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

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

Walter Zimmermann
Theoretische Physik I
Universität Bayreuth
Universitätsstrasse 30
95447 Bayreuth
walter.zimmermann@uni-bayreuth.de

Overview of Invited Talks and Sessions

(Lecture halls HÜL 186, ZEU 118, ZEU 160, and ZEU 147; Poster P1A and P1C)

Plenary and Prize talks

PLV II	Mon	8:30– 9:15	HSZ 01	**Bicontinuous Structures in Charged Polymer Blends** — •Timothy Lodge
PRV I	Mon	13:15–13:45	HSZ 01	**Quantum Dots for Quantum Technologies** — •Dieter Bimberg
PRV III	Tue	13:15–13:45	HSZ 01	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
PLV VII	Wed	8:30– 9:15	HSZ 01	**Physics of Morphogenesis** — •Stephan Grill
PLV IX	Wed	14:00–14:45	HSZ 02	**Stochastic thermodynamics: Concepts and applications** — •Udo Seifert
PLV XIV	Fri	8:30– 9:15	HSZ 01	**Machine Learning meets Quantum Physics** — •Klaus-Robert Müller

Invited Talks

DY 3.1	Mon	9:30–10:00	ZEU 118	**Disentangling Lagrangian Turbulence** — Lukas Bentkamp, Cristian Lalescu, •Michael Wilczek
DY 5.1	Mon	10:00–10:30	HÜL 186	**Dynamically probing winding numbers of Floquet toplogical insulators in optical lattices** — •André Eckardt
DY 11.1	Mon	15:00–15:30	HÜL 186	**A hydrodynamic view on the diffusion in membranes and dense solutions of proteins** — •Gerhard Hummer, Sören von Bülow, Martin Vögele, Lisa Pietrek, Marc Siggel, Max Linke, Jürgen Köfinger, Lukas Stelzl
DY 13.1	Mon	15:00–15:30	ZEU 118	**Shearing of glasses: new insight from studying model glasses of different system sizes** — •Andreas Heuer, Markus Blank-Burian, Lawrence Smith, Moumita Maiti
DY 14.1	Mon	15:00–15:30	ZEU 160	**Microswimmers in (semi-)dilute suspensions: binary mixtures, trapping, orientational ordering, collective motion, and imposed shear flows** — Christian Hoell, Giorgio Pessot, Hartmut Löwen, •Andreas M. Menzel
DY 21.1	Tue	9:30–10:00	HÜL 186	**From Non-normalizable Boltzmann-Gibbs statistics to infinite-ergodic theory** — •Eli Barkai
DY 23.1	Tue	9:30–10:00	ZEU 118	**Collective dynamics of cell-fate decision in the early embryo** — •Jordi Garcia-Ojalvo
DY 33.1	Wed	9:30–10:00	ZEU 118	**Statistical Mechanics of Granular Clogging** — •Douglas Durian
DY 34.1	Wed	9:30–10:00	ZEU 160	**Brownian systems with time-delay: non-equilibrium thermodynamics and connection to active systems** — •Sabine H.L. Klapp, Sarah A.M. Loos
DY 39.1	Wed	15:00–15:30	HÜL 186	**Supersymmetric Polarization Anomaly in Photonic Discrete-Time Quantum Walks** — •Sonja Barkhofen, Lennart Lorz, Thomas Nitsche, Christine Silberhorn, Henning Schomerus
DY 40.1	Wed	15:00–15:30	ZEU 118	**I want it all and I want it now!** — •Alexander K. Hartmann

DY 42.1	Wed	15:00–15:30	ZEU 160	**Light-regulated microbial dynamics and self-organization in complex geometries** — •Oliver Bäumchen
DY 46.1	Thu	9:30–10:00	HÜL 186	**Nanofriction in Ion Coulomb Systems** — •Tanja Mehlstäubler
DY 47.1	Thu	9:30–10:00	ZEU 118	**Nonlinear dynamics of cardiac arrhythmias in the long QT syndrome** — •Alain Karma
DY 47.6	Thu	11:15–11:45	ZEU 118	**Wave-particle duality of dissipative vortices and implications for cardiology** — •Irina V. Biktasheva
DY 51.1	Thu	14:00–14:30	ZEU 118	**Dyadic structure-function relationships in ventricular cardiac myocytes: from sparks to action potentials** — •Martin Falcke, Filippo G. Cosi, Wolfgang Giese, Wilhelm Neubert, Stefan Luther, Ulrich Parlitz
DY 61.1	Fri	9:30–10:00	HÜL 186	**Characterizing quantum chaos through adiabatic transformations** — •Anatoli Polkovnikov, Anushya Chandran, Pieter Claeys, Anatoly Dymarsky, Mohit Pandey, Tamiro Renzo, Dries Sels, Sho Sugiura, Jonathan Wurtz
DY 63.1	Fri	9:30–10:00	ZEU 160	**Coarse-grained descriptions of models of cell monolayers** — •Eric Bertin

Invited talks of the joint symposium SYSD (SKM Dissertation-Prize 2020)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:55	HSZ 02	**Disentangling transport in topological insulator thin films down to the nanoscale** — •Felix Lüpke
SYSD 1.2	Mon	9:55–10:20	HSZ 02	**Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies** — •Tom Sebastian Seifert, Tobias Kampfrath
SYSD 1.3	Mon	10:20–10:45	HSZ 02	**Non-radiative voltage losses in organic solar cells** — •Johannes Benduhn
SYSD 1.4	Mon	10:45–11:10	HSZ 02	**Multivalent ions for tuning the phase behaviour of protein solutions** — •Olga Matsarskaia
SYSD 1.5	Mon	11:10–11:35	HSZ 02	**Network Dynamics under Constraints** — •Malte Schröder
SYSD 1.6	Mon	11:35–12:00	HSZ 02	**Exciton spectroscopy of van der Waals heterostructures** — •Philipp Nagler

Invited talks of the joint symposium SYBD (Big data driven materials science)

See SYBD for the full program of the symposium.

SYBD 1.1	Tue	9:30–10:00	HSZ 02	**Materials innovation driven by data and knowledge systems** — •Surya Kalidindi
SYBD 1.2	Tue	10:00–10:30	HSZ 02	**Network Theory Meets Materials Science** — •Chris Wolverton, Murat Aykol, Vinay Hegde
SYBD 1.3	Tue	10:30–11:00	HSZ 02	**Verification and error estimates for ab initio data** — •Claudia Draxl
SYBD 1.4	Tue	11:15–11:45	HSZ 02	**Identifying Domains of Applicability of Machine Learning Models for Materials Science** — •Mario Boley, Christopher Sutton, Luca M. Ghiringhelli, Matthias Rupp, Jilles Vreeken, Matthias Scheffler
SYBD 1.5	Tue	11:45–12:15	HSZ 02	**Deep learning of low-dimensional latent space molecular simulators** — •Andrew Ferguson

Invited talks of the joint symposium SYCE (Climate and energy: Challenges and options from a physics perspective)

See SYCE for the full program of the symposium.

SYCE 1.1	Wed	9:30–10:00	HSZ 02	**Towards a carbon-free energy system: Expectations from R&D in renewable energy technologies** — •Bernd Rech, Rutger Schlatmann
SYCE 1.2	Wed	10:00–10:30	HSZ 02	**Decarbonizing the Heating Sector - Challenges and Solutions** — •Florian Weiser

SYCE 1.3	Wed	10:30–11:00	HSZ 02	**The challenge of anthropogenic climate change - Earth system analysis can guide climate mitigation policy** — •Matthias Hofmann
SYCE 1.4	Wed	11:15–11:45	HSZ 02	**A carbon-free Energy System in 2050: Modelling the Energy Transition** — •Christoph Kost, Philip Sterchele, Hans-Martin Henning
SYCE 1.5	Wed	11:45–12:15	HSZ 02	**The transition of the electricity system to 100% renewable energy: agent-based modeling of investment decisions under climate policies** — •Kristian Lindgren

Invited talks of the joint symposium SYES (Spain as Guest of Honor)

See SYES for the full program of the symposium.

SYES 1.1	Thu	9:30–10:00	HSZ 02	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs
SYES 1.2	Thu	10:00–10:30	HSZ 02	**Mechanics of life: Cellular forces and mechanics far from thermodynamic equilibrium** — •Timo Betz
SYES 1.3	Thu	10:30–11:00	HSZ 02	**A hydrodynamic approach to collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.4	Thu	11:15–11:45	HSZ 02	**The spindle is a composite of two permeating polar gels** — David Oriola, Benjamin Dalton, Franziska Decker, Frank Julicher, •Jan Brugues
SYES 1.5	Thu	11:45–12:15	HSZ 02	**Adding magnetic properties to epitaxial graphene** — •Rodolfo Miranda
SYES 2.1	Thu	15:00–15:30	HSZ 01	**Interactions in assemblies of surface-mounted magnetic molecules** — •Wolfgang Kuch
SYES 2.2	Thu	15:30–16:00	HSZ 01	**Towards phononic circuits based o optomechanics** — •Clivia M. Sotomayor-Torres
SYES 2.3	Thu	16:00–16:30	HSZ 01	**Optical properties of 2D materials and heterostructures** — •Janina Maultzsch
SYES 2.4	Thu	16:45–17:15	HSZ 01	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 2.5	Thu	17:15–17:45	HSZ 01	**Infrared signatures of the coupling between vibrational and plasmonic excitations** — •Annemarie Pucci

Invited talks of the joint symposium SYDW (Dynamical wetting of flexible, adaptive and switchable surfaces)

See SYDW for the full program of the symposium.

SYDW 1.1	Thu	15:00–15:30	HSZ 02	**Statics and Dynamics of Soft Wetting** — •Bruno Andreotti
SYDW 1.2	Thu	15:30–16:00	HSZ 02	**Modelling imbibition, dynamic wetting and evaporation on structured surfaces and porous coatings** — •Tatiana Gambaryan-Roisman, Noemi Ghillani
SYDW 1.3	Thu	16:00–16:30	HSZ 02	**Droplets on shaped liquid and electrically switchable surfaces** — •Glen McHale
SYDW 1.4	Thu	16:45–17:15	HSZ 02	**Liquid-liquid Dewetting: From Spinodal Breakup to Dewetting Morphologies and Rates** — •Ralf Seemann, Stefan Bommer, Roghayeh Shiri, Sebastian Jachalski, Dirk Peschka, Barbara Wagner
SYDW 1.5	Thu	17:15–17:45	HSZ 02	**Droplet durotaxis and engulfment on yielding viscoelastic gels** — •Anne Juel

Sessions

DY 1.1–1.3	Sun	16:00–18:30	HSZ 03	**Tutorials: Stochastic Processes from Financial Risk to Dynamics in Biology and Physics (joint session SOE/DY/TUT)**
DY 2.1–2.11	Mon	9:30–13:00	HÜL 386	**Active Matter I (joint session BP/DY/CPP)**
DY 3.1–3.10	Mon	9:30–12:30	ZEU 118	**Fluid Physics of Turbulence**
DY 4.1–4.6	Mon	9:30–11:15	ZEU 255	**Glasses and Glass Transition (joint session CPP/DY)**
DY 5.1–5.13	Mon	10:00–13:30	HÜL 186	**Many-body Systems: Equilibration, Chaos and Localization I (joint session DY/TT)**

DY 6.1–6.5	Mon	10:00–11:15	ZEU 147	**Nonlinear Dynamics, Synchronization and Chaos**
DY 7.1–7.10	Mon	10:00–12:45	ZEU 160	**Statistical Physics (General) I**
DY 8.1–8.4	Mon	11:30–12:30	ZEU 147	**Physics of Power Grids (joint session DY/SOE)**
DY 9.1–9.7	Mon	15:00–18:15	HSZ 03	**Focus Session: Simulating Quantum Many-Body Systems on Noisy Intermediate-Scale Quantum Computers (joint session TT/DY)**
DY 10.1–10.13	Mon	15:00–18:30	HSZ 201	**Graphene (jointly with DY, MA, HL, DS, O) (joint session TT/DY/HL)**
DY 11.1–11.1	Mon	15:00–15:30	HÜL 186	**Invited Talk**
DY 12.1–12.7	Mon	15:00–17:15	SCH A251	**Statistical Physics of Biological Systems I (joint session BP/DY)**
DY 13.1–13.10	Mon	15:00–18:00	ZEU 118	**Glasses and Glass Transition (joint session DY/CPP)**
DY 14.1–14.9	Mon	15:00–17:45	ZEU 160	**Microswimmers (joint session DY/CPP)**
DY 15.1–15.10	Mon	15:30–18:15	HÜL 186	**Condensed-matter simulations augmented by advanced statistical methodologies (joint session DY/CPP)**
DY 16.1–16.5	Mon	15:30–16:45	ZEU 147	**Convection**
DY 17.1–17.3	Mon	16:30–17:15	ZEU 260	**Interfaces and Thin Films I (joint session CPP/O/DY)**
DY 18.1–18.5	Mon	17:00–18:15	ZEU 147	**Delay and Feedback Dynamics**
DY 19.1–19.13	Tue	9:30–13:00	HSZ 204	**Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/DY)**
DY 20.1–20.11	Tue	9:30–13:15	GÖR 226	**Data analytics for dynamical systems I (Focus Session joint with DY and BP) (joint session SOE/DY/CPP/BP)**
DY 21.1–21.1	Tue	9:30–10:00	HÜL 186	**Invited Talk**
DY 22.1–22.11	Tue	9:30–13:00	HÜL 386	**Active Matter II (joint session BP/DY/CPP)**
DY 23.1–23.1	Tue	9:30–10:00	ZEU 118	**Invited Talk**
DY 24.1–24.13	Tue	9:30–13:00	ZEU 160	**Complex Fluids and Soft Matter (joint session DY/CPP)**
DY 25.1–25.12	Tue	9:30–13:00	ZEU 260	**Interfaces and Thin Films II (joint session CPP/O/DY)**
DY 26.1–26.12	Tue	10:00–13:15	HÜL 186	**Brownian Motion, Transport and Anomalous Diffusion**
DY 27.1–27.6	Tue	10:00–11:30	ZEU 118	**Statistical Physics II**
DY 28.1–28.9	Tue	10:00–12:30	ZEU 147	**Pattern Formation and Reaction-Diffusion Systems**
DY 29.1–29.8	Tue	14:00–16:00	HSZ 204	**Nonequilibrium Quantum Many-Body Systems 2 (joint session TT/DY)**
DY 30.1–30.8	Tue	14:00–16:00	ZEU 160	**Active Matter III (joint session DY/BP/CPP)**
DY 31.1–31.13	Wed	9:30–13:00	HÜL 186	**Many-body Systems: Equilibration, Chaos and Localization II (joint session DY/TT)**
DY 32.1–32.11	Wed	9:30–12:30	ZEU 114	**Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)**
DY 33.1–33.11	Wed	9:30–12:45	ZEU 118	**Granular Matter and Granular Dynamics I**
DY 34.1–34.1	Wed	9:30–10:00	ZEU 160	**Invited Talk**
DY 35.1–35.12	Wed	9:30–13:00	ZEU 255	**Modelling and Simulation of Soft Matter I (joint session CPP/DY)**
DY 36.1–36.6	Wed	10:00–11:30	ZEU 147	**Stochastic Thermodynamics**
DY 37.1–37.9	Wed	10:00–12:30	ZEU 160	**Active Matter IV (joint session DY/CPP/BP)**
DY 38.1–38.5	Wed	15:00–17:15	GÖR 226	**Partial Synchronization Patterns in Neuronal Networks I (Focus Session joint with DY / SOE / BP) (joint session SOE/DY)**
DY 39.1–39.14	Wed	15:00–19:00	HÜL 186	**Quantum Chaos (joint session DY/TT)**
DY 40.1–40.8	Wed	15:00–17:30	ZEU 118	**Data Analytics, Extreme Events, and Nonlinear Stochastic Systems (joint session DY/SOE)**
DY 41.1–41.7	Wed	15:00–16:45	ZEU 147	**Droplets and Wetting (joint session DY/CPP)**
DY 42.1–42.9	Wed	15:00–17:45	ZEU 160	**Fluid Physics of Life (joint session DY/BP)**
DY 43.1–43.8	Wed	15:00–17:30	ZEU 250	**Statistical Physics of Biological Systems II (joint session BP/DY)**
DY 44.1–44.7	Wed	15:00–16:45	ZEU 255	**Modelling and Simulation of Soft Matter II (joint session CPP/DY)**
DY 45.1–45.6	Wed	17:00–18:30	ZEU 147	**Microfluidics (joint session DY/CPP)**
DY 46.1–46.10	Thu	9:30–12:30	HÜL 186	**Many-body Quantum Dynamics I**
DY 47.1–47.10	Thu	9:30–12:45	ZEU 118	**Focus Session: Nonlinear Dynamics of the Heart I (joint session DY/BP)**
DY 48.1–48.10	Thu	9:30–12:15	ZEU 147	**Statistical Physics far from Thermal Equilibrium**

DY 49.1–49.13	Thu	9:30–13:00	ZEU 255	**Wetting and Liquids at Interfaces and Surfaces I (joint session CPP/O/DY)**
DY 50.1–50.7	Thu	10:00–11:45	ZEU 160	**Granular Matter and Granular Dynamics II**
DY 51.1–51.6	Thu	14:00–15:45	ZEU 118	**Focus Session: Nonlinear Dynamics of the Heart II (joint session DY/BP)**
DY 52.1–52.12	Thu	15:00–18:15	HÜL 186	**Quantum Dynamics, Decoherence and Quantum Information**
DY 53.1–53.21	Thu	15:00–18:00	P1A	**Poster: Quantum Dynamics, Chaos and Information; Many Body Systems**
DY 54.1–54.9	Thu	15:00–18:00	P1A	**Poster: Active Matter and Microswimmers (joint session DY/TT)**
DY 55.1–55.18	Thu	15:00–18:00	P1A	**Poster: Turbulence; Complex Fluids; Microfluidics; Droplets and Wetting**
DY 56.1–56.14	Thu	15:00–18:00	P1A	**Poster: Glasses; Granular Matter; Brownian Motion and Anomalous Diffusion**
DY 57.1–57.18	Thu	15:00–18:00	P1C	**Poster: Statistical Physics; Critical Phenomena; Stochastic Thermodynamics; Extreme Events; Data Analytics**
DY 58.1–58.15	Thu	15:00–18:00	P1C	**Poster: Nonlinear Dynamics; Pattern Formation; Networks; Delay Systems; Synchronization**
DY 59	Thu	18:15–19:15	ZEU 160	**Mitgliederversammlung**
DY 60.1–60.2	Fri	9:30–10:00	GÖR 226	**Data analytics for dynamical systems II (Focus Session joint with DY and BP) (joint session SOE/CPP/DY)**
DY 61.1–61.1	Fri	9:30–10:00	HÜL 186	**Invited Talk**
DY 62.1–62.8	Fri	9:30–11:45	ZEU 118	**Critical Phenomena and Phase Transitions**
DY 63.1–63.1	Fri	9:30–10:00	ZEU 160	**Invited Talk**
DY 64.1–64.9	Fri	9:30–12:15	ZEU 260	**Wetting and Liquids at Interfaces and Surfaces II (joint session CPP/DY/O)**
DY 65.1–65.6	Fri	10:00–12:00	GÖR 226	**Partial Synchronization Patterns in Neuronal Networks II (Focus Session joint with DY / SOE / BP) (joint session SOE/DY)**
DY 66.1–66.8	Fri	10:00–12:00	HÜL 186	**Many-body Quantum Dynamics II**
DY 67.1–67.6	Fri	10:00–11:30	ZEU 160	**Active Matter V (joint session DY/BP/CPP)**
DY 68.1–68.1	Fri	12:30–13:15	HSZ 02	**Closing Talk (joint session BP/DY/CPP)**

Annual General Meeting of the Dynamics and Statistical Physics Division

Thursday 18:15–19:15 ZEU 160

DY 1: Tutorials: Stochastic Processes from Financial Risk to Dynamics in Biology and Physics (joint session SOE/DY/TUT)

Stochastic Processes are an essential ingredient of models in biology, physics and chemistry, as well as in socio-economic systems where agents are often modeled by a simple set of rules. The tutorials first lay foundations, then introduce advanced concepts and finally demonstrate their application in turbulence, critical phenomena in socio-technical networks, and the dynamics of epidemic spreading. (Session organised by Jens Christian Claussen.)

Time: Sunday 16:00–18:30 Location: HSZ 03

Tutorial DY 1.1 Sun 16:00 HSZ 03

Stochastic models for particles in turbulence — •Bernhard Mehlig — Department of Physics, University of Gothenburg, Sweden

The subject of this tutorial is the dynamics of heavy particles in turbulence, such as water droplets in the turbulent air of a cumulus cloud, dust grains in the turbulent gas around a growing star, or motile microorganisms in the turbulent ocean. The analysis of such highly nonlinear and multi-scale problems poses formidable challenges, because any description of the dynamics must refer to the turbulent fluctuations that the particles experience as they move through the fluid. Experiments resolving the particle dynamics have only recently become possible, and direct numerical simulations of such systems are still immensely difficult.

In this tutorial I explain how to understand the fundamental mechanisms determining the dynamics of particles in turbulence in terms of statistical models that account for the symmetries and statistics of the turbulent flow. Using simple examples I illustrate how to solve such models with diffusion approximations, highlighting an analogy with Kramers' escape problem. I discuss the limitations of the approach, and summarise recent progress. I conclude by discussing open questions, arguing that the approach outlined provides a unique opportunity to make significant progress regarding this challenging and important problem.

