B as minimal continuum models for active matter undergoing a phase separation. The shape and chemical potential of droplets can be controlled through external potentials and activity patterns. We show how an asymmetric periodic activity pattern can drive a flow of active matter against an external force, thus acting as an autonomous engine. Moreover, we calculate and optimise the work that can be extracted by a cyclic engine that manipulates the activity and the potential landscape.

DY 51: Machine Learning in Dynamics and Statistical Physics (joint session DY/SOE)

Time: Friday 10:00–11:15 Location: H19

DY 51.1 Fri 10:00 H19

Reinforcement learning of optimal active particle navigation — •Mahdi Nasiri and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

In sufficiently complex environments, there is no simple way to determine the fastest route of an active particle that can freely steer towards a given target. In fact, while classical path planning algorithms (e.g. A*, Dijkstra) tend to fail to reach the global optimum, analytical approaches are incapable of handling generic complex environments. To overcome this gap in the literature, in the present work, we develop a policy gradient-based deep reinforcement learning method that employs a hybrid continuum-based representation of the environment and allows, for the first time, to determine the asymptotically optimal path in complex environments. Our results provide a key step forward towards a universal path planner for future intelligent active particles and nanorobots with potential applications in microsurgery as well as in drug and gene delivery.

DY 51.2 Fri 10:15 H19

Deep reinforcement learning for chemotactic active particles — •Edwin Loran, Mahdi Nasiri, and Benno Liebchen — Institute of Condensed Matter Physics, Technische Universität Darmstadt, D-64289 Darmstadt, Germany

Throughout evolution, microorganisms have developed efficient strategies for locating nutrients and avoiding toxins in complex environments. Understanding their adaptive policies can provide new key insights for the development of smart artificial active particles. Here, we use a machine learning approach, namely deep reinforcement learning, to develop smart foraging strategies for chemotactic active particles

which consume nutrients for their survival. Our method is able to devise efficient chemotactic navigation strategies guaranteeing "survival" inside unknown and complex landscapes while only having access to local sensory data. Our approach is based on deep Q-learning and uses the particle's observation of its surrounding chemical (nutrient) concentration as the input. The presented method highlights the extent of the capabilities of reinforcement learning approaches in mimicking (and going beyond) the evolutionary strategies learned by microorganisms.

DY 51.3 Fri 10:30 H19

Machine Learning the 2D percolation transition — •Djénabou Bayo[1,2], Andreas Honecker[2], and Rudolf A. Römer[1] — [1]Departement of Physics, University of Warwick, Coventry, CV47AL, United Kingdom — [2]Laboratoire de Physique Théorique et Modélisation (LPTM) (CNRS UMR8089), CY Cergy Paris Université, 95302 Cergy-Pontoise, France

The percolation model is one of the simplest models in statistical physics displaying a phase transition. A classical lattice is occupied randomly with a given probability at each site (or bond). A phase transition from a non-percolating to a percolating state appears around the so-called percolation threshold. Machine Learning (ML) and Deep Learning (DL) techniques are still relatively new methods when applied to physics. Recent work shows that ML/DL techniques seemingly detect the percolation transition from images of percolation clusters. We employ such supervised learning techniques, i.e., classification and regression for 2D site percolation. We find that the identification of spanning clusters provided by such methods does not fully correlate with their existence. Rather, the identification seems to rely on proxy measures such as the site occupation density. Furthermore, constructing challenging cluster distributions show scope for much misclassification when using even highly trained DL networks. Unsupervised ML strategies, such as variational autoencoders, might be able to reconstruct percolation clusters with acceptable spatial resolution, but in many cases struggle to reproduce the geometry of spanning clusters faithfully. Our work uses Python and the ML/DL libraries of PyTorch.

DY 51.4 Fri 10:45 H19

Exploring structure-property maps with kernel principal covariates regression — •Guillaume Fraux, Benjamin Helfrecht, Rose Cersonsky, and Michele Ceriotti — Institute of Materials, EPFL, Lausanne, Switzerland

Data analyses based on linear methods constitute the simplest, most robust, and transparent approaches to the automatic processing of large amounts of data for building supervised or unsupervised machine learning models. Principal covariates regression (PCovR) is an underappreciated method that interpolates between principal component analysis and linear regression and can be used conveniently to reveal structure-property relations in terms of simple-to-interpret, low-dimensional maps. We introduce a kernel version of PCovR (KPCovR), and demonstrate the performance of this approach in revealing and predicting structure-property relations in chemistry and materials science.

For large datasets, interactive exploration of the resulting map is a great tool to extract understanding. To this end, we introduce chemiscope, an open source software able to display and explore maps with hundred of thousands of points together with the corresponding molecular or crystal structure. Chemiscope is usable as an online tool, or locally through jupyter notebooks.

DY 51.5 Fri 11:00 H19

Investigation of plasticity in off-resonant delay-coupled reservoir computing — •Jonas Naujoks[1], Felix Köster[1], and Kathy Lüdge[2] — [1]Institute for Theoretical Physics, Technische Universität Berlin, 10559 Berlin, Germany — [2]Institute of Physics, Technische Universität Ilmenau, Weimarer Str. 25, 98693 Ilmenau, Germany

We analyse the effect of neuronal plasticity on the performance of a delay-based reservoir computer modelled by a generic oscillator with self-feedback. The memory capacity and task-specific performance are investigated in the case of non-resonant delay-clock-cycle configurations. By modifying the temporal multiplexing of the input, the responsiveness of the virtual nodes is maximised while promoting individual decorrelation. The training is done in an unsupervised manner. The effect on the task-specific performance is investigated, while we additionally demonstrate that the memory capacity can be tuned.