Tutorial DY 1.2 Sun 16:50 HSZ 03

From Percolation and Explosive Percolation to a unifying principle — •Jan Nagler — Frankfurt School of F&M, Frankfurt, Germany

The emergence of large-scale connectivity crucially underlies the structure, proper functioning, and failure of many complex socio-technical networks. For many decades, percolation was studied predominately as a second-order phase transition where at the critical threshold, the order parameter increases in a rapid but continuous way. In 2009, an explosive, i.e. extremely rapid, transition was found for a network growth process where links compete for addition. This observation of "explosive percolation" started an enormous surge of analyzing explosive phenomena and their consequences. Many models are now shown to yield discontinuous explosive percolation transitions, and some models exhibit a hybrid transition with a combination of second- and first- order features. Important mechanisms that achieve the required delay for explosive transitions include history dependence, non-self-averaging, and strong correlations. In this tutorial we will start to review standard percolation and end with "explosive phenomena" in networked systems. Examples include social systems, globalization, and the emergence of molecular life [D'Souza, Gomez-Gardenes, Nagler, Arenas, Explosive phenomena in complex networks, Advances in Physics 68(3):123, 2019]. We will close with some recent publication that provides a unifying framework for continuous, discontinuous and even hybrid phase transitions [Fan, Meng, Liu, Saberi, Kurths, Nagler, Universal gap scaling in percolation, Nature Physics, in press].

Tutorial DY 1.3 Sun 17:40 HSZ 03

Spreading dynamics on networks: from social interactions to epidemics and pandemics — •Fakhteh Ghanbarnejad — Sharif University of Technology, Tehran, Iran

Spreading of gossips, news, infectious diseases, computer viruses, new products, etc. are some examples of epidemic dynamics. In this tutorial, firstly we review the basic models for modelling such phenomena including deterministic and stochastic approaches. Also we address how social contacts and the underlying topology of interactions can affect the dynamics. Finally we discuss when and how a spreading dynamics may end to a widespread endemic or pandemic and if and how social interactions play a role.

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

Time: Monday 9:30–13:00 Location: HÜL 386

Invited Talk DY 2.1 Mon 9:30 HÜL 386

Spontaneous and driven active matter flows — •Eric Clement — PMMH-ESPCI-Sorbonne University, Paris, France

Understanding the individual and the macroscopic transport properties of motile micro-organisms in complex environments is a timely question, relevant to many ecological, medical and technological situations. At the fundamental level, this question is also receiving a lot of attention as fluids loaded with swimming micro-organisms has become a rich domain of applications and a conceptual playground for the statistical physics of active matter. The existence of microscopic sources of energy borne by the motile character of micro-swimmers is driving self-organization processes at the origin of original emergent phases and unconventional macroscopic properties leading to revisit many standard concepts in the physics of suspensions. In this presentation, I will report on a recent exploration on the question of collective motionspontaneous formation, in relation with the rheological response of active suspensions. I will also present new experiments showing how the motility of bacteria can be controlled such as to extract work macroscopically.

DY 2.2 Mon 10:00 HÜL 386

Light-regulated motility of microbial suspensions induces phase separation in confinement — •Alexandros Fragkopoulos[1], Jeremy Vachier[1], Johannes Frey[1], Flora-Maud Le Menn[1], Michael Wilczek[1], Marco Mazza[1,2], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), D-37077 Göttingen, Germany — [2]Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire LE11 3TU, United Kingdom

A highly concentrated suspension of self-propelled particles can form large-scale concentration patterns, separating into regions of high and low particle concentrations, due to the activity of the particles and their mutual interactions. However, such a phenomenon has so far been rarely seen in biological systems. Here, we present that a sufficiently concentrated suspension of *Chlamydomonas reinhardtii* cells, a model organism of puller-type microswimmers, forms such large-scale aggregations under confinement in specific light conditions. We find that cell-cell interactions need to be dominated by collisions for the aggregation to form, resulting to a generic coupling of the cell's motility and local cell density. In addition, the cell's motility decreases with decreasing light intensity, which regulates the cell aggregation. Through active Brownian particle simulations, we show that for our system the change of the motility is sufficient to induce the aggregation. Finally, we provide evidence that the photosynthetic activity controls the cell's motility, and consequentially, the separation of the active suspension into regions of high and low cell density.

DY 2.3 Mon 10:15 HÜL 386

Motility induced transport in microbial environments — •Jayabrata Dhar, Arkajyoti Ghoshal, and Anupam Sengupta

— Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg, 162 A, Avenue de la Faencerie, L-1511, Luxembourg City, Luxembourg

Despite their minuscule size, microbes mediate a range of processes in ecology, medicine and industry due to high local concentrations. Studies in aquatic ecosystems have demonstrated nutrient mixing via bioconvection by high concentrations of motile microbes [1] potentially impacts species distributions in natural settings. However, to date, we lack a systematic framework to capture the role of microbial traits (for instance, morphology or motility) on the onset and progression of bioconvection. Here, using different bloom-forming algal species as model organisms, we study how microbial traits underpin the onset of bioconvection and modulate mass transfer due to local density changes. Combining micro-PIV analysis of dispersed particles and auto-fluorescence imaging of algal cells, we quantify the emergent transport properties in real-time, revealing a plume-driven primary convective field. Interestingly, our results further capture relatively weak, secondary eddies that create local mixing patches with short lifetimes. Thus, bioconvection may alter the chemical environment of the microbes through distinct modes, impacting the distribution of nutrients, toxins or secondary metabolites, all of which could be vital for large-scale phenomena like harmful algal blooms.

[1] T. Sommer, et al., Geophysical Research Letters 44, 9424, 2017.

DY 2.4 Mon 10:30 HÜL 386

Reactivation of isolated axonemes by light-driven ATP regeneration system — Raheel Ahmed[1], Christin Kleinberg[2], Tanja Vidakovich-Koch[2], Kai Sundmacher[2], Eberhard Bodenschatz[1], and •Azam Gholami[1] — [1]MPI for Dynamics and Self-Organization — [2]MPI for Dynamics of Complex Technical Systems

Cilia and flagella are slender cellular appendages whose regular beating pattern pumps fluids, for example the mucus in mammalian airways, or propels unicellular organisms such as the green algae Chlamydomonas reinhardtii. Cilia and flagella have a microtubule-based structure called axoneme which performs whip-lash-like motion to provide motility. This oscillatory motion is powered by dynein molecular motors that generate active stresses for ciliary beat in the presence of ATP. In this work, we have successfully integrated light-driven energy module for continuous generation of ATP. This light-driven ATP regeneration system is built through bottom-up assembly of FOF1- ATP synthase and bacteriorhodopsin into two different types of artificial hybrid membranes based on a diblock copolymer (PBd-PEO) and a graft copolymer (PDMS- g-PEO). After illumination of the energy module with light, we mixed it with axonemes isolated from Chlamydomonas reinhardtii and observed actively beating axonemes for many hours. Interestingly, the axonemes beat even at low concentrations of ATP well below 50 μM.

DY 2.5 Mon 10:45 HÜL 386

Chemotaxis strategies of bacteria with multiple run-modes — •Zahra Alirezaeizanjani[1,2], Robert Grossmann[1], Veronika Pfeifer[1], Marius Hintsche[1], and Carsten Beta[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

Bacterial chemotaxis – a fundamental example of directional navigation in the living world – is key to many biological processes, including the spreading of bacterial infections. Many bacterial species were recently reported to exhibit several distinct swimming modes – the flagella may, for example, push the cell body or wrap around it. How do the different run modes shape the chemotaxis strategy of a multimode swimmer? Here, we investigate chemotactic motion of the soil bacterium *Pseudomonas putida* as a model organism. By simultaneously tracking the position of the cell body and the configuration of its flagella, we demonstrate that individual run modes show different chemotactic responses in nutrition gradients and thus constitute distinct behavioral states. Based on an active particle model, we demonstrate that switching between multiple run states that differ in their speed and responsiveness provide the basis for robust and efficient chemotaxis in complex natural habitats.

30 min. coffee break

DY 2.6 Mon 11:30 HÜL 386

Synthetic minimal active cilia — •Isabella Guido — Max Planck Institute for Dynamics and Self-Organization, Goettigen, Germany

Cilia and flagella are microtubule based filamentous organelles that protrude into the extracellular environment from the surface of many cells for promoting fluid transport or propelling organisms in fluids by producing rhythmic bending waves. The main contribution to their beating is due to motor proteins that drive sliding of the microtubule doublets. However, the fundamental mechanism of the motor-microtubule interaction is still a puzzle. Here we present a synthetic minimal active cilium, a two-filaments system, in which the beat is initiated by a buckling instability in one of the filaments. The system presents continuous beating through association and dissociation cycles, similar to the sliding of a pair of doublet microtubules observed in a Chlamydomonas flagellum. The analysis of the conformational dynamics gives us a quantification of dynein force, motor density and bending energy. We develop a theoretical model to study the dynamics of active elastic filaments induced by internal force in which the attachment and detachment kinetics of motors play as important a role as their force generation. The active stroke of the synthetic cilium occurs due to a buckling instability between two clamped filaments, while the recovery stroke follows a "catastrophic failure" of the bound motors.

This work is in collaboration with Prof. Ramin Golestanian and Dr. Andrej Vilfan.

DY 2.7 Mon 11:45 HÜL 386

Chiral stresses in nematic cell monolayers — •Ludwig A. Hoffmann[1], Koen Schakenraad[1,2], Roeland M. H. Merks[2,3], and Luca Giomi[1] — [1]Instituut-Lorentz, Leiden University, The Netherlands — [2]Mathematical Institute, Leiden University, The Netherlands — [3]Institute of Biology, Leiden University, The Netherlands

Recent experiments on monolayers of spindle-like cells have provided a convincing demonstration that certain types of collective phenomena in epithelia are well described by active nematic hydrodynamics. While recovering some of the predictions of this framework, however, these experiments have also revealed unexpected features that could be ascribed to the existence of chirality over length scales larger than the typical size of a cell.

We elaborate on the microscopic origin of chiral stresses in nematic cell monolayers and investigate how chirality affects the motion of topological defects, as well as the collective motion in stripe-shaped domains. We find that chirality introduces a characteristic asymmetry in the collective cellular flow, from which the ratio between chiral and non-chiral active stresses can be measured. Furthermore, we find that chirality changes the nature of the spontaneous flow transition under confinement and that, for specific anchoring conditions, the latter has the structure of an imperfect pitchfork bifurcation.

DY 2.8 Mon 12:00 HÜL 386

Self-organization of active surfaces — •Alexander Mietke[1,2,3,4,7], V. Jemseena[5], K. Vijay Kumar[5], Ivo F. Sbalzarini[2,3,4,6], and Frank Jülicher[1,3,6] — [1]MPI for the Physics of Complex Systems — [2]Faculty of Computer Science, TU Dresden — [3]Center for Systems Biology Dresden — [4]MPI of Molecular Cell Biology and Genetics — [5]ICTS-TIFR — [6]Cluster of Excellence PoL, TU Dresden — [7]Department of Mathematics, MIT, Cambridge, MA

Self-organization of morphogenetic events often arises through a feedback loop in which active forces, by inducing deformations and material flows, indirectly affect their own mechano-chemical regulation. In recent years, the existence of generic mechano-chemical patterning mechanisms in simple, fixed geometries has been demonstrated theoretically and experimentally. However, the interplay of mechano-chemical processes with the surface geometry remains to be explored. In our work, we employ the theory of active gels in complex geometries to study the properties of dynamically evolving active surfaces. Within those surfaces, diffusive and advective transport processes can redistribute molecules responsible for local stress generation. This resembles the interplay between active forces, the shape changes they imply and the effects this has on their regulation. Within our framework, a contractile ring formation, as well as the peristaltic motion of active tubular structures can be understood as natural emergent phenomena. Our approach provides novel opportunities to explore different scenarios of mechano-chemical self-organization and can help to better understand the role of shape as a regulatory element in morphogenetic processes.

DY 2.9 Mon 12:15 HÜL 386

Thin-Film Model of Resting and Moving Active Droplets

— •Fenna Stegemerten[1], Sarah Trinscheck[1,2], Karin John[2], and Uwe Thiele[1,3] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Münster, Germany — [2]Université Grenoble-Alpes, CNRS Laboratoire Interdisciplinaire de Physique, Grenoble, France — [3]Center for Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Münster, Germany

We propose a long-wave model for free-surface drops of polar active liquid on a solid substrate. The coupled evolution equations for the film height and the local polarization profile are written in the form of a gradient dynamics supplemented with active stresses and fluxes. A wetting energy for a partially wetting liquid is incorporated allowing for motion of the liquid-solid-gas contact line. This gives a consistent basis for the description of drops of dense bacterial suspensions or compact aggregates of living cells on solid substrates. As example, we analyze the dynamics of active drops and demonstrate how active forces compete with passive surface forces to shape droplets and drive contact line motion. We perform parameter continuation in the activity parameters discussing both, resting and moving droplets. Additional direct time simulations investigate transitions from non-uniformly to uniformly polarized states.

DY 2.10 Mon 12:30 HÜL 386

Fast vs. gradual death in assemblies of immotile growing cells — •Yoav G. Pollack, Philip Bittihn, and Ramin Golestanian — Max Planck Institute for Dynamics and Self-Organization (MPI-DS), Göttingen, Germany

Cell life-cycle processes such as growth, division and death, often all happen on a similar timescale, as do the resultant mechanical and dynamical responses of the cell assembly (such as a colony, biofilm or tissue). An archetypal example is *E. Coli* where growth, division and the subsequent relative motion of the daughter cells all happen at roughly the same rate. However there are also examples of another type of system showing abrupt processes, including 'snapping' cell division in *Actinobacteria* and 'explosive' bacterial lysis.

Here we test whether going from the first type of system to the other by introducing a second *fast* timescale in one of the microscopic processes can affect the macroscopic mechano-dynamics, such as the homeostatic pressure. Specifically we simulate a closed 1D channel of cells that grow and divide to fill up the channel and are removed (via death or extrusion) when pressure builds up. We focus on varying the timescale of the cell removal process, keeping growth and division timescales fixed. We show a clear distinction in the macroscopic system properties between abrupt vs. gradual cell removal, such as a significant increase in the homeostatic pressure.

DY 2.11 Mon 12:45 HÜL 386

Simulations of an active surface immersed in viscous fluids — •Lucas D. Wittwer and Sebastian Aland — Faculty of Informatics / Mathematics, University of Applied Science Dresden, Germany

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 surface immersed in viscous fluids. We show the resulting patterning and cell shape dynamics for different parameter configurations as well as the flow profiles in the surrounding fluids and compare it to results from other models.

DY 3: Fluid Physics of Turbulence

Time: Monday 9:30–12:30 Location: ZEU 118

Invited Talk DY 3.1 Mon 9:30 ZEU 118

Disentangling Lagrangian Turbulence — Lukas Bentkamp, Cristian Lalescu, and •Michael Wilczek — Max-Planck-Institut für Dynamik and Selbstorganisation, Göttingen

Turbulence remains a paradigmatic challenge for nonequilibrium statistical physics. The rapid evolution of computational power and experimental techniques, however, has brought significant progress over the past decades. In this presentation, I will discuss how simulations provide insights into the structure and dynamics of turbulence and inform the development of a statistical theory of turbulence. In particular, I will focus on Lagrangian tracer particles, which sample turbulence in space and time. On their roller-coaster ride through turbulence, tracer particles frequently encounter extreme accelerations which are closely related to the intermittent spatial distribution of intense flow structures such as vortex filaments. This mixed history of flow conditions leads to very complex particle statistics with a pronounced scale dependence. Categorizing Lagrangian particle data from simulations by means of their accelerations reveals that Lagrangian turbulence can be decomposed into much simpler, close-to-Gaussian sub-ensembles for a range of Reynolds numbers. Based on this observation, we develop a comprehensive theoretical framework for Lagrangian single-particle statistics that captures the acceleration, velocity increments as well as single-particle dispersion.

DY 3.2 Mon 10:00 ZEU 118

Statistical geometry of material loops in turbulence — •Lukas Bentkamp[1,2], Cristian Constantin Lalescu[1], Theodore Dimitrios Drivas[3], and Michael Wilczek[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077, Göttingen, Germany — [2]Faculty of Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077, Göttingen, Germany — [3]Department of Mathematics, Princeton University, Princeton, NJ 08544, United States of America

Understanding turbulent transport involves a close investigation of the multi-scale properties of turbulence, since they impose different transport mechanisms at each scale. At small scales, for example, chaos drives trajectories of initially close particles to diverge exponentially. By considering extended structures like material lines, which are passively advected and deformed by the flow, we probe not only this exponential separation, but the general stretch-and-fold mechanisms that lead to turbulent mixing at all scales. Here, we present a study of the statistical geometry of closed material lines. In particular, we complement fully resolved direct numerical simulations of homogeneous turbulence with the analytically tractable Kraichnan model, which allows, for example, for a closer investigation of the fractal dimension, length, curvature and torsion of the loops. By studying these quantities, we gain insight into the geometrical structure of the underlying turbulent flow.

DY 3.3 Mon 10:15 ZEU 118

Machine learning in subcritical plane Couette flow — •Stefan Zammert — Philipps-Universität Marburg

Plane Couette flow shows transient turbulence for Reynolds numbers where the laminar flow is linearly stable. In this so-called subcritical range the time evolution of the flow is deterministic but a turbulent trajectory eventually returns to the laminar state without any obvious precursor.

We study small periodic domains of plane Couette flow and use neural networks to predict if a turbulent trajectory returns to the laminar state within a fixed time T. The performances of the network for variations of the input variables are compared with the goal to minimize the amount of input variables necessary for a good prediction.

Having a reliable and fast method to predict the the decay of turbulence by using a limited set of input quantities which is also easily accessible in experiments might for example be helpful for active turbulence control.

DY 3.4 Mon 10:30 ZEU 118

Small scale structures of turbulence in terms of entropy and fluctuation theorems — Andre Fuchs[1], •Joachim Peinke[1], Matthias Waechter[1], Silvio M. Duarte Queiros[2], Alain Girard[3], and Pedro G. Lind[4] — [1]Institute of Physics and For-Wind, University of Oldenburg, — [2]Centro Brasileiro de Pesquisas Fisicas and National Institute of Science and Technology for Complex Systems, Rio de Janeiro - RJ, Brazil — [3]INAC-SBT, UMR CEA-

Grenoble, 38054 Grenoble, France — [4]Department of Computer Science, OsloMet - University, N-0130 Oslo, Norway

Experimental evidence that the integral fluctuation theorem as well as a detailed-like fluctuation theorem holds for large entropy values of the turbulent cascade processes. Stochastic equations describing the scale-dependent cascade process are derived. From individual cascade trajectories an entropy term can be determined. Since the statistical fluctuation theorems set the occurrence of positive and negative entropy events in strict relation, we are able to verify how cascade trajectories, defined by entropy-consumption or entropy-production are linked to turbulent structures: Where as trajectories with entropy-production show expected decreasing behavior; trajectories with entropy-consumption end at small scale velocity increments with finite size and show a lower bound for small scale increments. This indicates a tendency to local discontinuities in the velocity field.

DY 3.5 Mon 10:45 ZEU 118

The boundary zonal flow (BZF) in turbulent rotating convection — •Stephan Weiss[1,7], Xuan Zhang[1], Marcel Wedi[1], Dennis v. Gils[2], Robert E. Ecke[3], Lukas Zwirner[1], Guenter Ahlers[4], Susanne Horn[5], Eberhard Bodenschatz[1,6], and Olga Shishkina[1] — [1]MPI for Dyn. and Self-Org., Göttingen, Germany — [2]Twente University, NL — [3]Los Alamos National Lab., USA — [4]UCSB, USA — [5]Coventry University, UK — [6]Georg-August University Göttingen, Germany — [7]Max Planck – University Twente Center

Thermal convection under the influence of rotation is one of the main driving forces for flows in astro- and geophysical systems. There, Coriolis forces are usually larger then centrifugal forces and vertical scales (i.e., in the direction of the rotation axis) increases compared to horizontal scales. Therefore, experiments are often conducted in cylinders of rather small aspect ratios ($\Gamma = D/H$) between their diameter (D) and height (H), as then the centrifugal forces remain small. We show by using experiments and DNS that in rotating thermal convection in a confined domain with no-slip boundaries, a large-scale flow structure (boundary zonal flow - BZF) develops at the lateral sidewalls, which reaches from the bottom to the top of the cell. In the BZF the vertical velocity and thus the heat transport is severely enhanced. The BZF is periodic in azimuthal direction with a wave number of twice the aspect ratio Γ. While the fluid moves in cyclonic direction close to the sidewall, the entire structure drifts in anticyclonic direction. The BZF is crucial for extrapolating experimental results onto natural systems and also plays an important role in many engineering applications.

DY 3.6 Mon 11:00 ZEU 118

Transport and rotation statistics of self–propelled ellipsoids in turbulence — •José–Agustín Arguedas–Leiva and Michael Wilczek — Max Planck Institute for Dynamics and Self–Organization (MPI DS)

Many plankton species are motile. Motility is, for example, key for grazing and evading predation. Apart from the swimming speed, shape is a critical parameter in defining the response to hydrodynamic flows. A comprehensive understanding of the relation between the relevant particle parameters, shape and motility, and their transport properties and encounter rates in turbulent flows is still missing. Here, we study self–propelled ellipsoids in turbulence as a simple model for motile microorganisms in aquatic environments. Using direct numerical simulations we find non–trivial dispersion properties and rotation statistics as a result of a complex interplay between turbulent advection, motility, and particle spinning and tumbling rates. We show that one important aspect is the effect of rotation on particle transport. In contrast to spinning, tumbling constantly changes particle orientation. As tumbling rates are shape–dependent, this leads to intrinsically different transport properties for differently shaped particles. Our investigation thus helps to characterize the intricate dynamics of self–motile ellipsoids in turbulent flows and sheds light on the role played by shape and motility.

15 min. break.

DY 3.7 Mon 11:30 ZEU 118

Small-scale averaging coarse-grains passive scalar turbulence — •Tobias Bätge[1,2] and Michael Wilczek[1] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Faculty of Physics, University of Göttingen, Germany

Capturing the multi-scale dynamics of turbulent flows remains a theoretical and computational challenge. Therefore, many practical applications require a coarse-grained description, which treats the small scales effectively. How can we obtain such effective large-scale equations? Here, we address this problem at the example of a simple, one-dimensional model for the advection of a passive scalar field. Similar to the Kraichnan model, the scalar is advected by a Gaussian random field and subject to diffusion. Despite its simplicity and analytical tractability, this model shows non-trivial features such as intermittency, anomalous scaling and a dual scalar cascade. We propose that effective large-scale equations can be obtained by ensemble-averaging over the small-scale velocity fluctuations. We show that this procedure leads to an effective diffusivity reminiscent of phenomenological eddy viscosity models. To test our approach, we quantitatively compare the large-scale dynamics and statistics of fully resolved simulations with the ones obtained from our effective large-scale equation. This confirms the ability to reproduce the large scales of a fully resolved system.

DY 3.8 Mon 11:45 ZEU 118

Rayleigh-Taylor Instability in Merging Soap Bubbles — •Patricia Pfeiffer[1], Qingyun Zeng[2], Beng Hau Tan[3], and Claus-Dieter Pfeiffer[1] — [1]Otto von Guericke University Magdeburg, Germany — [2]Nanyang Technological University, Singapore — [3]MIT Alliance for Research and Technology, Singapore

The coalescence of centimeter-sized soap bubbles is studied using high-speed optical imaging. An interference pattern is observed in the area where the bubbles touch each other shortly before merging. This interference rings suggest that the bubbles are forming a dimple before merging and entrap a tiny volume of air between them. Upon merging a water bridge is formed between both bubbles at the crest of the dimpled region, where the distance between the two bubbles is smallest. The rim of the spreading film accelerates for a brief moment, simulations predict less than 1 *s and expands radially from the point of contact. During that time a Rayleigh-Taylor instability sets in resulting in an instability of the rim front. This instability is mainly visible in the area of the dimple since a higher curvature in that regime induces a higher velocity of the rim. At later times, the rim heals into a circular shape. Depending on the surfactant concentration the entrapment of gas pockets is possible with increasing surfactant concentration. However above the critical micelle concentration no further effect of the surfactant concentration on the instability of the rim is observed.

DY 3.9 Mon 12:00 ZEU 118

On the Inertial Range Scaling at Extreme Reyolds Numbers — •Christian Küchler[1,3], Gregory P. Bewley[2], and Eberhard Bodenschatz[1,2,3] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen — [2]Cornell University, Ithaca, NY, USA — [3]Georg August University Göttingen

Kolmogorov predicted in 1941 that universal scaling laws emerge in the increment statistics of turbulent velocities in the limit of infinite Reynolds numbers. In the past it has been found that this limit - if existent - requires extreme Reynolds numbers, which are difficult and expensive to create in a well-controlled turbulent flow. The Variable Density Turbulence Tunnel (Bodenschatz et al., 2014) is the first wind tunnel capable of producing such extreme Reynolds numbers finally allowing us to systematically study the long-standing Kolmogorov prediction and its refinements. The experiment combines the low kinematic viscosity of pressurized SF_6 and an active grid with individually controllable tiles (Griffin et al., 2019). With Nanoscale Thermal Anemometry Probes developed and generously provided by Princeton University (e.g. Bailey et al. (2009), Vallikivi et al. (2014)) we adequately resolve the small scale turbulence. We present results that logarithmic derivatives of structure functions differ from conventional scaling laws of isotropic turbulence. However, these local scaling exponents approach a universal form at some critical Reynolds number. We show that those results are well-described by the generalized self-similar spectrum of decaying turbulence introduced by Yang et al. (2018). It further allows us to extract the scaling exponent.

DY 3.10 Mon 12:15 ZEU 118

Asymmetries of Lagrangian Coherent Structures — •Gerrit Maik Horstmann[1,2], Jeffrey Tithof[2], and Douglas H. Kelley[2] — [1]Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Department of Mechanical Engineering, University of Rochester, Rochester, New York 14627, USA

Lagrangian coherent structures (LCSs) are the dominant barriers to mixing in a fluid flow. LCSs are either the most repelling or most attracting material surfaces in the flow over a given time interval and

are computed using velocity fields evolving either forward or backward in time, respectively. Using data from different 2D and 3D laboratory experiment and direct numerical simulations (DNS), an asymmetry between repelling and attracting LCSs growing with the Reynolds number is revealed. In 2D, this asymmetry is characterized by attracting LCSs occurring over a larger fraction of the spatial domain and moving in a more irregular way than repelling LCSs. Studying an analytical model that captures the salient features of this asymmetry, it can be argued that LCS asymmetry is tied to the direction of the energy cascade in turbulence and exhibits opposite trends in 2D versus 3D. In the 3D flows, it is further observed that attracting LCSs are stronger than repelling LCSs indicating the existence of a second, possibly independent, asymmetry. These results are partially connected to recent discoveries of temporal asymmetry in turbulence suggesting LCSs as an alternative analyzing tool for studying some fundamental properties of turbulent flows.

DY 4: Glasses and Glass Transition (joint session CPP/DY)

Time: Monday 9:30–11:15 Location: ZEU 255

Invited Talk DY 4.1 Mon 9:30 ZEU 255

Shear-stress fluctuations and relaxation in glassy liquids — Liudmyla Klochko, Ivan Kriuchevskyi, Joachim Wittmer, Alexander Semenov, Hendrik Meyer, and •Jörg Baschnagel — Institut Charles Sadron, University of Strasbourg & CNRS, 23 rue du Loess, 67034 Strasbourg Cedex, France

By means of molecular dynamics simulations we study the shear modulus μ and shear stress relaxation function $G(t)$ of a short-chain glass-forming liquid. We determine μ via the shear-stress fluctuation formalism as a function of temperature T and sampling time Δt. When cooling the system below the glass transition temperature T_g the shear modulus has a finite, T-dependent, value which depends on Δt. We show that this sampling time dependence can be traced back to the relaxation of $G(t)$, thereby establishing a relation between two often employed means—i.e. shear stress fluctuation formalism and $G(t)$—to characterize the shear response of glassy systems. We repeat the analysis for 100 independent configurations (samples) and find that the glass transition is accompanied by strong sample-to-sample fluctuations, implying that the standard deviation $\delta\mu$ of the (ensemble-averaged) modulus displays a peak near T_g and is of the same order of magnitude as μ itself. We propose a theory which explains this behavior.

DY 4.2 Mon 10:00 ZEU 255

Molecular dynamics study of 1,4-polybutadiene supported film — •Fedir Demydiuk[1], Hendrik Meyer[1], Joerg Baschnagel[1], Mathieu Solar[1], and Wolfgang Paul[2] — [1]Institute Charles Sadron, University of Strasbourg, UPR22 CNRS, 67034 Strasbourg, France — [2]Institut für Physik, University of Halle, 06120 Halle (Saale), Germany

Our work is dedicated to studying the influence of realistic intrachain constraints imposed due to the presence of torsional barriers on the glass transition in thin polymer films of supported geometry by means of classical molecular dynamics simulations. In order to do so, we use the well-established united-atom model of 1,4-polybutadiene, that has been developed by W. Paul and coworkers (G. D. Smith and W. Paul, *J. Phys. Chem. A*, 102, 1200 (1998)) and studied in confined systems (M. Solar, K. Binder and W. Paul, *J. Chem. Phys*, 146, 203308 (2017)). In our case, the model had to be adapted for usage in systems with free surface.

Focusing on dynamics of united atoms and shear-stress relaxation, we first discuss our results for bulk polybutadiene and then present first extensions of bulk simulations to supported films. First analysis of the supported films shows that dynamics is enhanced at the free surface and slowed down at the substrate.

DY 4.3 Mon 10:15 ZEU 255

Dynamics of an arrested phase transition in a protein system — •Anita Girelli[1], Hendrik Rahmann[2], Nafisa Begam[1], Anastasia Ragulskaya[1], Fabian Westermeier[3], Fajun Zhang[1], Christian Gutt[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Universität Siegen, Germany — [3]DESY, Germany

The interest in phase transitions in biological systems has attracted much effort because of their numerous applications and its role as a mechanism underlying intracellular organization [1]. In this study the development of the spinodal decomposition near the gel/glass transition in a globular protein system was studied using X-Ray Photon Correlation Spectroscopy (XPCS) in the ultra small angle X-Ray scattering (USAXS) regime. The dynamics was probed at different quench depth, exhibiting two regimes: the first regime shows a single exponential decay of the correlation function, and the corresponding decorrelation time increases exponentially with waiting time t_w. In the second regime, a second relaxation channel appears and the associated non-ergodicity parameter increases with t_w until it becomes the dominating decay. The corresponding decorrelation time increases as a power law in t_w. The dynamics was compared to simulations, which were performed by solving numerically the Cahn-Hilliard equation coupled with a gel transition. The effect of nanoscale arrested dynamics can be seen on the microscopic dynamics. Aging with quench depth dependence is visible and can be connected to real space parameters such as final concentration and mobility.

[1] Berry et al., *Rep. Prog. Phys.*, **81**, 046601, 2018

DY 4.4 Mon 10:30 ZEU 255

molecular dynamics of glassy polynorbornenes bearing flexible side substituents: nanophase separation and glass transition — •Mohamed Aejaz Kolmangadi[1], Paulina Szymoniak[1], Glen Jacob Smales[1], Brian Pauw[1], Maxim Bermeshev[2], Martin Böhning[1], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]A.V. Topchiev Institute of Petrochemical Synthesis of Russian Academy of Science, Leninskii prospect, 29, 119991 Moscow, Russia

Polynorbornenes are latest among the high-performance polymers in the field of membrane gas separation. Not much has been studied regarding their molecular dynamics till now. In the present work, we report dielectric and calorimetric investigations of series of polynorbornenes with rigid main backbone and flexible (AlkO)3Si side groups with different length (Al = Propyl, Butyl, Octyl, Decyl). Two dielectrically active α and β relaxations observed are assigned to localized fluctuations and segmental relaxation of the flexible side groups of the polymer. A nanophase separation between the main and side chain parts is concluded from the presence of two dynamic glass transitions of the polymer, is confirmed by means of small and wide-angle X-ray scattering. Furthermore, for the first time, the glass transition temperatures of these polymers which are beyond or near to their degradation temperature are determined using Fast Scanning calorimetry employing high heating and cooling rates. The glass transition temperatures of the polymers decrease with increasing length of the alkyl side chain.

DY 4.5 Mon 10:45 ZEU 255

Controlled crystallisation of luminescent borate-based glasses — •Marc Bürger[1], A. Charlotte Rimbach[1], and Stefan Schweizer[1,2] — [1]Faculty of Electrical Engineering, South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Lübecker Ring 2, 59494 Soest

Luminescent borate glasses and glass ceramics offer a broad spectrum of optical applications. Here, the optical properties of the glass as well as the glass ceramic strongly depend on their composition and the production process. In this work, two different glass systems and their crystallization processes therein are analysed: (i) Lithium borate glass comprised of Li_2O-Al_2O_3-B_2O_3 and (ii) barium borate glass with BaO-B_2O_3. For optical activation, the lanthanide ion Dy^{3+} is added in the form of Dy_2O_3 to enable for a bright green-yellowish luminescence. To initiate the crystallization process in the glass, the samples are thermally-processed at a temperature above the glass transition temperature. The number and size as well as the phase of the grown crystallites depend significantly on annealing temperature and time as well as the heating rate. The crystallite growth is investigated and analysed in detail by differential scanning calorimetry and *in situ* x-ray diffractometry. In addition, the samples are optically characterized

for transmittance, reflectance and scattering.

DY 4.6 Mon 11:00 ZEU 255

X-ray computed tomography of glass foams with controlled bi-modal pore size distribution — •Cristine S. de Oliveira[1], Richard Kohns[2], Felix Meyerhoefer[2], Matthias Neumann[3], Dirk Enke[2], Volker Schmidt[3], Ralf B. Wehrspohn[1], and Juliana Martins de S. e Silva[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Institut für Technische Chemie, Universität Leipzig, Germany — [3]Institut für Stochastik, Universität Ulm, Germany

Glass foams are materials consisting of a light-weight porous glass structure of special importance in the fields of civil engineering and bio-implants. Typically, their synthesis involves the thermal foaming of a powder mixture of glass with a foaming agent that decomposes at the foaming temperature, resulting in a solid glass skeleton permeated by empty pores. In our work, we synthesized a series of glass foams followed by a phase-separation procedure and acid leaching. We used a powdered mixture of silica-based glasses, MnO_2 and C which we submitted to a foaming process at 815 °C. Afterwards, the material was left to cool inside the oven to temperatures around 500 °C and maintained at a constant temperature for phase separation. We then acid leached, washed and dried the samples. Based on the results obtained using X-ray CT at the micro and nanometer scales we observed that slight changes in the preparation procedure resulted in foams with different porosity, pore sizes, pore volumes and sphericity.

DY 5: Many-body Systems: Equilibration, Chaos and Localization I (joint session DY/TT)

Time: Monday 10:00–13:30 Location: HÜL 186

Invited Talk DY 5.1 Mon 10:00 HÜL 186

Dynamically probing winding numbers of Floquet toplogical insulators in optical lattices — •André Eckardt — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden

The classification of topological Floquet systems with time-periodic Hamiltonians transcends that of static systems. For example, spinless fermions in periodically driven two-dimensional lattices are not completely characterized by the Chern numbers of the quasienergy bands, but rather by a set of winding numbers associated with the quasienergy gaps [Phys. Rev. X 3, 031005 (2013)]. I will present two schemes for probing these winding numbers in experiments with ultracold atoms in driven optical lattices. The first one relies on the quench-based tomography [PRL 113, 045303 (2014), Science 352, 1091 (2016)] of band-touching singularities occurring, when adiabatically connecting the driven system to a trivial high-frequency regime [PRL 122, 253601 (2019)]. The second one is based on observing the far-from equilibrium micromotion of the driven system within two driving periods after a sudden quench into the target Hamiltonian and relies on the identification of the winding numbers with an Hopf invariant characterizing the micromotion operator [Phys. Rev. Research 1, 022003(R) (2019)]. Together with the measurement of Chern numbers from the far-from equilibrium dynamics monitored in stroboscopic steps of the driving period [Nat. Comms. 10, 1728 (2019)], it provides a full characterization of the system.

DY 5.2 Mon 10:30 HÜL 186

Evaporative cooling and self-thermalization in an open system of interacting fermions — •Andrey Kolovsky[1,2] and Dima Shepelyansky[3] — [1]Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia — [2]Siberian Federal University, 660041 Krasnoyarsk, Russia — [3]Université de Toulouse, CNRS, 31062 Toulouse, France

We study depletion dynamics of an open system of weakly interacting fermions with two-body random interactions. In this model fermions are escaping from the high-energy one-particle orbitals, that mimics the evaporation process used in laboratory experiments with neutral atoms to cool them to ultra-low temperatures. It is shown that due to self-thermalization the system instantaneously adjusts to the new chemical potential and temperature which decreases in course of time.

DY 5.3 Mon 10:45 HÜL 186

Entanglement entropy of fractal states — •Giuseppe De Tomasi[1] and Ivan Khaymovich[2] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187-Dresden, Germany

In this talk we will discuss the relations between entanglement (and Renyi) entropies and fractal dimensions D_q of many-body wavefunctions.

As a simple example we introduce a new class of *sparse* random pure states being fractal in the corresponding computational basis and show that their entropies grow linearly with for fractal dimension smaller than the subsystem size ($D_q < 0.5$ for equipartitioning) and reach the upper bound of Page value otherwise, far below the ergodic limit $D_q = 1$. The latter shows that Page value entanglement entropy does not guarantee ETH.

Moreover this D_q-dependence poses an upper bound for entanglement and Renyi entropies of any multifractal states and uncovers the relation between multifractality and entanglement properties of many-body wave-functions.

DY 5.4 Mon 11:00 HÜL 186

Tripartite information, scrambling, and the role of Hilbert space partitioning in quantum lattice models — Oskar Schnaack[1], •Niklas Bölter[1], Sebastian Paeckel[1], Salvatore R. Manmana[1], Stefan Kehrein[1], and Markus Schmitt[2,3,1] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Department of Physics, University of California, Berkeley — [3]Max-Planck-Institute for the Physics of Complex Systems, Dresden

For the characterization of the dynamics in quantum many-body systems the question how information spreads and becomes distributed over the constituent degrees of freedom is of fundamental interest. We investigate the time-evolution of tripartite information as a natural operator-independent measure of scrambling, which quantifies to which extent the initially localized information can only be recovered by global measurements. Studying the dynamics of quantum lattice models we demonstrate that in contrast to quadratic models generic interacting systems scramble information irrespective of the chosen partitioning of the Hilbert space, which justifies the characterization as scrambler.

DY 5.5 Mon 11:15 HÜL 186

Moire Localization in Two Dimensional Quasi-Periodic Systems — •Biao Huang[1,2] and W Vincent Liu[1] — [1]University of Pittsburgh — [2]Max Planck Institute for the Physics of Complex Systems

Moire reconstructions of Bloch waves have led to exciting development recently, where bilayer systems with small twist angles produce new periodic structures including the flat-band induced superconductivity. Here, we point out that an incommensurate, large twist angle, realized in a recent bilayer graphene experiment, may imply a qualitatively new localized system. This includes a rapidly changing mobility edge with respect to energy distinguishing from quasi-periodic systems in 1D and 3D, and scaling exponents saturating the Harris bound formulated for a purely random system in the localization transition. Methods for engineering and signatures for detections in cold atom simulations are also discussed.

Ref: B. Huang and W. V. Liu, Phys. Rev. B 100, 144202 (2019).

DY 5.6 Mon 11:30 HÜL 186

Hierarchy of relaxation timescales in local random Liouvillians — Kevin Wang[1], •Francesco Piazza[2], and David Luitz[2] — [1]Department of Physics, Stanford University, Stanford, California 94305, USA — [2]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, Dresden, Germany

To characterize the generic behavior of open quantum systems, we consider random, purely dissipative Liouvillians with a notion of locality. We find that the positivity of the map implies a sharp separation of the relaxation timescales according to the locality of observables. Specifically, we analyze a spin-1/2 system of size ℓ with up to n-body Lindblad operators, which are n-local in the complexity-theory sense. Without locality ($n = \ell$), the complex Liouvillian spectrum densely

covers a "lemon"-shaped support, in agreement with recent findings [*Phys. Rev. Lett.* **123**, 140403;arXiv:1905.02155]. However, for *local Liouvillians* ($n < \ell$), we find that the spectrum is composed of several dense clusters with random matrix spacing statistics, each featuring a lemon-shaped support wherein all eigenvectors correspond to n-body decay modes. This implies a hierarchy of relaxation timescales of n-body observables, which we verify to be robust in the thermodynamic limit.

DY 5.7 Mon 11:45 HÜL 186

Decay of spin-spin correlations in disordered quantum and classical spin chains — •Dennis Schubert, Jonas Richter, and Robin Steinigeweg — University of Osnabrück, Germany

The real-time dynamics of equal-site correlation functions is studied for one-dimensional spin models with quenched disorder. Focusing on infinite temperature, we present a comparison between the dynamics of models with different quantum numbers $s = 1/2, 1, 3/2$, as well as of chains consisting of classical spins. Based on this comparison as well as by analysing the statistics of energy-level spacings, we show that the putative many-body localization transition is shifted to considerably stronger values of disorder for increasing s . In this context, we intro- duce an effective disorder strength, which provides a mapping between the dynamics for different spin quantum numbers. For small values of the effective disorder, we show that the real-time correlations become essentially independent of s , and are moreover very well captured by the dynamics of classical spins. Particularly for $s = 3/2$, the agreement between quantum and classical dynamics is remarkably observed even for very strong values of disorder. This behaviour also reflects itself in the appropriate spectral functions, which are obtained via a Fourier transform from the time to the frequency domain. As an aside, we also comment on the self-averaging properties of the correlation function at weak and strong disorder.
[1] arXiv:1911.09917

DY 5.8 Mon 12:00 HÜL 186

Statistics of correlations functions in the random Heisenberg chain — •Luis Colmenarez[1], David Luitz[1], Paul McClarty[1], and Masudul Haque[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, Dresden, Germany — [2]Department of Theoretical Physics, Maynooth University, Co. Kildare, Ireland

Ergodic quantum many-body systems satisfy the eigenstate thermalization hypothesis (ETH). However, strong disorder can destroy ergodicity through many-body localization (MBL) – at least in one dimensional systems – leading to a clear signal of the MBL transition in the probability distributions of energy eigenstate expectation values of local operators. We consider the full probability distribution of eigenstate correlation functions across the entire phase diagram. At intermediate disorder – in the thermal phase – we find further evidence for anomalous thermalization in the form of heavy tails of the distributions. In the MBL phase, we observe peculiar features of the correlator distributions: a strong asymmetry in $S^z_i S^z_{i+r}$ correlators skewed towards negative values; and a multimodal distribution for spin-flip correlators. A quantitative quasi-degenerate perturbation theory calculation of these correlators yields a surprising agreement of the full distribution with the exact results, revealing, in particular, the origin of the multiple peaks in the spin-flip correlator distribution as arising from the resonant and off-resonant admixture of spin configurations. The distribution of the $S^z_i S^z_{i+r}$ correlator exhibits striking differences between the MBL and Anderson insulator cases.

DY 5.9 Mon 12:15 HÜL 186

Quantum coherent dynamical extension to RKKY interaction — •Stephanie Matern and Bernd Braunecker — School of Physics and Astronomy, University of St Andrews, UK

We study the full time evolution of a pair of impurity spins coupled to a bath of itinerant electrons. Even if the spins do not interact directly they can be coupled through the bath. In its simplest form this corresponds to the RKKY interaction. However, the RKKY interaction is considered as instantaneous and disregards that the spins are not just affected by the response of the bath but have an influence on the bath itself. To capture this effect on the dynamics we take into account all temporal correlations, particularly the quantum coherent correlations building up between the spins and the bath. This immediately leads to non-Markovian dynamics and to a coupling between the spins induced by the coherent quantum excitations of the electron bath. This effective coupling can be considered as a dynamical quantum coherent extension to the RKKY interaction.

Our approach is based on a self-consistent projection operator calculation for generalised quantum master equations. This method allows us to keep track of the time evolution of both the spins and the electron bath, and therefore for the bath to go beyond the usual assumption that it is represented by a Gibbs equilibrium state.