DY 52: Nonlinear Dynamics 2: Stochastic and Complex Systems, Networks (joint session DY/SOE)

Time: Friday 11:30–12:45 Location: H19

DY 52.1 Fri 11:30 H19

Thermodynamic uncertainty relations for many-body systems with fast jump rates and large occupancies — •Ohad Shpielberg[1] and Arnab Pal[2] — [1]University of Haifa, Haifa, Israel. — [2]Department of Physics, Indian Institute of Technology, Kanpur, India

The thermodynamic uncertainty relations constitute an important inequality, bounding the entropy production through current fluctuations. The results have been successfully applied, in particular for single body dynamics. Here we present uncertainty relations and other useful inequalities for the many body systems, in the limit of highly occupied systems. The resulting coarse grained theory also accounts for tighter inequalities than the single body case.

DY 52.2 Fri 11:45 H19

Effects of measures on phase transitions in two cooperative susceptible-infectious-recovered dynamics — Adib Khazaee[1] and •Fakhteh Ghanbarnejad[1,2] — [1]Sharif University of Technology, Tehran, Iran — [2]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed),Technical University of Dresden, 01062 Dresden, Germany

In recent studies, it has been shown that a cooperative interaction in a co-infection spread can lead to a discontinuous transition at a decreased threshold. Here, we investigate effects of immunization with a rate proportional to the extent of the infection on phase transitions of a cooperative co-infection. We use the mean-field approximation to illustrate how measures that remove a portion of the susceptible compartment, like vaccination, with high enough rates can change discontinuous transitions in two coupled susceptible-infectious-recovered dynamics into continuous ones while increasing the threshold of transitions. First, we introduce vaccination with a fixed rate into a symmetric spread of two diseases and investigate the numerical results. Second, we set the rate of measures proportional to the size of the infectious compartment and scrutinize the dynamics. We solve the equations numerically and analytically and probe the transitions for a wide range of parameters. We also determine transition points from the analytical solutions. Third, we adopt a heterogeneous mean-field approach to include heterogeneity and asymmetry in the dynamics and see if the results corresponding to homogeneous symmetric case stand. (Physical Review E 105 (3), 034311)

DY 52.3 Fri 12:00 H19

ANDOR and beyond: Dynamically switchable logic gates as modules for flexible information processing in biochemical regulatory networks — •Mohammadreza Bahadorian[1,2] and Carl D. Modes[1,2,3] — [1]Max Planck Institut for Molecular Cell Biology and Genetics (MPI-CBG), 01307 Dresden, Germany — [2]Center for Systems Biology Dresden (CSBD), 01307 Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, 01069 Dresden, Germany

Understanding how complex (bio-)chemical regulatory networks may be capable of processing information in flexible, yet robust ways is a key question with implications in biology and dynamical systems theory. Considerable effort has been focused on identification and characterization of structural and dynamical motifs of biological information processing, but a framework for studying flexibility and robustness of the motifs is lacking. We here propose a small set of effective modules capable of performing different logical operations based on the basin of attraction in which the system resides. These dynamically switchable logic gates require fewer components than their traditional

analogs where static, separate gates are used for each desired function. We demonstrate the applicability and limits of these circuits by determining a robust range of parameters over which they correctly operate and then characterize their resilience against intrinsic noise of the constituent reactions using the theory of large deviations. Tradeoffs between multi-functionality and robustness against various types of noise are shown.

DY 52.4 Fri 12:15 H19

Memory formation in adaptive networks — •Komal Bhattacharyya[1], David Zwicker[1], and Karen Alim[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany

Continuous adaptation of networks like our vasculature ensures optimal network performance when challenged with changing loads. Here, we show that adaptation dynamics allow a network to memorize the position of an applied load within its network morphology. We identify that the irreversible dynamics of vanishing network links encode memory. Our analytical theory successfully predicts the role of all system parameters during memory formation, including parameter values which which prvent memory formation. We thus provide an analytically tractable theory of memory formation in disordered systems.

DY 52.5 Fri 12:30 H19

Inference of fractional nonlinear models from temperature time series and application to predictions — •Johannes A. Kassel and Holger Kantz — MPI for the Physics of Complex Systems, Dresden, Germany

We introduce a method to reconstruct macroscopic models of one-dimensional nonlinear stochastic processes with long-range correlations from sparsely sampled time series by combining fractional calculus and discrete-time Langevin equations. We reconstruct a model for daily mean temperature data recorded at Potsdam (Germany) and use it to predict the first frost date. Including the Arctic Oscillation Index as an external driver into our model, we predict extreme temperatures for several European weather stations, illustrating the potential of long-memory models for predictions in the subseasonal-to-seasonal range.

[1] Johannes A. Kassel and Holger Kantz, Phys. Rev. Research 4, 013206