DY 5.10 Mon 12:30 HÜL 186

Entanglement Negativity at Localization Transition — •Gergő Roosz[1], Robert Juhasz[2], and Zoltan Zimboras[2] — [1]TU Dresden — [2]Wigner RCP

We study the entanglement negativity and entanglement entropy asymptotic at the localization transition of the quasi-periodic Harper model. In the delocalized phase the scaling is identical with the scaling of the homogeneous system $S \sim \frac{1}{3} \ln l$ and $\mathcal{E} \sim \frac{1}{4} \ln l$. In the critical point the scaling is different, $S \sim \frac{\tilde{c}}{3} \ln L$ and $\mathcal{E} \sim \frac{\tilde{c}}{4} \ln L$, with $\tilde{c} \approx 0.78$ In the localized phase the length scale is set by the localization length l_{loc} and we find $S \sim \frac{\tilde{c}}{3} \ln l_{loc}$ and $\mathcal{E} \sim \frac{\tilde{c}}{4} \ln l_{loc}$. Unlike the random and aperiodic singlet phases, where the ratio of the entanglement entropy and negativity prefactor is 2, in the Harper model this ratio is identical with the homogeneous case, 3/4.

DY 5.11 Mon 12:45 HÜL 186

Signatures of excited-state quantum phase transitions in quench dynamics — •Michal Kloc — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Excited-state quantum phase transitions manifest themselves as singularities in the level density of the excited states. In the case of integrable or weakly chaotic systems, we show that equilibration after a rapid quantum quench is affected by these singularities. The specific features of the equilibration process are analyzed using both purely quantum and quasiclassical approaches.

DY 5.12 Mon 13:00 HÜL 186

Density dynamics in the mass-imbalanced Hubbard model — •Tjark Heitmann, Jonas Richter, and Robin Steinigeweg — Physics Department, University of Osnabrück, Germany

We consider two mutually interacting particle species on a onedimensional lattice and study how the mass ratio between the two species affects the (equilibration) dynamics of the particles. While initial nonequilibrium density distributions are known to decay for equal masses (by diffusion [1]), the lighter particles localize in an effective disorder potential when the heavy particles become infinitely heavy and thus immobile. Knowing that, what behavior can we expect in the case of intermediate mass-imbalance ratios [2,3]? To investigate this question, we prepare pure initial states featuring a sharp nonequilibrium density profile and study their real-time dynamics which, by means of dynamical quantum typicality, can be related to equilibrium correlation functions. We observe that anomalous diffusion impedes localization as soon as the heavy particles become mobile.

[1] R. Steinigeweg et al., Phys. Rev. E 96, 020105(R) (2017).
[2] N. Y. Yao et al., Phys. Rev. Lett. 117, 240601 (2016).
[3] J. Sirker, Phys. Rev. B 99, 075162 (2019).

DY 5.13 Mon 13:15 HÜL 186

Thermalization properties of closed quantum systems in linear response — •Christian Bartsch — Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, D-33615 Bielefeld

Linear response theory provides a useful tool to describe nonequilibrium dynamics not too far away from equilibrium. We are able to identify different long time behavior for certain types of nonequilibrium initial conditions also with respect to the eigenstate thermalization hypothesis (ETH). Additionally, we investigate the stability of long time dynamics in driven quantum systems and its dependence on, e.g., the driving frequency. Along these lines we analyze the average energy input per driving period.

DY 6: Nonlinear Dynamics, Synchronization and Chaos

Time: Monday 10:00–11:15 Location: ZEU 147

DY 6.1 Mon 10:00 ZEU 147

Estimating Lyapunov exponents in billiards — George Datseris[1,2], •Lukas Hupe[1,2], and Ragnar Fleischmann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen — [2]Faculty of Physics, Georg-August-Universität Göttingen, 37077, Göttingen, Germany

Dynamical billiards are paradigmatic examples of chaotic Hamiltonian dynamical systems with widespread applications in physics. We study how well their Lyapunov exponent, characterizing the chaotic dynamics, and its dependence on external parameters can be estimated from phase space volume arguments, with emphasis on billiards with mixed regular and chaotic phase spaces. We show that in the very diverse billiards considered here the leading contribution to the Lyapunov exponent is inversely proportional to the chaotic phase space volume, and subsequently discuss the generality of this relationship. We also extend the well established formalism by Dellago, Posch, and Hoover to calculate the Lyapunov exponents of billiards to include external magnetic fields and provide a software implementation of it.

DY 6.2 Mon 10:15 ZEU 147

Dynamics of discrete light bullets in passively mode-locked semiconductor lasers — •Thomas Seidel[1], Julien Javaloyes[2], and Svetlana Gurevich[1,3] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Straße 9, 48149 Münster, Germany — [2]Departament de Física, Universitat de les Illes Balears, Carretera Valldemossa km 7.5, 07122 Palma, Spain — [3]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstraße 2, 48149 Münster, Germany

We study the emergence and stability of discrete light bullets in the output of a passively mode-locked semiconductor laser array coupled to a distant saturable absorber. Fist, we investigate the dynamics of the tranverse field which can be modeled by a discretised version of the generalised Rosanov equation and next, we also include the longitudinal direction and thus, show the existence of three-dimensional dissipative localized structures with one discrete (transverse) and two continuous (longitudinal) directions. In both situations, we find the presence of multistability between solution branches consisting of different numbers of lasing lasers by numerical time integration. For the transverse case, a detailed bifurcation analysis by means of path continuation was conducted in order to study the transition between different solution branches.

DY 6.3 Mon 10:30 ZEU 147

Laminar Chaos in Experiments: Nonlinear Systems with Time-Varying Delays and Noise — Joseph D. Hart[1,2], Rajarshi Roy[1,2,3], •David Müller-Bender[4], Andreas Otto[4], and Günter Radons[4] — [1]Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, Maryland 20742, USA — [2]Department of Physics, University of Maryland, College Park, Maryland 20742, USA — [3]Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742, USA — [4]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

A new type of dynamics called laminar chaos was discovered theoretically in scalar systems with time-varying delay [1]. It is a low-dimensional dynamics characterized by laminar phases of nearly constant intensity with periodic durations and a chaotic variation of the intensity from phase to phase. This is in contrast to the typically observed higher-dimensional turbulent chaos, which is characterized by strong fluctuations. In our present work [2] we provide the first experimental observation of laminar chaos by studying an optoelectronic setup. The noise inherent in the experiment requires the development of a nonlinear Langevin equation with variable delay. We show that laminar chaos can be observed in higher-order systems, and that it is robust to noise and a digital implementation of the variable time delay.

[1] Müller, Otto, and Radons, Phys. Rev. Lett. 120, 084102 (2018).
[2] Hart, Roy, Müller-Bender, Otto, and Radons, Phys. Rev. Lett. 123, 154101 (2019).

DY 6.4 Mon 10:45 ZEU 147

Synchronization and Frequency Pulling in Mutually Coupled Mode-Locked Lasers — •Clara R. Roca-Sastre, Jakob Eberhardt, Stefan Meinecke, and Kathy Lüdge — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Monolithic passively mode-locked semiconductors lasers (PMLLs) are simple and compact sources of high-frequency ultra-short light pulses. These devices can be utilized in novel secure communication schemes or optical clock synchronization. However, due to the absence of an external reference clock, this class of MLLs exhibits higher timing jitter than their active counterparts [1]. In order to overcome this detrimental effect, a mutual all-optical coupling can be introduced to reduce the timing jitter. This technique also gives access to different synchronization regimes of the laser outputs. In pursuance of a better understanding of the synchronization regime, we model numerically a coupled system by using delay differential equations [3]. For the mutual coupling of two non-identical lasers, frequency pulling in addition to a wide range of interesting dynamics can be found. At delay times around half of the cold cavity roundtrip time and in an intermediate feedback strength regime, regions of leap frogging arise where the lasers show an effective doubling of the pulse repetition rate, emitting pulses alternately at the fundamental repetition frequency.

[1] Otto et al., New J. Phys. 14, 113033 (2012).
[2] Simos et al., IEEE JQE 54, 2001106 (2018)
[3] Vladimirov et al., Phys. Rev. A 72, 3, 033808 (2005).

DY 6.5 Mon 11:00 ZEU 147

Dimensional Reduction in Coupled Heteroclinic Cycles — •Maximilian Voit and Hildegard Meyer-Ortmanns — Jacobs University Bremen, Bremen, Deutschland

Modeling complex systems as networks has recently received much attention, as real world systems usually consist of many coupled units. The dynamics of such coupled systems generically differs from the individual dynamics of single units and collective effects are in the focus of interest. Although heteroclinic cycles emerge robustly in various scenarios (e.g. in population dynamics, fluid dynamics, or game theory), systems of coupled heteroclinic cycles have not been extensively studied up to now. Here, we present results on small networks of coupled heteroclinic systems. In spite of their simple structure, they exhibit rich dynamics. Different kinds of dimensional reduction are identified, most prominently generalized synchronization. In addition, we investigate the arising chaotic transients and their scaling behaviour.

DY 7: Statistical Physics (General) I

Time: Monday 10:00–12:45 Location: ZEU 160

DY 7.1 Mon 10:00 ZEU 160

Climbing the Jacob's ladder of path integral approaches: quantum effects by classical polymer theory — •Péter Szabó and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

Path integral formalism provides an elegant way to evaluate thermal quantum expectation values in the language of classical physics. In ring polymer path integral methods a quantum object is mapped into a classical polymer ring in an extended, high dimensional phase space, where the beads of the polymer are the replicas of the classical system. The equilibrium averages of this polymer give the corresponding thermal properties of the quantum mechanical system.[1]

We have developed a classical polymer theory for imaginary path integrals to get an exact, low dimensional phase space representation of thermal quantum systems. This new picture preserves the classical description, but it allows us to get rid of the curse of dimensionality. The computational complexity of the problem does not depend anymore on the number of replicas. The quantum expectation values

can be evaluated by the sampling of the original, classical phase space. The performance of this method is tested in molecular systems, where we calculated the quantum partition functions and compared them to the exact results.

[1] D. Chandler and P. G. Wolynes, J. Chem. Phys. **74**, 4078 (1981)

DY 7.2 Mon 10:15 ZEU 160

The Five Problems of Irreversibility — •Michael te Vrugt — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

Macroscopic thermodynamics has a clear arrow of time: Systems irreversibly approach equilibrium accompanied by a monotonous increase of entropy. This stands in contrast to the laws of microscopic theories, which are invariant under time-reversal. The question how this difference can be explained has created a long debate, with suggestions involving coarse-graining methods as well as cosmological considerations about the entropy of the early universe. In this talk, I will show that a part of the difficulty in solving the problem of irreversibility arises from the fact that it actually consists of five different sub-problems, which are mixed in most discussions. Understanding why these problems have to be distinguished and how they are related to each other then allows to solve them on the basis of modern nonequilibrium statistical mechanics.

DY 7.3 Mon 10:30 ZEU 160

Nonconservative forces and the fluctuation-dissipation theorem — •Kiryl Asheichyk[1,2] and Matthias Krüger[3] — [1]4th Institute for Theoretical Physics, University of Stuttgart, Germany — [2]Max Planck Institute for Intelligent Systems, Germany — [3]Institute for Theoretical Physics, University of Göttingen, Germany

An equilibrium system which is perturbed by an external potential relaxes to a new equilibrium state, a process obeying the fluctuation-dissipation theorem (FDT). In contrast, perturbing by nonconservative forces yields a nonequilibrium steady state, and FDT can in general not be applied. Here we exploit a freedom inherent to linear response theory: Force fields which perform work that does not couple statistically to the considered observable can be added without changing the response. Using this freedom, we demonstrate that FDT can be applied for certain nonconservative forces. In particular, for the case of shear perturbation, this yields a response formula, alternative to and advantageous over the known Green-Kubo relation.

[1] K. Asheichyk and M. Krüger, arXiv:1908.11287.

[2] K. Asheichyk, A. P. Solon, C. M. Rohwer, and M. Krüger, J. Chem. Phys. 150, 144111 (2019).

DY 7.4 Mon 10:45 ZEU 160

Entanglement entropy of random partitioning — •Gergö Roosz[1], Istvan Kovacs[2], and Ferenc Igloi[3] — [1]TU Dresden — [2]Northwestern University, USA — [3]Wigner RCP, Budapest

We study the entanglement entropy of random partitions in one- and two-dimensional critical fermionic systems. In an infinite system we consider a finite, connected (hypercubic) domain of linear extent L, the points of which with probability p belong to the subsystem. The leading contribution to the average entanglement entropy is found to scale with the volume as $a(p)L^D$, where $a(p)$ is a non-universal function, to which there is a logarithmic correction term, $b(p)L^{D-1}\ln L$. In $1D$ the prefactor is given by $b(p) = \frac{c}{3}f(p)$, where c is the central charge of the model and $f(p)$ is a universal function. In $2D$ the prefactor has a different functional form of p below and above the percolation threshold.

DY 7.5 Mon 11:00 ZEU 160

A microscopic model for the computation of dielectric relaxation phenomena in composite systems — •Sujith Reddy Varakantham and Herbert Kliem — Institute of Electrical Engineering Physics, Saarland University, Saarbrücken, Germany

Dielectric relaxation in single phase and composite systems is computed using a microscopic model comprised of thermally activated dipoles fluctuating in double well (DW) potentials. The dipoles interact with each other by their Coulomb forces, thereby influencing mutually the properties of the DWs. To find the time dependent polarization response, a Monte-Carlo simulation method is employed by combining deterministic calculation of potentials with a probabilistic random number. By the interaction, the polarization response changes from Debye to stretched exponential. Afterwards, the time dependent polarization is transformed into the frequency domain. Two single systems with different DW barrier heights, i.e., different relaxation times and also with different distribution of barrier heights are computed first. Then the systems are combined in series connection as well as in embedded systems. While the individual systems exhibit stretched exponential responses with varied stretching factors corresponding to fixed and distributed barrier heights of the DWs, composed systems, on the other hand, show an intermediate behavior comprising both responses. To validate our simulation results, experiments are carried out using a series combination of aluminium and hafnium oxides, each having different dielectric responses. Our simulation results are in agreement with the experimental findings

DY 7.6 Mon 11:15 ZEU 160

Extreme value statistics of ergodic Markov processes from first passage times in the large deviation limit — •David Hartich and Aljaz Godec — Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany

Extreme value functionals of stochastic processes are inverse functionals of the first passage time — a connection that renders their probability distribution functions equivalent. Here, we deepen this link and establish a framework for analyzing extreme value statistics of ergodic reversible Markov processes in confining potentials on the hand of the underlying relaxation eigenspectra. We derive a chain of inequalities, which bounds the long-time asymptotics of first passage densities, and thereby extrema, from above and from below [1]. The bounds involve a time integral of the transition probability density describing the relaxation towards equilibrium. We apply our general results to the analysis of extreme value statistics at long times in the case of Ornstein-Uhlenbeck process and a 3D Brownian motion confined to a sphere, also known as Bessel process. We find that even on time-scales that are shorter than the equilibration time, the large deviation limit characterizing long-time asymptotics can approximate the statistics of extreme values remarkably well. Our findings provide a novel perspective on the study of extrema beyond the established limit theorems for sequences of independent random variables and for asymmetric diffusion processes beyond a constant drift.

[1] D. Hartich and A. Godec, J. Phys. A, 52 (2019) 244001.

15 min. break.

DY 7.7 Mon 11:45 ZEU 160

Microscopic reweighting for non-equilibrium steady states dynamics — •Marius Bause, Timon Wittenstein, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

Computer simulations generate trajectories at a single, well-defined thermodynamic state point. Statistical reweighting offers the means to reweight static and dynamical properties to different equilibrium state points by means of analytic relations. We extend these ideas to non-equilibrium steady states by relying on a maximum path entropy formalism subject to physical constraints. Stochastic thermodynamics analytically relates the forward and backward probabilities of any pathway through the external non-conservative force, enabling reweighting both in and out of equilibrium. We avoid the combinatorial explosion of microtrajectories by systematically constructing pathways through Markovian transitions. We further identify a quantity that is invariant to dynamical reweighting, analogous to the density of states in equilibrium reweighting.(M.Bause,T.Wittenstein,K.Kremer,T.Bereau, PRE(in press))

DY 7.8 Mon 12:00 ZEU 160

The quantum first detection problem — •Felix Thiel[1,2], David A. Kessler[2], and Eli Barkai[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany — [2]Department of Physics, Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan 52900, Israel

An observer prepares a quantum particle at position x_{in} on a lattice and wants to find its (random) time of arrival T in the target position x_{d}. To avoid complications related to wave function collapse and the quantum Zeno effect, he must adhere to a detection protocol. That means he attempts to detect the particle in the target at the times $\tau, 2\tau, 3\tau, \ldots$, where τ is the detection period, a free parameter. The time T of the first successful detection attempt is the first detection time that generalizes a classical random walker's first-passage time to the quantum realm. Such a situation can easily be implemented in

optical quantum walk or waveguide experiments.

In this contribution, we outline the quantum first detection theory and its similarities to first passage theory. We obtain the probability F_n of first detection at the n-th attempt and focus on its asymptotic decay for large times. We present numerical and analytical results for tight-binding quantum walks on one or higher-dimensional simple-cubic lattices.

DY 7.9 Mon 12:15 ZEU 160

Non-Flat Histogram Techniques for Spin Glasses — •Fabio Mueller, Stefan Schnabel, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany

We study the bimodal Edwards-Anderson spin glass comparing established methods, namely the multicanonical method, the 1/k-ensemble and parallel tempering, to an approach where the ensemble is modified by simulating power-law-shaped histograms in energy instead of flat histograms as in the standard multicanonical case. We show that by this modification a significant speed-up in terms of mean round-trip times can be achieved for all lattice sizes taken into consideration.

DY 7.10 Mon 12:30 ZEU 160

Asymmetric nascent Dirac delta functions and their application to probability and mechanics — •Jens Christian Claussen — Department of Mathematics, Aston University, Birmingham B4 7ET, U.K.

The Dirac delta distribution is ubiquitious from quantum mechanics and statistical physics to Fourier analysis. In theoretical physics lectures, a commonly presented approach uses a series of nascent delta functions which are normalized and localized and converge point-wise to zero except at the origin. For simplicity, nascent delta functions are usually chosen to be even, i.e. $\delta_n(x) = \delta_n(-x)$. However, this is not a necessary assumption, and in physical interactions as the inelastic collision of two rigid bodies, the force between the particles as a function of time may follow an asymmetric profile; nevertheless with the total momentum transferred in a Dirac delta pulse in the limit of an infinesimal short interaction time.

Here I discuss asymmetric nascent Dirac delta functions and their implications in probability and physics. The gross advantage of asymmetric nascent delta functions is found in their application to probability theory. By introduction of totally asymmetric nascent delta functions, the inconsistencies of using the Dirac delta in mixed discrete-continuous probability spaces when arriving at the cumulative distribution function are resolved. It is anticipated that asymmetric nascent delta functions find further applications in mathematical physics and the theory of measurement.

DY 8: Physics of Power Grids (joint session DY/SOE)

Time: Monday 11:30–12:30 Location: ZEU 147

DY 8.1 Mon 11:30 ZEU 147

Dynamic Vulnerability of Oscillatory Networks and Power Grids — •Xiaozhu Zhang[1], Cheng Ma[2], and Marc Timme[1] — [1]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), Cluster of Excellence Physics of Life, Technical University of Dresden, 01062 Dresden, Germany — [2]School of Physics, Nankai University, Tianjin 300071, China

Driven by dynamic fluctuations, oscillatory networks such as AC power grids exhibit highly heterogeneous, nontrivial resonant patterns that jointly depend on the driving frequency, the interaction topology of the network and the nodes driven [1,2]. However, it remains an open problem to identify which nodes are most susceptible and may make entire systems vulnerable to dynamic driving signals. Here we propose a Dynamic Vulnerability Index (DVI) [3] for identifying those nodes that exhibit largest amplitude responses to dynamic driving signals with given power spectra, and thus are most vulnerable. The DVI is easy to compute and enables robust high-quality predictions. It shows potential for a wide range of applications across dynamically driven networks, e.g. for identifying the vulnerable nodes in AC power grids driven by power fluctuations from renewable energy sources and customers' behaviour.

[1] X. Zhang et al., Science Advances 5:eaav1027 (2019).
[2] S. Tamrakar et al., Scientific Reports 8:6459 (2018).
[3] X. Zhang et al., arXiv:1908.00957 (2019).

DY 8.2 Mon 11:45 ZEU 147

Message Passing for State Estimation of Power Grids — •Tim Ritmeester and Hildegard Meyer-Ortmanns — Jacobs University, Bremen

The method of message passing is known from statistical physics and computer science. Here we use it to estimate the state of power grids in terms of the generator production and power flow, based on redundant error-prone measurements. We illustrate the method on the IEEE300-grid, and show that it outperforms standard least-squares approaches if the influence from distant nodes matters. We perform our analysis in this regime and show under what circumstances missing data can reliably be retrieved and how placement of modern measurement devices such as PMUs (Phasor Measurement Units) affects the accuracy of the estimate.

DY 8.3 Mon 12:00 ZEU 147

Large-deviation properties of the basin stability of power grids — •Yannick Feld and Alexander K. Hartmann — Institute of Physics, University of Oldenburg, Germany

Due to climate change the usage of fossil power sources has to be reduced. This results in more and more fluctuating power sources, which makes maintaining a stable energy grid more challenging and the properties of extremely stable (or unstable) power grid typologies are of interest. We use a dynamic model of power grids, specifically the Kuramoto-like model [1].

An advanced, however, nonlinear way to characterize the stability of power grids against (possibly large) fluctuations is the *basin stability*. Thus, we study numerically [2] the probability distribution of the basin stability for two random graph ensembles, namely an *Erdős-Rényi* and a *small-world* ensemble. Using *large deviation techniques* [3], we were able to measure [4] the probability distribution ranging over eight decades in probability, which is considerably larger than possible using standard sampling. Additionally we investigated the correlations of the basin stability with other measurable quantities like *backup capacity* [3] and number of leafs (dead ends).

[1] G. Filatrella, A.H. Nielsen, and N.F. Pedersen, Eur. Phys. J. B **61** 485-491 (2008)
[2] A.K. Hartmann, *Big Practical Guide to Computer Simulations* (World Scientific, 2015).
[3] T. Dewenter and A.K. Hartmann, New J. Phys. **17**, 015005 (2015)
[4] Y. Feld and A.K. Hartmann, Chaos **29**, 113103 (2019).

DY 8.4 Mon 12:15 ZEU 147

Enhancing power grid synchronization and stability through time delayed feedback control — Halgurd Taher[1], •Simona Olmi[1], and Eckehard Schöll[2] — [1]Inria Sophia Antipolis Mediterranee Research Centre, 2004 Route des Lucioles, 06902 Valbonne, France — [2]Institut fuer Theoretische Physik, Technische Universitaet Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

We study the synchronization and stability of power grids within the Kuramoto phase oscillator model with inertia with a bimodal natural frequency distribution representing the generators and the loads. We identify critical nodes through solitary frequency deviations and Lyapunov vectors corresponding to unstable Lyapunov exponents. To cure dangerous deviations from synchronization we propose time-delayed feedback control, which is an efficient control concept in nonlinear dynamic systems. Different control strategies are tested and compared with respect to the minimum number of controlled nodes required to achieve synchronization and Lyapunov stability. As a proof of principle, this fast-acting control method is demonstrated for different networks (the German and the Italian power transmission grid), operating points, configurations, and models.

DY 9: Focus Session: Simulating Quantum Many-Body Systems on Noisy Intermediate-Scale Quantum Computers (joint session TT/DY)

Time: Monday 15:00–18:15 Location: HSZ 03

Invited Talk DY 9.1 Mon 15:00 HSZ 03

Quantum simulations with linear ion crystals interacting with laser light — •Christian Roos — IQOQI Innsbruck, Innsbruck, Austria

I will describe recent quantum simulation experiments with linear ion crystals. In these experiments, ion crystals are laser-cooled to low temperatures and subjected to laser pulses that induce interactions between qubits encoded in the ions, which can be modeled as a long-range Ising interaction. I will discuss our efforts to characterize the complex entangled states that results from the non-equilibrium dynamics induced by the laser field and to apply such states for computational tasks.

Invited Talk DY 9.2 Mon 15:30 HSZ 03

Entanglement spectroscopy on the IBM quantum computer — •Titus Neupert — University of Zurich, Zurich, Switzerland

Entanglement properties are routinely used to characterize phases of quantum matter in theoretical computations. For example, the spectrum of the reduced density matrix, or so-called "entanglement spectrum", has become a widely used diagnostic for universal topological properties of quantum phases. However, while being convenient to calculate theoretically, it is notoriously hard to measure in experiments. I will discuss how IBM quantum computers allow the measurement of the entanglement spectrum using various states of one-dimensional spin systems as examples. This way, it is possible to distinguish topological states via their entanglement spectrum from paramagnetic and long-range ordered states. I will also remark on the challenges connected to the simulation of a simple interacting many-body Hamiltonian, such as the Hubbard model, on a NISQC device.

Invited Talk DY 9.3 Mon 16:00 HSZ 03

Simulating quantum many-body systems on a quantum computer — •Adam Smith[1,2], Bernhard Jobst[1], Andrew G. Green[3], and Frank Pollmann[1,4] — [1]Technical University Munich, Garching, Germany — [2]Imperial College London, London, UK — [3]University College London, London, UK — [4]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Universal quantum computers are potentially an ideal setting for simulating many-body quantum systems out of reach for classical computers. Here we discuss the practical applications to two main problems: the simulation of far out-of-equilibrium dynamics and the study of topological ground states of static Hamiltonians. In the former we demonstrate that on small scales current devices are already capable of capturing the correct qualitative physics of quantum quenches with the presence of disorder and interactions. In the latter we represent the ground states of Hamiltonians using shallow quantum circuits and observe a topological phase transition on a quantum device. Looking to the near-future, we discuss the utility of these devices for dynamics and the efficient representation of physical quantum states as we enter the noisy intermediate-scale quantum (NISQ) era.

15 min. break.

Invited Talk DY 9.4 Mon 16:45 HSZ 03

Quantum computing and its applications in chemistry and physics — •Ivano Tavernelli — IBM Research - Zurich

Quantum computing is emerging as a new paradigm for the solution of a wide class of problems that are not accessible by conventional high performance computers based on classical algorithms. In the last few years, several interesting problems with potential quantum speedup have been brought forward in the domain of quantum physics, like eigenvalue-search using quantum phase estimation algorithms and evaluation of observables in quantum chemistry, e.g. by means of the hybrid variational quantum eigensolver (VQE) algorithm. The simulation of the electronic structure of molecular and condensed matter systems is a challenging computational task as the cost of resources increases exponentially with the number of electrons when accurate solutions are required. With the deeper understanding of complex quantum systems acquired over the last decades this exponential barrier bottleneck may be overcome by the use of quantum computing hardware. To achieve this goal, new quantum algorithms need to be develop that are able to best exploit the potential of quantum speed-up. While this effort should target the design of quantum algorithms for the future fault-tolerant quantum hardware, there is pressing need to develop algorithms that can be implemented in present-day NISQ (noisy intermediate scale quantum) devices with limited coherence times. In this talk, I will introduce the basics of quantum computing using superconducting qubits, focusing on those aspects that are crucial for the implementation of quantum chemistry/physics algorithms.

Invited Talk DY 9.5 Mon 17:15 HSZ 03

Randomized measurements: A toolbox for probing quantum simulators and quantum computers — •Benoit Vermersch[1,2,8], Andreas Elben[1,2], Jinlong Yu[1,2], Lukas Sieberer[1,2], Guanyu Zhu[3], Marcello Dalmonte[4], Frank Pollmann[5], Mohammad Hafezi[3], Norman Yao[6], Ignacio Cirac[7], Peter Zoller[1,2], Tiff Brydges[1,2], Manoj Joshi[1,2], Christine Maier[1,2], Petar Jurcevic[1,2], Ben Lanyon[1,2], Christian Roos[1,2], and Rainer Blatt[1,2] — [1]Center for Quantum Physics and Institute for Experimental Physics, University of Innsbruck, Austria — [2]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, Innsbruck, Austria — [3]JQI - University of Maryland, USA — [4]ICTP, Trieste, Italy — [5]TU Munich, Garching, Germany — [6]LBL - University of California, Berkley, USA — [7]Max-Planck-Institut fur Quantenoptik, Garching, Germany — [8]LPMMC CNRS/Universite Grenoble Alpes, Grenoble, France

Randomized measurements have emerged as a new tool to probe the properties of quantum simulators and quantum computers beyond standard observables. In the talk I will present our recent results including randomized measurement protocols to measure entanglement [1], out-of-time-ordered correlations [2], and many-body topological invariants [3]. I will also show some experimental results [4,5] obtained in collaboration with the group of Rainer Blatt (IQOQI Innsbruck).

[1] Phys. Rev. Lett. 120 (2018) 050406
[2] Phys. Rev. X 9 (2019) 021061
[3] arXiv:1906.05011
[4] Science 364.6437 (2019), pp. 260-263
[5] M. Joshi et al., in preparation

DY 9.6 Mon 17:45 HSZ 03

Crossing a topological phase transition with a quantum computer — •Bernhard Jobst[1], Adam Smith[1,2], Andrew Green[3], and Frank Pollmann[1,4] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom — [3]London Centre for Nanotechnology, University College London, Gordon St., London WC1H 0AH, United Kingdom — [4]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, D-80799 München, Germany

Quantum computers promise to perform computations beyond the reach of modern computers with profound implications for scientific research. Due to remarkable technological advances, small scale devices are now becoming available for use. One of the most apparent applications for such a device is the study of complex many-body quantum systems, where classical computers are unable to deal with the generic exponential complexity of quantum states. Even zero-temperature equilibrium phases of matter and the transitions between them have yet to be fully classified, with topologically protected phases presenting major difficulties. We construct and measure a continuously parametrized family of states crossing a symmetry protected topological phase transition on the IBM Q quantum computers. The simulation that we perform is easily scalable and is a practical demonstration of the utility of near-term quantum computers for the study of quantum phases of matter and their transitions.

DY 9.7 Mon 18:00 HSZ 03

analysis of probabilistic error cancellation method on NISQ quantum computers — •Jiasheng Xie[1,2], Sebastian Zanker[1], and Michael Marthaler[1] — [1]HQS Quantum Simulations GmbH, Haid-und-Neu Straße 7, 76131 Kralsruhe, Germany — [2]Freie Uiversität Berlin, 14195 Berlin, Germany

Noisy Intermediate-Scale Quantum (NISQ) technologies are likely to be developed in the near future with the possibility of building devices with 50 to a few hundred physical qubits. NISQ devices are very useful in simulating quantum many body systems and may be able to perform tasks beyond the capability of classical computers. However, these devices are very noisy and lack fault tolerance. In order to reduce the noise level in the NISQ devices, it is useful to implement quantum error mitigation scheme. We have tested probabilistic error cancellation (PEC) method, a quantum error mitigation protocol that utilizes gate set tomography and quasiprobability decomposition. We have benchmarked the noiseless system and noisy systems with basic types of decoherences for 4 qubit case and will compare them with the noise mitigated circuit using Richardson linear extrapolation and PEC method from simulation. This will provide us a good understanding of the usefulness of this particular error mitigation protocol for the NISQ quantum computer algorithms.

DY 10: Graphene (jointly with DY, MA, HL, DS, O) (joint session TT/DY/HL)

Time: Monday 15:00–18:30 Location: HSZ 201

DY 10.1 Mon 15:00 HSZ 201

Edge state crossing behaviour in a multi-band tight-binding model of graphene — •Thorben Schmirander, Marta Prada, and Daniela Pfannkuche — I. Institut für theoretische Physik Universität Hamburg, Hamburg, Deutschland

The description of Dirac electrons in the band structure of graphene is commonly performed using effective tight binding models [1]. These effective models use single-orbital Hamiltonians with modified hopping parameters in order to account for the influence of the higher energy orbitals in graphene. We go beyond such effective models by including d-orbitals in an atomistic tight-binding model. The inclusion of the d-orbitals results in a breaking of electron-hole symmetry which in turn changes the dispersion of the states around the Fermi energy. When considering a finite graphene sample, edge states occur, which cross the band gap and connect the Dirac cones at the K and K' point. These edge states are the key to the topological properties of graphene, because they may exhibit the Spin Hall effect [3]. The band gap crossing is discussed by comparing different expectation values computed from the edge states. These expectation values change under different influences, such as strain or an external electric field. Apart from qualitatively treating these influences on the crossing of the band gap, electron-electron interactions are included via a self-consistent mean-field approach.

[1] van Miert, G., Juricic, V. and Morais Smith, C. Phys. Rev. B 90 195414 (2014)
[2] van Gelderen, R. and Morais Smith, C., Phys. Rev. B 81 125435 (2010)
[3] Kane, C. L . and Mele, E. J., Phys. Rev. Lett. 95, 226801 (2005)

DY 10.2 Mon 15:15 HSZ 201

Graphene grain boundaries for strain sensing: a computational study — •Delwin Perera and Jochen Rohrer — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Graphene has been celebrated as a material with exceptional properties at various fronts of electronics. In this contribution we investigate the strain sensing capabilities of graphene containing grain boundaries by using the non-equilibrium Green function formalism. Our work is inspired by an enhanced piezoresistivity of nanocrystalline graphene found experimentally in 2015 [1]. We investigate how different structural realizations of the grain boundary impact the transport properties. In particular, we compute strain gauge factors solely from *ab initio* electronic structure calculations as a function of the grain boundary topology. Thereby, we can compare this popular figure of merit for strain gauges with experimental values.

[1] Riaz *et al.*, Nanotechnology **26**, 325202 (2015)

DY 10.3 Mon 15:30 HSZ 201

Virtual experiments on negative refraction across graphene pn junctions — •Wun-Hao Kang and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

Graphene is a promising 2D material exhibiting optics-like properties due to its relativistic electronic structure linear in momentum. When charge carriers pass through a bipolar junction, the group velocity component parallel to the interface changes sign, leading to a negative refraction angle and hence effectively a negative refraction index in Snell's law. Many groups have been working on negative refraction in graphene, both theoretically and experimentally. However, most studies focus on the design of Veselago lensing. Here, we revisit a recent experiment [1] and perform quantum transport simulations for the same device geometry, based on the scalable tight-binding model [2]. Under ideal conditions, our result shows clear conductance peaks due to electron focusing, which is a combined effect of Klein tunneling and negative refraction. To single out the effect of negative refraction, we have further proposed a simpler design for future experiments.

[1] G.-H. Lee et al., Nat. Phys. **11**, 925–929 (2015)
[2] M.-H. Liu et al., Phys. Rev. Lett. **114**, 036601 (2015)

DY 10.4 Mon 15:45 HSZ 201

Electronic properties in a Bernal bilayer graphene monitored by selective functionalization — •Ahmed Missaoui[1,3], Jouda khabthani[1], Didier Mayou[2], and Guy Trambly de Laissardière[3] — [1]Laboratoire de la Physique de la Matière Condensée, Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunis, Tunisia — [2]Institut Néel, CNRS, Univ. Grenoble Alpes, France — [3]Laboratoire de Physique théorique et Modélisation, CNRS , Univ. de Cergy- Pontoise, France

The absence of a band gap in the monolayer graphene presents a great limitation of the fields of application. In a Bernal bilayer of graphene we can exceed its limits with induce a tunable band gap here by applying a gate voltage. In this context, we study the electronic properties of bilayer graphene in the presence of adsorbates such as hydrogene. We used a tight binding modelisation and DFT calculations for our study. We analyze [1] the effects of a selective distribution of adosrbats between the two sublattices A and B [2] on band structure and the microscopic conductivity with Kubo formalisim. The results show that in some cases depending on Fermi energy value and specific adsorbate distribution a gap appears, and in others cases, a linear dispersion with an increase in conductivity with the concentrations is reported.

[1] Jyoti. Katoch et al., Phys. Rev. Lett. 121, 136801 (2018)
[2] A. Missaoui et al., J. Phys. : Condens. Matter 30, 195701 (2018)

DY 10.5 Mon 16:00 HSZ 201

Zero-magnetic-field Hall effects in artificially corrugated bilayer graphene — •Sheng-Chin Ho[1], Ching-Hao Chang[1,2], Yu-Chiang Heish[1], Shun-Tsung Lo[1], Botsz Huang[1], Carmine Ortix[3,4], and Tse-Ming Chen[1,2] — [1]Department of Physics, National Cheng Kung University, Tainan, Taiwan — [2]Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 701, Taiwan — [3]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University, Princetonplein 5, NL-3584 CC Utrecht, Netherlands — [4]Dipartimento di Fisica E. R. Caianiello, Universita di Salerno, IT-84084 Fisciano, Italy

We propose a new scheme that uses a lithographically-defined strain technology to modify the interlayer coupling and intralayer interaction of bilayer graphene (BLG). In this deformed BLG system, we demonstrate an unusual pseudo-magnetoresistance anisotropy and the so-called nonlinear Hall effect. These observations are the consequence of the Fermi surface anisotropy and tilted mini-Dirac cones, which originate from the non-zero first-order moments of the pseudo-magnetic field in both real- and momentum-spaces, i.e., the pseudo-magnetic field dipole and Berry curvature dipole. This new approach enables us to turn a simple bilayer graphene into an exotic phase of matter with nontrivial band dispersion generated by the strain engineering, on par with the creation of metamaterials or state-of-art twistronics engineering.

DY 10.6 Mon 16:15 HSZ 201

Spin-caloritronic transport in hexagonal graphene nanodots — Thi Thu Phùng[1], Robert Peters[2], •Andreas Honecker[1], Guy Trambly de Laissardière[1], and Javad Vahedi[1,3] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France — [2]Department of

Physics, Kyoto University, Japan — [3]Department of Physics and Earth Sciences, Jacobs University Bremen, Germany

First, we investigate magnetism in the Hubbard model for hexagonal graphene dots. Employing static respectively dynamic mean-field theory (DMFT) we show that magnetism can be generated at the zigzag edges beyond a critical interaction of the on-site Coulomb interaction U that decreases with increasing dot size. Building on these results, we apply the Landauer formalism in the framework of the non-equilibrium Green function method to calculate the spin and charge currents through these dots as a function of temperature. We show that in the "*meta*" configuration of a hexagonal dot subject to weak Coulomb interactions, a pure spin current can be driven just by a temperature gradient in a temperature range that is promising for device applications.

15 min. break.

DY 10.7 Mon 16:45 HSZ 201

Lévy flights and Hydrodynamic Superdiffusion on the Dirac Cone of Graphene — •Egor Kiselev[1] and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

We show that the hydrodynamic collision processes of graphene electrons at the neutrality point can be described in terms of a Fokker-Planck equation with a fractional derivative, corresponding to a Lévy flight in momentum space. Thus, electron-electron collisions give rise to frequent small-angle scattering processes that are interrupted by rare large-angle events. The latter give rise to superdiffusive dynamics of collective excitations. We discuss the relevance of our results to experiments with injected electron beams, and show how the superdiffusive behavior makes it possible to obtain analytical results for transport coefficients relevant to the hydrodynamics of graphene electrons.

DY 10.8 Mon 17:00 HSZ 201

Gate-controllable graphene superlattices: Numerical aspects — •Szu-Chao Chen, Wun-Hao Kang, and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

We study transport properties of gate-controllable graphene superlattices by performing quantum transport simulations based on the scalable tight-binding model and calculations of miniband structures within the continuum method [1]. Good agreement between transport simulations and the corresponding miniband structures confirms the reliability of our calculations for electrostatic superlattices in graphene. Combined with realistic potential profiles obtained from finite-element-based electrostatic simulations, our transport simulations agree well with recent transport experiments for gate-controllable square superlattices. This work therefore paves the way toward exploring gate-controllable graphene superlattices of arbitrary lattices, such as honeycomb or Lieb.
[1] S.-C. Chen et al., arXiv:1907.03288 (2019).

DY 10.9 Mon 17:15 HSZ 201

Localization at the Van Hove singularity — •Peter Silvestrov[1] and Jakub Tworzydło[2] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Institute of Theoretical Physics, Warsaw University, Hoża 69, 00–681 Warsaw, Poland

Van Hove singularities are found in the electron spectrum of many 2-dimensional materials of current interest, including graphene systems (twisted bilayer and monolayer on a substrate), transitional dichalcogenides, and 2-dimensional superconductors. They appear due to saddle points in the energy bands at certain momenta. Even though the effective kinetic energy corresponding to such saddle point is unbounded from both above and below, we show that exponentially localized electronic states generically appear here in the presence of a smooth potential $U(x, y)$ with sufficiently diverse landscape. We also consider high order Van Hove singularities, where we predict a discrete spectrum of non-exponentially localized states.

DY 10.10 Mon 17:30 HSZ 201

The optical conductivity of strongly interacting Dirac fermions: a bosonization approach to the Kadanoff-Baym self-consistent resummation — •Sebastián Mantilla and Inti Sodemann — Max Planck Institute for the Physics of Complex Systems

The optical conductivity of 2D Dirac fermions at low energies is controlled by fundamental constants of nature $\sigma_0 = e^2/16\hbar$. However, Coulomb interactions produce a non-trivial dependence of the conductivity with the frequency. We use a bosonization approach to implement exactly a self-consistent Kadanoff-Baym resummation of the electron-hole propagator by mapping the momentum space lattice onto a Heisenberg-type model of interacting spins and employ this approach to determine the frequency dependence of the optical conductivity for Coulomb repulsions. We recover the perturbative renormalization group results at small coupling and extend its predictions to strong coupling. We discuss the relevance of our results to Dirac materials such as graphene and 3D topological insulator surface states.

DY 10.11 Mon 17:45 HSZ 201

Geometric-dissipative origin of the light-induced Hall current in graphene I — •Marlon Nuske[1,3], Lukas Broers[1], and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]CUI: Advanced Imaging of Matter, 22761 Hamburg, Germany

We determine the origin of the light-induced Hall current in graphene recently reported by J. McIver, et al., Nature Physics (2019). The Hall current derives from the total Berry curvature of the occupied states of the light-induced Floquet bands, in addition to the kinetic contribution deriving from the band velocities. The occupation of these states of the light-driven material emerges as a steady state that is determined by dissipative processes balancing out the optical driving force. For low electric field strength we propose an intuitive explanation of the Hall current within a two-level Rabi picture.

DY 10.12 Mon 18:00 HSZ 201

Geometric-dissipative origin of the light-induced Hall current in graphene II — •Lukas Broers[1], Marlon Nuske[1,3], and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]CUI: Advanced Imaging of Matter, 22761 Hamburg, Germany

Inspired by the recent experiments by J. McIver, et al., Nature Physics (2019), we investigate the light-induced Hall current in graphene. We show that this Hall current derives from the Berry curvature and band velocity contributions of the occupied Floquet-states. To support this proposal we determine the energy and momentum resolved single particle correlation function. The resulting steady state momentum and energy distribution supports the interpretation as a Floquet induced mechanism. We find that for low driving intensity the main contribution to the Hall current emerges from the resonantly driven electron states of the Dirac cone. With increasing driving intensity, additional higher order resonances contribute, giving rise to the full Floquet-driven effect. We demonstrate this within a Master equation formalism, and obtain good quantitative agreement with the experimentally measured Hall current.

DY 10.13 Mon 18:15 HSZ 201

Lightwave valleytronics in graphene — •Hamed Koochaki Kelardeh[1], Alexandra Landsman[2], and Takashi Oka[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Ohio State University, Columbus, USA

We propose a valley-selective device based on graphene at a few-femtosecond timescale with charge separation at different sublattices, and correspondingly at nonequivalent valleys. We characterize the maximality condition of valley polarization and investigate the parameters and condition upon which we can coherently control the carriers and store data via valley degree of freedom. The valley polarization is controlled by the amplitude as well as the carrier-envelope phase of the pulse - one cycle optical field - and the curvature of the electron trajectory in the reciprocal space. We believe the results of our study will step forward the Valleytronics and shed light on ultrafast data storage and processing with uttermost reliability and robustness.

DY 11: Invited Talk

Time: Monday 15:00–15:30 Location: HÜL 186

Invited Talk DY 11.1 Mon 15:00 HÜL 186

A hydrodynamic view on the diffusion in membranes and dense solutions of proteins — •Gerhard Hummer[1,2], Sören von Bülow[1], Martin Vögele[1,3], Lisa Pietrek[1], Marc Siggel[1], Max Linke[1], Jürgen Köfinger[1], and Lukas Stelzl[1] — [1]Department of Theoretical Biophysics, Max Planck Institute of Biophysics, 60438 Frankfurt am Main, Germany — [2]Institute for Biophysics, Goethe University Frankfurt, 60438 Frankfurt am Main, Germany — [3]Computer Science Department, Stanford University, Stanford, CA 94305-9025, USA

Molecular dynamics simulations of the diffusion of proteins and other macromolecules in dense solutions and in lipid membranes revealed unexpected complexities. In systems mimicking the interior of a living cell, with densely packed proteins, the translational and rotational diffusion of proteins slow down dramatically at high protein concentrations, and the Stokes-Einstein relation appears to break down. In membranes, the apparent diffusion coefficient appears to grow without bound as the box size is increased. We resolve these issues by showing, first, that transient clustering of proteins explains quantitatively the increase in the apparent Stokes radius and the rise in the viscosity. Second, we show that the divergence of membrane diffusion is the result of the unusual hydrodynamics under periodic boundary conditions. Hydrodynamics also plays a central role in rotational diffusion, both in the bulk and within membranes. Accounting for hydrodynamics, we obtain diffusion coefficients that can be interpreted meaningfully and compared to experiment.

DY 12: Statistical Physics of Biological Systems I (joint session BP/DY)

Time: Monday 15:00–17:15 Location: SCH A251

DY 12.1 Mon 15:00 SCH A251

Stability and diversity in random Lotka-Volterra systems with non-linear feedback — •Laura Sidhom and Tobias Galla — The University of Manchester, Oxford Road, Manchester, M13 9Pl

Ecosystem stability is important for maintaining a healthy microbiome, so understanding the factors that contribute to stability is of great relevance. In this talk I will discuss an ecosystem of many interacting species, that evolve according to Lotka-Volterra dynamics, with interaction coefficients drawn from a random distribution. We investigate the effects of sigmoidal nonlinear feedback on the stability of the ecosystem, and on its diversity. We find that nonlinear feedback causes species growth to be bounded, increasing ecosystem stability. In the talk I will illustrate the model parameters, using examples of interactions found in nature. We also investigate how pairwise interactions, and the introduction of higher-order interactions affect ecosystem stability, and how this relates to ecosystems in nature. I will briefly discuss the generating-functional path integral approach and the linear stability analysis, and discuss these results in terms of the human microbiome and explain how attributes of the host can influence its stability.

DY 12.2 Mon 15:15 SCH A251

Towards a grammar of probabilistic models for large biological networks — •Philipp Fleig[1] and Ilya M. Nemenman[2] — [1]University of Pennsylvania, Philadelphia, USA — [2]Emory University, Atlanta, USA

Biological interaction networks such as biological neural networks, amino acid sequences in proteins, etc. are critical to the functioning of any living system. The trend of modern experiments is to record data with a rapidly increasing number of simultaneously measured network variables. Inferring models for such complex data is becoming increasingly more difficult, since one is confronted with a combinatorial explosion in the number of possible interactions between variables. Here we present first steps of an approach to overcome this obstacle. We investigate the question whether a small set of carefully chosen statistical models suffices to describe rich phenomenology in data of biological networks. As candidate models for this grammar we consider low-rank approximation, clustering, sparsity, etc.. We discuss the distribution of eigenvalues and pairwise correlations characteristic for each model, working under the assumption that they serve as key indicators for the phenomenology described by a model. We provide examples of modelling data of Ising spin systems and outline a vision for how combinations of models in the grammar cover a large part of model space occupied by biological networks.

DY 12.3 Mon 15:30 SCH A251

Kauffman NK models interpolated between K=2 and K=3 — James E. Sullivan, Dmitry Nerukh, and •Jens Christian Claussen — Department of Mathematics, Aston University, Birmingham B4 7ET, U.K.

The NK model was introduced by Stuart Kauffman and coworkers [1] as a model for fitness landscapes with tunable ruggedness, to understand epistasis and pleiotropy in evolutionary biology. In the original formulation, fitness is defined as a sum of fitness functions for each locus, each depending on the locus itself and K other loci. Varying K from $K = 0$ to $K = N - 1$ leads to different ruggedness of the landscape. In previous work we introduced a generalization that allows to interpolate between integer values of K by allowing K_i to assume different values for each locus. We focus on the interpolation between the most widely studied cases of $K = 2$ and $K = 3$ and characterize the landscapes by study of their local minima. Here we transfer this approach to Random Boolean Networks and investigate attractor basins and limit cycles where the average K assumes integer and noninteger values. Relaxing the assumption of degree-homogeneity is an important step towards more realistic boolean network models, relevant to a broad range of applications in the dynamics of social systems and in systems biology.

[1] Kauffman, S.; Levin, S., Journal of Theoretical Biology. 128, 11 (1987); Kauffman, S.; Weinberger, E., Journal of Theoretical Biology. 141, 211 (1989).

Invited Talk DY 12.4 Mon 15:45 SCH A251

Density waves, jamming and dynamic arrest in growing microbial communities — •Oskar Hallatschek — University of California, Berkeley, USA

Microbes often colonize spatially-constrained habitats, such as pores in the skin or crypts in the colon. The resulting micro-communities are often stable and contribute to the genetic diversity and function of our microbiomes. It is, however, unclear how spatial constraints influence microbial community assembly. By monitoring and modeling microbial populations under controlled microfluidic confinement, we find a rich spectrum of dynamical patterns that are controlled by the competition between density-dependent outflow and population growth. Our results show that density-dependent passive diffusion can drive a reproducing populations to a jamming threshold, which entails a total loss of mixing and intra-species competition.

15 min. coffee break

DY 12.5 Mon 16:30 SCH A251

Effect of alternating between sexual and asexual reproduction on the number of expected mating types in isogamous species — •Ernesto Berríos-Caro[1], George W. A. Constable[2], and Tobias Galla[1] — [1]The University of Manchester — [2]University of York

The number of mating types of sexually reproducing isogamous species can range from two to thousands. The latter case is highly unusual and contradicts the argument that new types are sexually advantaged, which would imply a consistent growth of the number of types. Recent works based on a Moran-type individual-based model seem to suggest that the rate of sexual reproduction plays a crucial role in the low number of mating types observed in nature. Motivated by species that alternate between sexual and asexual reproduction, we subject the reproduction events to a switching environment of both states.

We explore how the distribution of the number of mating types is affected by different switching regimes. When the environments switch slowly, we find that the distribution of mating types can become bimodal if the population size is large enough and the time spent in both environments (on average) is similar. When the switching is fast, we find that the system behaves as if it were in an effective single-fixed environment, where the sex is facultative. Also, we investigate the transition from slow to fast switching environments by calculating the distributions of the number of types in each environment based on the Kolmogorov equations of the system.

DY 12.6 Mon 16:45 SCH A251

Specialisation and plasticity in a primitive social insect — •Adolfo Alsina[1], Solenn Patalano[2], Martin Bachman[3], Irene Gonzalez-Navarrete[4], Stephanie Dreier[5], Shankar Balasubramanian[3], Seirian Sumner[5], Carlos Gregorio-Rodriguez[6], Wolf Reik[2], and Steffen Rulands[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]The Babraham Institute, Cambridge, UK — [3]University of Cambridge, Cambridge , UK — [4]Centre for Genomic Regulation (CRG), Barcelona , Spain — [5]Institute of Zoology, London , UK — [6]Universidad Complutense de Madrid (UCM), Madrid, Spain

Biological systems not only have the remarkable capacity to build and maintain complex spatio-temporal structures in noisy environments, they can also rapidly break up and rebuild such structures. How can such systems can simultaneously achieve both robust specialisation and plasticity is poorly understood. Here we use primitive societies of Polistes wasps as a model system where we experimentally perturb the social structure by removing the queen and follow the relaxation dynamics back to the social steady state over time. We combine a unique experimental strategy correlating measurements across vastly different spatial scales with a theoretical approach. We show that Polistes integrates antagonistic processes on multiple scales to distinguish between extrinsic and intrinsic perturbations and thereby achieve both robust specialisation and rapid plasticity. Such dynamics provide a general principle of how both specialization and plasticity can be achieved in biological systems.

DY 12.7 Mon 17:00 SCH A251

Coarse graining of biochemical systems described by discrete stochastic dynamics — •David Seiferth and Stefan Klumpp — Institute for the Dynamics of Complex Systems, University of Göttingen, Friedrich Hund Platz 1, 37077 Göttingen, Germany

Many biological systems can be described by finite Markov models. A general method for simplifying master equations will be presented by merging two adjacent states. The method preserves the steady-state probability distribution and all steady-state fluxes disregarding the one between the merged states. As the order of merging states is not important, different levels of coarse-grained models of the underlying microscopic dynamics can be obtained. Different criteria for the level of coarse graining or the resolution of the process will be proposed. The application of the method will be discussed for specific biochemical examples.

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

Time: Monday 15:00–18:00 Location: ZEU 118

Invited Talk DY 13.1 Mon 15:00 ZEU 118

Shearing of glasses: new insight from studying model glasses of different system sizes — •Andreas Heuer, Markus Blank-Burian, Lawrence Smith, and Moumita Maiti — Inst. Phys. Chemie, WWU Muenster, Germany

Upon shearing of glasses a large variety of different phenomena can be observed. This includes, e.g., the stress overshoot and the emergence of shear bands. Many properties have been related to the presence of shear transformation zones (STZs).

In previous work on quiescent glasses important information about the physical mechanisms could be extracted from studying the dependence of dynamical properties on the system size. Here it was essential to study system sizes between approx. 60 and a few thousand [1]. Furthermore, an appropriate discretization of the dynamics in terms of metabasins was essential.

Here we study the properties of sheared systems in an analogous setting. Formally, shearing corresponds to a time-dependent energy landscape, requiring a generalization of the metabasin concept [2]. Interestingly, when studying the size dependence upon shearing at low temperatures, it turns out that macroscopically relevant behavior starts to be observed for system sizes above (approx.) 10.000. Important properties of the dynamic heterogeneities as reflected, e.g., by the emergence of shear bands, is extracted from these dependencies and related to the STZs.

[1] C. Rehwald, A. Heuer, Phys. Rev. E, 86, 051504 (2012). [2] M. Blank-Burian. A. Heuer, Phys. Rev. E 98, 033002 (2018).

DY 13.2 Mon 15:30 ZEU 118

Nonlinear dielectric response: molecular reorientation models — •Gregor Diezemann — Institut für Physikalische Chemie, JGU Mainz, Duesbergweg 10-14, 55128 Mainz

The nonlinear dielectric response of supercooled liquids has been intensively studied, both experimentally and theoretically during the last decade. Since an analogue of the well known fluctuation dissipation theorem for nonlinear responses is missing, one has to rely on the results of model calculations. A number of different models have been used for the calculation of the nonlinear (third order) response and some of them exhibit features also observed experimentally.

I will present the results of calculations of the third order and the fifth order response for models of molecular reorientations. Sofar, one important point in the interpretation of the peaks observed in the modulus of the nonlinear response was that rotational Brownian motion does not give rise to such a peak. However, it is well known that this model of isotropic rotational diffusion is also not able to reproduce important features of the linear dielectric response of glassforming systems.

Here, I will show that very simple models like the model of random rotational jumps or anisotropic rotational diffusion also exhibit a so-called hump in the modulus of the nonlinear response functions. Also the relation between the third order response and the fifth order repsonse is obeyed to some extent. What is missing in this kind of models is a temperature dependence of the features observed. I will discuss the results in the context of recent experimental observations.

DY 13.3 Mon 15:45 ZEU 118

Efficient algorithm to study dynamics in the transition between quasiperiodic and disordered environments — •Alan Rodrigo Mendoza Sosa and Atahualpa Kraemer — Universidad Nacional Autónoma de México, Mexico City, Mexico

Crystals have translational and rotational symmetries while quasicrystals have rotational symmetry in a single point, and glasses have none. This is revealed in the diffraction pattern, where crystals and quasicrystals have a discrete pattern, but quasicrystals exhibit forbidden symmetries, while glasses have a continuous pattern. Increment the rotational symmetry of quasicrystals should produce a denser diffraction pattern, closer to the continuous pattern exhibit in glasses. Motivated with the previous arguments we propose to study the structure of a quasiperiodic array and the dynamics of particles in quasiperiodic environments when the folding symmetry increases. However, the usual techniques to produce quasiperiodic arrays are aimed at producing arrays of low symmetries and near to the center of symmetry, then it becomes time expensive to perform simulations. In this work, we present an algorithm to produce quasiperiodic arrays with arbitrary symmetry around any point in the space, based on the generalized dual method. Also, using the Voronoi tessellation of the quasiperiodic array, and the incremental algorithm to track particles, we made an algorithm to perform simulations of particles moving in a quasiperiodic potential with arbitrary symmetry. We apply this algorithm to a quasiperiodic Lorentz gas with high symmetry to study diffusion and compare it with the random Lorentz Gas.

DY 13.4 Mon 16:00 ZEU 118

Interpreting the Types of Derivatives in Fractional Relaxation Models — •Tillmann Kleiner and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

The excess wing of α-relaxation peaks and the phenomenon of nearly constant loss that have been observed in dielectric spectra of glass forming materials [1] are predicted by susceptibility functions that involve stretching exponents derived from fractional dynamics [2,3]. The relaxation motions predicted by such models can be described by initial value problems involving fractional derivatives with a type parameter. Special choices for the type parameter yield Liouville-Caputo and Riemann-Liouville derivatives.

Using a translation invariant fractional derivative the fractional initial value problems are reformulated as linear response equations. The influence of the type parameter is then described by additional fractional derivative expressions. The reformulation brings the advantage that the mathematical external force term coincides with the physical external force term which is not guaranteed for all types in the initial value problem formulation. Further, predictions for realistic spectroscopy and relaxation experiments are now described in a unified way and physical predictions depend continuously and more transparently on the parameters of the model.

[1] F. Kremer and A. Loidl, The Scaling of Relaxation Processes, Springer, (2018)
[2] R. Hilfer, Analysis **36**, 49-64 (2016)
[3] R. Hilfer, J. Stat. Mech. (2019) 104007

DY 13.5 Mon 16:15 ZEU 118

Dynamic properties of quasi-confined colloidal hard-sphere liquids near the glass transition — •Lukas Schrack, Charlotte Petersen, and Thomas Franosch — Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, 6020 Innsbruck, Austria

The complex behavior of confined fluids arising due to a competition between layering and local packing can be disentangled by considering quasi-confined liquids with translational invariance along the confined direction. We provide a mode-coupling theory (MCT) for quasi-confined liquids using multiple relaxation channels and elaborate an efficient method for the numerical implementation.

Investigating both the collective and tagged-particle motion near the glass transition we focus on the non-monotonic behavior of the glass-form factor as well as of the intermediate scattering functions comparing numerical MCT results and simulations. We also provide a non-equilibrium state diagram as a function of the confinement length.

DY 13.6 Mon 16:30 ZEU 118

Broadband Dielectric and Nuclear Magnetic Resonance Spectroscopy Studies on Dynamics of Ethylene Glycol in Soft and Hard Confinement — •Melanie Reuhl, Max Weigler, and Michael Vogel — Institut für Physik kondensierter Materie, Technische Universität Darmstadt

As hydrogen-bond networks are often restricted or confined in nature and technology, we investigate the influence of the type of confinement on hydrogen-bonded systems. Using nuclear magnetic resonance (NMR) and broadband dielectric spectroscopy (BDS), we analyse the dynamics of ethylene glycol (EG) in nanoporous silica, elastin and Ficoll matrices over broad temperature ranges. For all investigated systems, BDS and NMR results consistently indicate a slowdown and an enhanced heterogeneity of dynamics due to confinement. For EG in silica pores, calorimetric studies reveal partial freezing at temperatures below the bulk freezing point, indicating substantial freezing point suppression. We study changes in the dynamical behaviour when the confined liquid evolves into coexisting liquid and solid phases upon cooling. The dynamical behaviour of both EG phases in silica confinement is independent of pore size for diameters below 6 nm. In the studied soft confinements, fractional freezing does not occur. Still, two dynamically distinguishable EG species occur, which can be assigned to free EG and interfacial EG at elastin/sugar surfaces.

15 min. break.

DY 13.7 Mon 17:00 ZEU 118

Dynamics of Ethylene Glycol Water Mixtures in Bulk and Mesoporous Silica Studied by Nuclear Magnetic Resonance and Dielectric Spectroscopy — •Philipp Monnard, Melanie Reuhl, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Hydrogen bonds remain a topic of scientific interested because of their key role in countless chemical systems. Aqueous solutions of ethylene glycol (EG) create complex networks of hydrogen bonds, because of EGs ability to form both intramolecular and intermolecular bonds. Those solutions are also widely used in heating, cooling and deicing applications, since their freezing point is significantly lower than that of their components. Using nuclear magnetic resonance (NMR) and dielectric spectroscopy (DS), we analyze the effect of silica confinement on the dynamics of EG-water mixtures with different concentrations. In particular, we determine the dependence of correlation times on the pore diameter over a broad temperature range. In doing so, we exploit the isotope selectivity of NMR to observe only the partially deuterated EG-d4(C2D4(OH)2) molecules. Further, we prepared solutions, with heavy water and EG-d2(C2H4(OD)2) to measure the dynamics of the counterpart. We found that the dynamics depend on the mixing ratio, explicitly there is a slowdown with higher concentrations of EG. Moreover, we observe strong dynamical heterogeneity and, for solutions of 30 wt.% EG, the relaxation is even bimodal at intermediate temperatures.

DY 13.8 Mon 17:15 ZEU 118

Aging of SiO_2: Scaling of Dynamic Heterogeneities and Cluster Analysis of Single Particle Jumps — •Katharina Vollmayr-Lee[1], Horacio E. Castillo[2], Christopher H. Gorman[3], and Taylor S. Cookmeyer[4] — [1]Bucknell University, Lewisburg, PA, USA — [2]Ohio University, Athens, OH, USA — [3]University of California, Santa Barbara, CA, USA — [4]University of California, Berkeley, CA, USA

We study the aging dynamics of the strong glass former SiO_2 via molecular dynamics simulations. We quench the system from a high to a low temperature, and then investigate the dynamics of the system as a function of waiting time, the time elapsed since the quench. For a system of 336 atoms, we find that both the dynamic susceptibility and the probability distribution of the local incoherent intermediate scattering function can be described by simple scaling forms in terms of the global incoherent intermediate scattering function. We also find for the scaling of these dynamic heterogeneities that the aging dynamics is controlled by a unique aging clock which is the same for Si and O atoms. Furthermore, we present results for a system of 115248 atoms for which we use single particle trajectories to identify single particle jump events when a particle escapes its cage formed by its neighbors. To study how these jump events are correlated in space and time, we find clusters of jumping particles. We will present cluster size distributions of both simultaneously jumping particles, as well as space-time clusters (jump events which are neighbors in space and time).

DY 13.9 Mon 17:30 ZEU 118

Residual stress distributions and mechanical noise in athermally deformed amorphous solids from atomistic simulations — •Céline Ruscher[1,2] and Jörg Rottler[2] — [1]Institut Charles Sadron, Strasbourg, France — [2]Department of Physics and Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, Canada

The distribution $P(x)$ of local residual stresses in amorphous packings governs the statistical properties of global collective failure events at the yielding transition. We reveal the evolution of $P(x)$ upon deformation by combining atomistic simulations with the frozen matrix approach. A pseudogap form $P(x) \sim x^\theta$ is observed in the freshly quenched state and in the early stages of deformation. After a few percent strain, however, $P(x)$ starts to develop a plateau p_0 in the small x limit, where $p_0 \sim L^{-p}$ with L the system size. A direct comparison with the system size scaling of the stress drops shows that the distribution of avalanche sizes are controlled by θ in the transient regime and the plateau exponent p in the steady state flow. The broad distribution of mechanical noise $P(\Delta x) \sim |\Delta x|^{-1-\mu}$ is characterized by a Levy-exponent μ and can be related to the behavior of $P(x)$ via a mean-field description.

DY 13.10 Mon 17:45 ZEU 118

AGE-INDEPENDENT PROCESS IN AGING HARD-SPHERE SUSPENSIONS: THE BETA PROCESS AND ITS RAMIFICATIONS — •Hans Joachim Schöpe[1] and William van Megen[2] — [1]Universität Tübingen — [2]RMIT University Melbourne

We consider the dynamics of a suspension of hard sphere-like particles in the proximity of its glass transition, the region where the intermediate scattering functions show significant aging. The time correlation function of the longitudinal particle current shows no dependence on age and reveals behaviour of ideal super-packed fluid and glass. The power laws of the beta process of the idealised mode coupling theory are exposed directly without reliance on fitting parameters. We proffer a mechanism linking the reversible/ageless dynamics, which constitutes the beta-process, and the irreversible aging dynamics.

DY 14: Microswimmers (joint session DY/CPP)

Time: Monday 15:00–17:45 Location: ZEU 160

Invited Talk DY 14.1 Mon 15:00 ZEU 160

Microswimmers in (semi-)dilute suspensions: binary mixtures, trapping, orientational ordering, collective motion, and imposed shear flows — Christian Hoell, Giorgio Pessot, Hartmut Löwen, and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Active microswimmers self-propel while setting the surrounding fluid into motion. This leads to hydrodynamic swimmer interactions and can enable emergent collective behavior. Extending our corresponding statistical characterization of (semi-)dilute microswimmer suspensions, we have derived a dynamical density functional theory to describe binary microswimmer mixtures [1]. First, we address mixtures of pushers and pullers of otherwise identical properties [1]. We find that the majority species hydrodynamically imposes its behavior onto the minority species, both under spherical confinement and for unbounded planar motion [1,2]. Particularly, this concerns emergent polar orientational order. Second, we consider trapped active microswimmers confined by a ring of driven passive particles [1]. Through resulting imposed hydrodynamic fluid flows, the enclosed microswimmers concentrate in a centered spot, mimicking the behavior of active circle swimmers [3]. Since frequently in nature many active species interact with each other under confinement, we consider our extensions essential on the path of statistically characterizing corresponding biological systems.

[1] C. Hoell et al., *J. Chem. Phys.* **151**, 064902 (2019).
[2] G. Pessot et al., *Mol. Phys.* **116**, 3401 (2018).
[3] C. Hoell et al., *New J. Phys.* **19**, 125004 (2017).

DY 14.2 Mon 15:30 ZEU 160

Fine balance of chemotactic and hydrodynamic torques: When microswimmers orbit a pillar just once — •Chenyu Jin[1,2], Jérémy Vachier[1], Soumya Bandyopadhyay[3], Tamara Macharashvili[4], and Corinna Maass[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany. — [2]University of Bayreuth, Bayreuth, Germany — [3]Purdue University, West Lafayette, USA — [4]Princeton University, Princeton, USA

Self-propelling liquid crystal droplets in an aquaeous surfactant solution is an excellent model system for biological microswimmers: they exhibit chemotaxis and negative autochemotaxis, and they interact with boundaries. Here we study the detention statistics of these droplet microswimmers attaching to microfluidic pillars. The repulsive trail of spent fuel shed by themselves biases them to detach from pillars in a specific size range after orbiting the pillars just once. We have designed a microfluidic assay recording microswimmers in pillar arrays of varying diameter, derived detention statistics via digital image analysis, and interpreted these statistics via the Langevin dynamics of an active Brownian particle model. By comparing data from orbits with and without residual chemical field, we can independently estimate quantities such as hydrodynamic and chemorepulsive torques, chemical coupling constants and diffusion coefficients, as well as their dependence on environmental factors such as wall curvature. This type of analysis is generalizable to many kinds of microswimmers.

DY 14.3 Mon 15:45 ZEU 160

Active dynamics of microalgae in an anisotropic porous environment — •Florian von Rüling and Alexey Eremin — Otto von Guericke University Magdeburg

Understanding the motion of active colloids in porous media is essential for fundamental physics and a wide range of biological and medical applications. Cell growth and motion is often restricted by complex environments such as the cytoskeleton. Here, we report experimental studies on the motion of the unicellular microalgae Chlamydomonas reinhardtii through a flexible anisotropic lattice of chains formed by magnetic particles. In a thin cell or capillary, the microalgae interact with chain-like aggregates that form in a magnetic field. Shape-anisotropic structures guide the swimmers or initiate tumbling. They affect the persistence time of the microswimmer's motion. As the chains of magnetic particles disintegrate quickly after turning off the magnetic field, the system transforms into an unperturbed state. We investigate the effect of the chains on the orientational velocity correlations in the active dynamics of the algae.

DY 14.4 Mon 16:00 ZEU 160

Percolation transition of pusher-type microswimmers — •Fabian Jan Schwarzendahl[1,2] and Marco G. Mazza[2,3] — [1]Department of Physics, University of California, Merced,5200 N. Lake Road, Merced, California 95343, USA — [2]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [3]Interdisciplinary Centre for Mathematical Modelling and Department of Mathematical Sciences,Loughborough University, Loughborough, Leicestershire LE11 3TU, United Kingdom

In this talk I will present the presence of a continuum percolation transition in model suspensions of pusher-type microswimmers. The clusters dynamically aggregate and disaggregate resulting from a competition of attractive and repulsive hydrodynamic and steric interactions. As the microswimmers' filling fraction increases, the cluster size distribution approaches a scale-free form and there emerge large clusters spanning the entire system. We characterize this microswimmer percolation transition via the critical exponents, analytical arguments, and scaling relations known from percolation theory. This finding opens new vistas on microswimmers' congregative processes.

DY 14.5 Mon 16:15 ZEU 160

Self-assembling complex and functional structures at the (sub)millimeter scale — •Nicolas Vandewalle — GRASP, Institut de Physique B5a, Sart Tilman, Universite de Liege, B4000 Liege, Belgium

When soft ferromagnetic particles are suspended at air-water interfaces in the presence of a vertical magnetic field, dipole-dipole repulsion competes with capillary attraction such that structures self-assemble. The complex arrangements of such floating bodies are emphasized. By adding a horizontal and oscillating magnetic field, periodic deformations of the assembly are induced. We show herein that collective particle motions induce locomotion at low Reynolds number. The physical mechanisms and geometrical ingredients behind this cooperative locomotion are identified. These physical mechanisms can be exploited to much smaller scales, offering the possibility to create artificial and versatile microscopic swimmers. Moreover, we show that it is possible to generate complex structures that are able to capture particles, perform cargo transport, fluid mixing, etc...

15 min. break.

DY 14.6 Mon 16:45 ZEU 160

Shape-anisotropic microswimmers: Influence of hydrodynamics — •Arne W. Zantop and Holger Stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Constituents of active matter, e.g. bacteria or active filaments, are often elongated in shape. The shape and the stiffness of the active components clearly influence their individual dynamics and collective pattern formation. On length scales much larger than the size of the constituents, active materials exhibit many fascinating phenomena such as the formation of vortices or turbulent structures [1,2]. To identify how steric and hydrodynamic interactions as well as thermal fluctuations influence collective behavior is subject of current research.

In this context, we model shape-anisotropic microswimmers with rod shape by composing them of overlapping spherical squirmers [3]. We simulate their hydrodynamic flow fields using the method of multi-particle collision dynamics. With increasing aspect ratio of the rods, we find that a force quadrupole moment dominates the hydrodynamic flow field, whereas in quasi-2D confinement between two parallel plates (Hele-Shaw geometry) the far field is determined by a two-dimensional source dipole moment. Investigating the collective dynamics of the squirmer rods, we identify with increasing density and aspect ratio of the rods a disordered, a swarming, and a jamming state.

[1] Dunkel *et al.*, PRL 110.22 (2013): 228102.
[2] Wensink *et al.*, PNAS 109.36 (2012): 14308-14313.
[3] Downton *et al.*, J. of Ph.: Cond. Mat. 21.20 (2009): 204101.

DY 14.7 Mon 17:00 ZEU 160

Chemokinesis causes trapping and avoidance by dynamic scattering — •Justus Kromer — Stanford University, Stanford, United States of America

A minimal control strategy for artificial microswimmers with limited

information processing capabilities is chemokinesis: the regulation of random directional fluctuations or speed as function of local, non-directional cues. In contrast to chemotaxis, it is not well understood whether chemokinesis is beneficial for the search for hidden targets.

We present a general theory of chemokinetic search agents that regulate directional fluctuations according to distance to a target. We characterize a dynamic scattering effect that reduces the probability to penetrate regions with strong directional fluctuations. If the target is surrounded by such a region, dynamic scattering causes beneficial inward-scattering of agents that had just missed the target, but also disadvantageous outward-scattering of agents approaching the target for the first time. If agents respond instantaneously to positional cues, outward-scattering dominates and chemokinetic agents perform worse than simple ballistic search. Yet, agents with just two internal states can decouple both effects and increase the probability to find the target significantly. Interestingly, these agents violate a mean-chord-length theorem. We apply our analytical theory to the biological example of sperm chemotaxis of marine invertebrates. Sperm cells need to pass a 'noise zone' surrounding the egg, where chemokinesis masks chemotaxis.

Kromer et al. arXiv:1904.11020

DY 14.8 Mon 17:15 ZEU 160

Feedback Control of Multiple Active Microswimmers — •Alexander Fischer and Frank Cichos — Uni Leipzig

Collective motion created by the interaction of autonomous individuals plays a major role in flocks of birds, bacterial growth or the motion of robotic swarms. Sensing and reacting to signals is a fundamental issue of life. Microswimmers, which are artificial objects that mimic the active motion of biological systems, do not have such sensing and response features built in yet, but may gain them through an external control of their propulsion. Here we explore the emergent collective behavior as a result of an information exchange between artificial microswimmers by computer-controlled feedback processes. We have created a setup where multiple active microswimmers can react to their position in space or their distance to other microswimmers [1]. Our system consists of autonomous agents performing directed motion in a plane and their orientation is subject to noise. We study in particular the delayed response of the swimmers to environmental signals, where the swimmers remember previous information on a signaling landscape or infer future signals from the experience. We find that this type of delayed response is changing the collective behavior.

[1] U. Khadka, V. Holubec, H. Yang, F. Cichos, Nat. Commun. 9, 3864 (2018)

DY 14.9 Mon 17:30 ZEU 160

Viscosity destabilizes the propulsion dynamics of active droplets — •Babak Vajdi Hokmabad[1], Maziyar Jalaal[2], Ranabir Dey[1], Kyle Baldwin[1,3], Detlef Lohse[1,2], and Corinna Maass[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Physics of Fluids Group, Max Planck Center for Complex Fluid Dynamics, Enschede, The Netherlands — [3]Nottingham Trent University, Nottingham, United Kingdom

Biological micro-organisms have developed sophisticated swimming behaviors such as run-and-tumble or switch-and-flick. These complex functions depend on their complicated biophysical machinery. In efforts to develop artificial micro-swimmers, the aim is to build a minimal system based on the principles of out-of-equilibrium physics that is able to mimic such complex behaviors. In this work, we show that an active droplet, undergoing micellar solubilization, experiences unsteady self-propulsion in response to an increase in the viscosity of the swimming medium. The origins of this seemingly counterintuitive behavior is explained using theory in conjunction with a novel experimental technique to simultaneously visualize the hydrodynamic and chemical fields around the droplet. By varying the viscosity we can tune the propulsion dynamics and observe behaviors reminiscent of natural micro-swimmers.

DY 15: Condensed-matter simulations augmented by advanced statistical methodologies (joint session DY/CPP)

Time: Monday 15:30–18:15 Location: HÜL 186

DY 15.1 Mon 15:30 HÜL 186

Funnel Hopping Monte Carlo: An efficient method to overcome broken ergodicity — •Jonas Alexander Finkler and Stefan Goedecker — University of Basel, Switzerland

Monte Carlo simulations are a powerful tool in the investigation of thermodynamic properties of atomic systems. In practice however sampling of the complete configuration space is often hindered by high energy barriers between different regions of configuration space which can make ergodic sampling completely infeasible within accessible simulation time.

We present a novel method called Funnel Hopping Monte Carlo (FHMC) to overcome broken ergodicity in Monte Carlo simulations. The method requires a priory knowledge of the funnel structure of the potential energy surface. This information does not have to be obtained from expensive Monte Carlo simulations but can be obtained very cheaply from a Minima Hopping [1] run. By approximating the Boltzmann distribution around local minima using Gaussian mixtures high quality Monte Carlo moves can be proposed that allow the simulation to directly jump between different funnels, circumventing the energy barriers in between.

The methods performance is demonstrated on the example of the 38 and 75 atom Lennard-Jones clusters which are well known for their double funnel energy landscapes that completely prevent ergodic sampling with conventional Monte Carlo simulations.

[1] S. Goedecker, J. Chem. Phys. 120, 9911 (2004)

DY 15.2 Mon 15:45 HÜL 186

Second-principles investigation of the electrocaloric properties of $PbTiO_3$ — •Monica Graf[1] and Jorge Iñiguez[1,2] — [1]Luxembourg Institute of Science and Technology - LIST — [2]University of Luxembourg

Electrocaloric effects attract increasing attention as they provide an ecologically-friendly alternative for solid-state cooling [1] . Here we investigate the electrocaloric response of prototype ferroelectric $PbTiO_3$, using a second-principles approach that has already proved its ability to reproduce qualitatively the properties of this compound in bulk [2] and when embedded in various heterostructures [3]. More precisely, we perform Monte Carlo simulations at finite temperature and under applied electric field to obtain the first- and second-order electrocaloric tensor of $PbTiO_3$, in a temperature range including the ferroelectric transition. The first-order electrocaloric tensor can be computed from the thermal fluctuations of polarization and energy, as obtained from simulations in absence of electric field, taking advantage of Maxwell's relations in the same way that is done in "indirect" experimental measurements of the electrocaloric effect. To access the second-order tensor, we simulate the material subject to electric fields of varying magnitude, parallel and perpendicular to the polarization. In this talk we will present and discuss our results.

References:
1. Nat Commun 9, 1827 (2018)
2. Phys. Rev. Lett. 112, 247603 (2014)
3. Nature 534, 524 (2016)

DY 15.3 Mon 16:00 HÜL 186

Exploring Chemical Reaction Space with Machine Learning — •Sina Stocker[1], Gábor Csányi[2], Karsten Reuter[1], and Johannes T. Margraf[1] — [1]Chair of Theoretical Chemistry, Technical University Munich, Germany — [2]Department of Engineering, University of Cambridge, United Kingdom

Reaction networks are essential tools for the analysis, visualization and understanding of chemical processes in such diverse fields as catalysis, combustion and the origin of life. For complex processes, the number of individual reaction steps in such a network is so large that an exhaustive first-principles calculation of all reaction energies and rates becomes prohibitively expensive. In this contribution, we use machine learning (ML) to accelerate the exploration of chemical reaction space, in analogy to the more established ML-based exploration of chemical space. To this end, we generated a new *reactive* reference database

of open- and closed-shell organic molecules. This allows us to apply "chemical space" ML methods to predict the thermochemistry of reaction networks. We also develop explicitly "reaction space" based ML approaches to directly predict reaction properties. The performance of these methods confirms the potential of ML for the high-throughput screening of large reaction networks.

DY 15.4 Mon 16:15 HÜL 186

Kernel-based machine learning for efficient molecular liquid simulations — •Christoph Scherer[1], René Scheid[1], Tristan Bereau[1,2], and Denis Andrienko[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]University of Amsterdam, Netherlands

Most current force fields based on machine learning (ML) techniques result in high computational cost at every integration time step of an MD simulation. We describe a number of practical and computationally-efficient strategies to parametrize force fields for molecular liquids with kernel-based ML. We employ a particle decomposition ansatz to two- and three-body force fields and covariant kernels. Binning techniques allow to incorporate significantly more training data. Tabulation of the kernel predictions lead to MD simulations with the same computational cost than analytic three-body potentials. Results are presented for model molecular liquids: pairwise Lennard-Jones and three-body Stillinger-Weber systems, as well as an example from bottom-up coarse-graining of liquid water [1]. Many-body representations, decomposition, and kernel regression schemes are implemented in the open-source software package VOTCA [2].

[1] Scherer, Andrienko, PCCP, 20, 22387 (2018); [2] Rühle, Junghans, Lukyanov, Kremer, Andrienko, JCTC, 5, 3211 (2009)

DY 15.5 Mon 16:30 HÜL 186

Anharmonic phonons sampled from large scale molecular dynamics based on on-the-fly machine- learning force fields — •Jonathan Lahnsteiner and Menno Bokdam — Computational materials physics University of Vienna, Sensengasse 8/12 1090 Wien

The phonon spectrum for complex dynamic solids at elevated temperatures is often ill-described by the harmonic approximation. In this talk, I will present a molecular dynamics (MD) study of the Caesium Lead Bromide perovskite (CsPbBr3) in its orthorhombic and cubic phase. In the cubic phase, the Cs cation displays 'rattling' motion and (surrogate) structures are dynamically unstable, as indicated by imaginary phonon modes obtained in the harmonic approximation. For high accuracy and efficiency, the on-the-fly machine-learning force field (MLFF) method [1] is applied. This method generates a force-field with near first-principles accuracy and is trained to mimic the potential energy surface described by the SCAN density functional. Large scale microcanonical ensembles are generated with the MLFF and the finite-temperature dynamic structure factors are computed from the Fourier transform of the ionic density-density correlation functions. The intensities of the dynamic structure factor directly give insight in the phonon properties by taking into account phonon scattering events up to infinite order. These fully dynamic phonon spectra are compared to the phonons in the harmonic approximation. With this we are able to discuss the importance of anharmonic lattice vibrations to the stabilization of CsPbBr3 perovskite phases at finite temperature.

[1] Jinnouchi et.al. Phys.Rev.Let.10.1103/PhysRevLett.122.225701

15 min. break.

DY 15.6 Mon 17:00 HÜL 186

Edgy and Parallel – Efficient Equilibration of Anisotropic Hard Particulate Systems — •Marco Klement and Michael Engel — Institute for Multiscale Simulation, FAU Erlangen, Erlangen, Germany

Particle simulations are an important method to study the phase behavior of fluids and solids. A common task is structure prediction via thermal equilibration. Examples are crystallization or melting and the aging of glasses. Near the liquid-solid phase transition of hard spheres event driven molecular dynamics (EDMD) is known as most efficient. Correlated movement of particles in EDMD aids the equilibration. For Monte Carlo methods event-chains [1] introduce a correlation of particle updates. Particles move until the next collision. One of several collision rules determines the new particle to continue the chain and the new direction of the chain. The recently published Newtonian event-chain (NEC) algorithm [2] is an advanced statistical methodology that assigns velocities to particles and performs collisions elastically. It is a close competitor in efficiency to EDMD. In this contribution we present the extension of NEC to polyhedral particles. We also discuss how parallelization strategies [3] can be adapted to this algorithm. Our implementation has been added to the software package HOOMD-blue. [4]

[1] Bernard et al., Phys. Rev. E 80, 056704 (2009)
[2] Klement et al., J. Chem. Phys. 150, 174108 (2019)
[3] Kampmann et al., J. Comput. Phys. 281, 864-875 (2015)
[4] http://glotzerlab.engin.umich.edu/hoomd-blue/

DY 15.7 Mon 17:15 HÜL 186

Machine-learning force fields trained on-the-fly with bayesian inference — Ryosuke Jinnouchi[1,2], Jonathan Lahnsteiner[1], Ferenc Karsai[3], Georg Kresse[1], and •Menno Bokdam[1] — [1]University of Vienna, Vienna, Austria — [2]oyota Central R&D Labs, Inc., Aichi, Japan — [3]VASP Software GmbH, Vienna, Austria

Realistic finite temperature simulations of matter are a formidable challenge for first principles methods. Long simulation times and large length scales are required, demanding years of compute time. We present an on-the-fly machine learning scheme that generates force fields automatically during molecular dynamics simulations[1]. This opens up the required time and length scales, while retaining the distinctive chemical precision of first-principles methods and minimizing the need for human intervention. The method is widely applicable to multi-element complex systems and implemented in the VASP code. We demonstrate its predictive power on the entropy-driven phase transitions of hybrid perovskites (CH3NH3PbI3), which have never been accurately described in simulations.

[1] R. Jinnouchi et al., Phys. Rev. Lett. 122, 225701 (2019)

DY 15.8 Mon 17:30 HÜL 186

Learning effective collective variables for biasing via t-distributed stochastic neighbor embedding — •Omar Valsson[1] and Jakub Rydzewski[2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Torun, Poland

A common strategy to overcome the time scale problem of molecular dynamics (MD) simulations is to employ collective variable (CV) based enhanced sampling methods [1]. However, the efficiency of such approaches depends critically on the quality of the chosen CVs that must describe all the slow degrees of freedom. While physical and chemical intuition has proven generally successful in achieving this, there is a growing need for methods that can automatically find good CVs. An appealing option to accomplish this is to use ideas from the field of machine learning.

Here we show how dimensionality reduction via t-distributed stochastic neighbor embedding (t-SNE) [2] can be employed to learn effective CVs for biasing. We have implemented t-SNE directly in the PLUMED plug-in, which allows us to use it directly in numerous MD codes.

[1] O. Valsson, P. Tiwary, and M. Parrinello, Ann. Rev. Phys. Chem. 67, 159 (2016)
[2] L. van der Maaten and G. Hinton, J. Mach. Learn. Res. 9, 2579 (2008)

DY 15.9 Mon 17:45 HÜL 186

Variational autoencoders as a tool to learn collective variables from simulation snapshots — •Miriam Klopotek and Martin Oettel — Institut für Angewandte Phsyik, Eberhard Karls Universität Tübingen, Tübingen, Germany

Variational autoencoders (VAEs) are powerful neural-network architectures capable of learning abstract representations of data (distributions of latent variables) in an unsupervised fashion. We apply a standard formulation of VAEs [1,2] to equilibrium configurations obtained by grand canonical Monte Carlo simulations and formulate a probabilistic model for the VAE which shows that the latent variables are collective variables, and their variances are generalized susceptibilities. Upon application to a lattice model with sticky rods which shows competing gas, liquid and nematic phases we find that the leading collective variables are akin to the two order parameters of the model. Furthermore, the collective variables define coarse-grained configurations. Increasing the number of latent variables leads to finer spatial resolution of the coarse-grained configurations and increasingly preciser physical observables obtained from them. Finally, we discover there is an optimal hyperparameter β in so-called β-VAEs [3] where the collective variables become disentangled with respect to structural

correlation length-scales: These disentangled collective variables hence form a hierarchy of different levels-of-detail.
[1] Kingma, D. P. & Welling, M. (2013). arXiv:1312.6114. [2] Rezende, D. J., Mohamed, S., & Wierstra, D. (2014). arXiv:1401.4082. [3] Higgins, I. et al. (2017). ICLR, 2(5), 6.

DY 15.10 Mon 18:00 HÜL 186

Adversarial Reverse Mapping of Equilibrated Condensed-Phase Molecular Structures — •Marc Stieffenhofer[1], Michael Wand[2], and Tristan Bereau[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz — [2]JGU Mainz, Institute of Computer Science, Staudingerweg 9, 55128 Mainz

Coarse-grained molecular dynamics simulations circumvent prohibitively long equilibration times by averaging out degrees of freedom. However to consistently link the scales a reverse mapping scheme is needed to reintroduce higher resolution details. Traditional schemes propose a rough coarse-to-fine mapping and rely on further energy minimization and molecular dynamics simulations to re-equilibrate the system. In this study we introduce DeepBackmap: A deep neural network based approach to predict equilibrated molecular structures without running molecular dynamics simulations. We use generative adversarial networks to learn the Boltzmann distribution from training data and realize reverse mapping by using the coarse-grained structure as a conditional input. Our method can be used for condensed-phase systems of arbitrary sizes. The model uses only local information and reconstructs the atomistic structure autoregressively. We test our method on syndiotactic polystyrene molecules and show that the model trained in a melt shows remarkable transferability to the crystalline phase. The learned local correlations appear to be temperature independent indicating a separation of the scales.

DY 16: Convection

Time: Monday 15:30–16:45 Location: ZEU 147

DY 16.1 Mon 15:30 ZEU 147

Resolved energy budget of superstructures in Rayleigh-Bénard convection — •Gerrit Green[1,2], Dimitar G. Vlaykov[1,3], Juan Pedro Mellado[4], and Michael Wilczek[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Faculty of Physics, University of Göttingen, Göttingen, Germany — [3]Astrophysics Group, University of Exeter, Exeter, UK — [4]Department of Physics, Universitat Politècnica de Catalunya, Barcelona, Spain

Coherent large-scale flow patterns in the presence of turbulent small-scale fluctuations are a ubiquitous phenomenon in natural flows. Currently, the interaction of these so-called turbulent superstructures with small-scale fluctuations is not understood in detail. In order to clarify this interaction, we study superstructures by means of direct numerical simulations in Rayleigh-Bénard convection. This idealized model system shows a complex coexistence of turbulent fluctuations and superstructures. Here, we employ a filtering approach to separate the superstructures from the small-scale fluctuations. We study the resolved energy budget at the scale of the superstructures and characterize the different contributions to the budget, such as the energy input by buoyancy, the direct dissipation, and the energy transfer between scales. We find that the energy transfer primarily acts as an energy sink but exhibits a complex structure in the boundary layer. Our detailed analysis of the energy budget sheds light on the interaction between superstructures and small-scale fluctuations and may help to guide the development of reduced-order models.

DY 16.2 Mon 15:45 ZEU 147

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

Direct numerical simulations of an incompressible fluid are used to investigate differences between exact 2D and 3D simulations. The fluid is rotated about a direction perpendicular to the direction of gravity. The Prandtl number is 0.7 and the convection is controlled by a Rayleigh number ranging from 10^4 to 10^9. Rotation is characterised by the Ekman number ranging from 10^{-1} down to 10^{-6}. The convective flow will be restrained to the plane perpendicular to the direction of rotation at strong enough rotation due to the Taylor-Proudman theorem. This behaviour will break up once convective driving is strong enough. Thermal transport and kinetic energy density depart noticeably from the 2D scaling. In the regime of 3D isotropic turbulence the scaling of the Nusselt number is different from the 2D scaling by a constant factor.

DY 16.3 Mon 16:00 ZEU 147

Moist Rayleigh-Bérnard Convection in conditionally unstable environments — •Florian Heyder, Jörg Schumacher und Martina Hentschel — Technische Universität Ilmenau, 98693 Ilmenau, Germany

The presence of water vapour and liquid water leads to cloud formation in the turbulent atmosphere. The boost of buoyancy due to latent heat release by condensation at cloud level implies different dynamics for dry unsaturated and moist saturated air parcels. We investigate their motion by direct numerical simulations in a moist Rayleigh-Bénard (RB) model in the Boussinesq approximation. Our setup takes moist and dry dynamics into account by linearising the equation of state on both sides of the phase boundary. This simplified model allows us to study differences to classical RB systems without phase changes, as well as the formation of clouds in extended horizontal domains. Special emphasis is given to conditionally unstable environments where dry air is stably and moist air unstably stratified.

DY 16.4 Mon 16:15 ZEU 147

Heat and momentum transport enhancement in liquid metal convection exposed to horizontal magnetic fields — •Tobias Vogt[1], Juancheng Yang[2], Felix Schindler[1], and Sven Eckert[1] — [1]Helmholtz Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Xi'an Jiaotong University, Xi'an, China

We investigate the effect of a static, horizontal magnetic field on a liquid metal Rayleigh-Bénard convection by means of laboratory experiments. Although a static magnetic field acts as a stabilizing force on the fluid, we find that self-organized convective flow structures reach an optimal state where the heat transport significantly increases and convective velocities reach the theoretical free-fall limit. Our measurements show that the application of the magnetic field leads to an anisotropic, highly ordered flow structure and a decrease of the turbulent fluctuations. When the magnetic field strength is increased beyond the optimum, Hartmann braking becomes dominant and leads to a reduction of the heat and momentum transport. The results are relevant for magneto-hydrodynamic convective flows in stellar interiors and planetary cores.

DY 16.5 Mon 16:30 ZEU 147

Helical Rayleigh-Benard Convection — •Philipp Reiter[1], Rodion Stepanov[2], and Olga Shishkina[1] — [1]Max-Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute of Continuos Media Mechanics, Perm, Russia

Helicity is known to play a key role in generation of large coherent flow structures in a large class of geophysical and astrophysical flows. Here we suggest a new way to inject helicity in convective systems through coupling of the temperature and vertical vorticity via the temperature boundary conditions under the requirement that the area-averaged temperatures of the heated and cooled plates are kept constant.

Using 3D direct numerical simulations, we verify the impact of these boundary conditions on the mean-flow helicity, analyze the global flow structures and the heat transport and investigate their dependencies on the particular parameters of the boundary conditions. For a certain set of parameters, when a significant amount of helicity is injected, we observe generation of the mean vertical angular momentum. In that case, after an initial transitional phase, the flow enters a state of a well-pronounced stable rotation.

DY 17: Interfaces and Thin Films I (joint session CPP/O/DY)

Time: Monday 16:30–17:15 Location: ZEU 260

DY 17.1 Mon 16:30 ZEU 260

In Situ Monitoring Mesoscopic Deformation of Nanostructured Porous Titania Films Caused by Water Ingression — Lin Song[1,2], Monika Rawolle[1], Nuri Hohn[1], Jochen S. Gutmann[3], Henrich Frielinghaus[4], and •Peter Müller-Buschbaum[1,5] — [1]Lehrstuhl für funktionelle Materialien, Physik Department, TU München, 85748 Garching, Germany — [2]Xian Institute of Flexible Electronics, Northwestern Polytechnical University, Xian 710072, Shaanxi, China — [3]Fakultät für Chemie, Universität Duisburg-Essen, 45141, Essen, Germany — [4]JCNS at MLZ, Forschungszentrum Jülich GmbH, 85748 Garching, Germany — [5]MLZ, TU München, 85748 Garching, Germany

Nanostructured porous titania films are used in many energy related applications. We investigate the temporal evolution of the mesoscopic deformation of mesoporous titania films synthesized via block copolymer assisted sol-gel chemistry with in situ grazing incidence small-angle neutron scattering (GISANS) during exposure to water vapor. Two types of mesoporous titania films are compared, which have a different degree of structural stability, depending on the applied annealing temperature in nitrogen atmosphere. Water ingression causes a gradual structure deformation in terms of decreasing center-to-center distances and broadening of the size distribution of the titania nanostructures. Based on the evolution of the mesopore size obtained from in situ GISANS measurements, the results show which type of titania structure is more stable against water infiltration.

DY 17.2 Mon 16:45 ZEU 260

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

Responsive block copolymer thin films are of interest for many applications, e.g. as fast sensors or switchable membranes. In the present work, we investigate a pH and temperature responsive pentablock quaterpolymer in thin films during solvent vapor annealing (SVA). The end blocks are temperature-responsive and hydrophobic while the midblock is pH-responsive and hydrophilic. Structural information was obtained by employing in situ grazing-incidence small-angle X-ray scattering (GISAXS) and by model fitting the obtained 2D patterns. We find that, varying the pH value of the solution for spin-coating as well as the nature of the solvent used for SVA gives the opportunity to tune the structures in a wide range.

DY 17.3 Mon 17:00 ZEU 260

Self-assembly of large magnetic nanoparticles in ultrahigh molecular weight linear diblock copolymer films — •Wei Cao[1], Senlin Xia[1], Xinyu Jiang[1], Markus Gallei[2], Matthias Opel[3], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Saarland University, Chair in Polymer Chemistry, 66123 Saarbrücken — [3]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [4]DESY, Notkestrasse 85, 22603 Hamburg — [5]KTH Royal Institute of Technology, FPT, SE-100 44 Stockholm, Sweden

The fabrication of diblock copolymer nanocomposite films that consist of magnetic nanoparticles (NPs) with diameters (D) of more than 20 nm is a challenging task. Herein, ultrahigh molecular weight (UHMW) linear polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) diblock copolymer is spin-coated as a template for the self-assembly of large iron oxide NPs (D = 27 nm), and the morphology of hybrid nanocomposites is governed by the concentration of the iron oxide NPs. The NPs are functionalized with carboxylic acid groups showing an affinity to the PMMA blocks. Due to the rearrangement of the polymer chains for accommodating the NPs, well-ordered spherical nanostructures are readily generated at a NP concentration of 0.5 wt%. Most interestingly, a chain-like network appears inside the hybrid films at a high NP loading. All hybrid films show ferromagnetism at room temperature, proven with a superconducting quantum interference device magnetometer.

DY 18: Delay and Feedback Dynamics

Time: Monday 17:00–18:15 Location: ZEU 147

DY 18.1 Mon 17:00 ZEU 147

Satellite instability in Passively Mode-Locked Integrated External-Cavity Surface Emitting Lasers — Christian Schelte[1,2], •Denis Hessel[2], Julien Javaloyes[1], and Svetlana Gurevich[2,3] — [1]Departament de Física, Universitat de les Illes Balears & Institute of Applied Computing and Community Code (IAC-3), Cra. de Valldemossa, km 7.5, E-07122 Palma de Mallorca, Spain — [2]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany — [3]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, D-48149 Münster, Germany

We are interested in a pulse instability appearing in passively mode-locked integrated external-cavity surface-emitting lasers (MIXSELs) modelled by delayed algebraic differential equations (DADEs). The micro-cavity geometry induces third order dispersion (TOD) that can lead to a train of satellites on the leading edge of a pulse. We show that those can become unstable due to carrier interaction. The resulting limit cycle is born in a global bifurcation of the saddle-node infinite period (SNIPER) type and exhibits behavior characteristic of excitable systems.

DY 18.2 Mon 17:15 ZEU 147

Analysing and Optimizing the Nonlinear Memory Capacity of Photonic Reservoir Computing — •Felix Köster and Kathy Lüdge — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, 10623 Berlin

Reservoir computing is a neuromorphic inspired machine learning paradigm that utilizes the naturally occurring computational capabilites of dynamical systems. In this work, we investigate the linear and nonlinear memory capacity of a delay-based class-A-laser reservoir computer via numerical simulations. We show that the reservoir computing performance is deeply connected to the total memory capacity and that resonances between the information injection rate and the delay time of the laser system play a crucial role in optimizing the reservoir. Additionally, we study the method of speed gradient descent as an optimization scheme for a delay based reservoir computer. By applying this method we can force our reservoir into having certain memory capacities tailored for a specific task.

DY 18.3 Mon 17:30 ZEU 147

Non-local effects in external cavity passively mode-locked lasers — •Jan Hausen[1], Christian Schelte[2,3], Julien Javaloyes[2], Svetlana V. Gurevich[2,3], and Kathy Lüdge[1] — [1]TU Berlin, Hardenbergstrasse 36, 10623 Berlin — [2]Universitat de les Illes Balears, Cra. de Valldemossa, km 7.5. Palma (Illes Balears) — [3]WWU Münster, Wilhelm-Klemm-Strasse 9, 48149 Münster

Asymmetrical geometries can improve the performances of passively mode-locked vertical external-cavity surface-emitting lasers and give rise to non-equidistant pulse patterns. We show that these geometries create non-local effects; by analyzing a previously developed delay differential equation model, we derive rigorously a Master equation from the pulse evolution that contains such non-local terms. Setting adequate boundary conditions, we extend our analysis to the dynamics of intermediate cavities (600ps), particularly relevant for high perfor-

mance mode-locking. We study the influence of the non-locality stemming from the asymmetric position of the elements in the cavity and we recover the bifurcation structure of non-equidistant pulse patterns.

DY 18.4 Mon 17:45 ZEU 147

Optimale Regeleigenschaften eines Zufluss-Abfluss-Systems fern vom Gleichgewicht — •Claus Fütterer[1,2] und Katja Prasol[1,2] — [1]Biophysical Tools GmbH — [2]Labor für Biophysik, Leipzig

Die Regelung einer intensiven Größe in einem vorgegebenen Volumen kann durch Anpassung von Zufluss und Abflusswiderständen für eine dieses Volumen durchströmende extensive Größe erreicht werden. Dies ist ein Muster, das man in zahlreichen biologischen Systemen und in vielen technologischen Anwendungen wiederfindet.

Als konkrete Anwendung diskutieren wir die Regelung des pneumatischen Drucks für die mikro-und mesofluidische Strömungskontrolle. Hierzu modellieren wir ein System mit einem kleinen Druckvolumen, welches über Ventile mit konstanter Quelle und Senke verbunden ist. Das diskutierte Verfahren ist eine Weiterentwicklung des "PI"-Reglers.

Wir präsentieren eine kurze Herleitung der durch Gegenkopplung linearisierten Gleichungen und diskutieren Eigeschaften der analytischen Lösungen, wie Anstiegszeit und Stabilität. Wir können hierbei Formeln für optimale Regelparameter für schnellste, überschwingerfreie Einregelzeit ableiten. Hierbei unterscheiden wir zwischen statischen Sollwerten, nicht-stetigen und stetigen Sollwertfunktionen, wie z.B. einer Sinusfunktion. Die Analogie zum Federpendel hilft bei der Interpretation der Zusammenhänge.

Zuletzt betrachten wir noch Optimierungsmöglichkeiten sowie in Anwendungen häufig auftretende endliche Regelstrecken und nichtlineare Effekte.

DY 18.5 Mon 18:00 ZEU 147

An event-based model for synchronization in digital phase locked loops — •Sara Ameli Kalkhouran, Lucas Wetzel, and Frank Jülicher — Max Planck Institute for physics of complex systems, Dresden, Germany

We study synchronization in digital phase-locked loops, which are two state oscillators in a feedback loop. The state of the oscillator, either high or low, is represented by sets of discrete event-times at which signals switch between these states and a low pass filter acts as the controlling element. One advantage of this model is that the implementation of noise, so-called timing-jitter, can be done in a physically sound way as it can be added directly to the event-times.

We have developed a numeric and analytic framework within which one can study the case of free-running oscillation (oscillator in open loop) as well as entrainment with an external reference (closed-loop). This model can be generalized for variety of discrete-continuous systems; Having the response function of a system, e.g. obtained from experiments, our approach can be used to analyse the dynamics of a variety of systems in which the timing of an event is controlled in a self-tuned manner; like cell division, or firing in a neural population.

DY 19: Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/DY)

Time: Tuesday 9:30–13:00 Location: HSZ 204

DY 19.1 Tue 9:30 HSZ 204

Exponential damping in perturbed quantum many-body systems — •Jonas Richter[1], Fengping Jin[2], Lars Knipschild[1], Hans De Raedt[3], Kristel Michielsen[2], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]University of Osnabrück, Germany — [2]Forschungszentrum Jülich, Germany — [3]University of Groningen, The Netherlands

Given a quantum many-body system and the expectation-value dynamics of some operator, we study how this reference dynamics is altered due to a perturbation of the system's Hamiltonian. Based on projection operator techniques, we unveil that if the perturbation exhibits a random-matrix structure in the eigenbasis of the unperturbed Hamiltonian, then this perturbation effectively leads to an exponential damping of the original dynamics. Employing a combination of dynamical quantum typicality and numerical linked cluster expansions, we demonstrate that our theoretical findings are relevant for the dynamics of realistic quantum many-body models. Specifically, we study the decay of current autocorrelation functions in spin-1/2 ladder systems, where the rungs of the ladder are treated as a perturbation to the otherwise uncoupled legs. We find a convincing agreement between the exact dynamics and the lowest-order prediction over a wide range of interchain couplings, even if the perturbation is not weak.
[1] J. Richter et al., arXiv:1906.09268.

DY 19.2 Tue 9:45 HSZ 204

Slow quantum thermalization and many body revivals from mixed phase space — •Alex Michailidis[1], Chris Turner[2], Dimitry Abanin[3], Zlatko Papic[2], and Maksym Serbyn[1] — [1]IST Austria, Klosterneuburg, Austria — [2]University of Leeds, Leeds, United Kingdom — [3]University of Geneva, Geneva, Switzerland

Isolated, interacting quantum systems thermalize when local measurements are distributed according to the Gibbs ensemble. The ability of an isolated quantum many body system to thermalize is tied to the absence of an extensive set of integrals of motion. The thermalization rate may, however, depend strongly on the initial state. A class of kinetically constraint systems [Nat. Phys. 14, 745 (2018)] displays such features, due to a set of quasi-eigenmodes, known as "quantum many body scars", which form a slowly thermalizing subspace. The slow thermalization is also associated to an unstable periodic orbit in a slightly entangled manifold of matrix product states (MPS) [PRL 122, 040603 (2019)] .

First, by using tensor tree states (TTS) and ideas from standard mean field theory, we generalize the MPS ansatz to higher dimensions. We employ the time-dependent-variational-principle to analytically calculate the equations of motion for lattices of arbitrary connectivity. We find that the coherent oscillations in the quantum system are associated to stable periodic orbits in a mixed phase space. This method provides a new way to identify entangled states which display coherent dynamics. Finally, we associate slowly thermalizing states to regular "islands" in the mixed phase space.

DY 19.3 Tue 10:00 HSZ 204

Collective behavior of an excitonic insulator in the quantum electromagnetic field — •Katharina Lenk and Martin Eckstein — Department of Physics, University of Erlangen-Nuremnberg, 91058 Erlangen, Germany

The strong coupling of light and matter in cavity quantum electrodynamics provides new avenues to engineer properties of complex materials. In this talk, we investigate the behavior of a so-called excitonic insulator (EI) in a cavity. The EI is a phase driven by the Coulomb interaction, in which two bands of a semiconductor or semimetal spontaneously hybridize, leading to the opening of a gap. We consider the particular case in which the EI implies a breaking of the U(1) symmetry related to the conservation of charge in the individual bands. The coupling of a generic bosonic mode, such as the coordinate of a phonon, reduces the symmetry, adds a mass to the phase mode, and stabilizes the symmetry-broken phase. While this suggests that a similar mechanism may be at work for the coupling of the EI to a cavity mode, we show that the balancing of dipolar interactions and the dipolar light-matter coupling leaves the phase mode massless, in spite of the breaking of the U(1) symmetry.

DY 19.4 Tue 10:15 HSZ 204

A memory truncation scheme to investigate long-time dynamics in correlated systems — •Antonio Picano and Martin Eckstein — Friedrich-Alexander-Universität Erlangen-Nürnberg

We present an approach to follow the evolution of many-body systems up to previously unaccessible long time scales. Provided only that the system of interest shows a self-energy that is short-range in time, its time evolution can be determined by solving a simplified version of the full Kadanoff-Baym equations. The computational effort scales only linearly with the number of time-steps, and the computer memory is independent of the propagation time.

We have applied the method to investigate the dynamical phase transitions from antiferromagnetic to paramagnetic states driven by an interaction quench in the fermionic Hubbard model, using the nonequilibrium dynamical mean-field theory. We have observed the presence

of two dynamical transition points: one is related to the thermal phase transition, the other is connected to the existence of a transient non-thermal antiferromagnetic order above the thermal critical temperature. The non-thermal order displays a slow decay, which is followed by a faster thermalization process, and thermalization is significantly delayed by the trapping of the system in the nonthermal state.

DY 19.5 Tue 10:30 HSZ 204

Critical quenches in the attractive Hubbard model — •Christopher Stahl and Martin Eckstein — Lehrstuhl für Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Deutschland

We investigate critical quenches from a paramagnetic phase in a three dimensional attractive Hubbard model towards the ordered superconducting phase using a two-time Green's function formalism on the Keldysh contour and the fluctuation exchange approximation (FLEX). This self-consistent approach gives access to the coupled dynamics of single particle properties and collective fluctuations in the transient state, and allows to study the growth of order in the initially disordered system. By truncating the two-time self-energy with respect to relative time we set up a long-time multi-scale simulation which resolves the dynamics of both the fast electronic and slow bosonic degrees of freedom. This may help to close the gap between short time microscopic simulations and predictions for the long time behavior based on Ginzburg-Landau-theory and the theory of dynamic critical phenomena.

DY 19.6 Tue 10:45 HSZ 204

Thermalization of a two-species condensate — •Jan Louw[1], Michael Kastner[2], and Johannes Kriel[2] — [1]University of Goettingen, Goettingen, Germany — [2]Stellenbosch University, Stellenbosch, South Africa

Motivated by recent experiments, we study the time evolution of a two-species Bose-Einstein condensate which is coupled to a bosonic bath. For the particular condensate, unconventional thermodynamics have recently been predicted. To study these thermal properties we find the conditions under which this open quantum system thermalizes—equilibrates to the Gibbs state describing the canonical ensemble. We do this in a semi-classical picture with corrections scaling with the inverse system size.

DY 19.7 Tue 11:00 HSZ 204

Exceptional points and the topology of quantum many-body spectra — •David Luitz and Francesco Piazza — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We show that in a generic, ergodic quantum many-body system the interactions induce a nontrivial topology for an arbitrarily small non-Hermitian component of the Hamiltonian. This is due to an exponential-in-system-size proliferation of exceptional points which have the Hermitian limit as an accumulation (hyper)surface. The nearest-neighbor level repulsion characterizing Hermitian ergodic many-body systems is thus shown to be a projection of a richer phenomenology, where actually all the exponentially many eigenvalues are pairwise connected in a topologically robust fashion via exceptional points.

15 min. break.

DY 19.8 Tue 11:30 HSZ 204

η–paired hidden phase in photodoped Mott insulators — •Jiajun Li[1], Denis Golez[2], Philipp Werner[3], and Martin Eckstein[1] — [1]University of Erlangen-Nuremberg, Germany — [2]Flatiron Institute, New York, US — [3]University of Fribourg, Switzerland

We show that a metastable η–pairing superconducting phase can be induced by photodoping doublons and holes into a strongly repulsive fermionic Hubbard model. The doublon-hole condensate extends over a wide range of doublon densities and effective temperatures. Different non-equilibrium protocols to realize this state are proposed and numerically tested. We also study the optical conductivity in the superconducting phase, which exhibits ideal metallic behavior, i.e., a delta function at zero-frequency in the conductivity, in conjunction with negative conductivity at large frequencies. These characteristic optical properties can provide a fingerprint of the η-pairing phase in pump-probe experiments.

DY 19.9 Tue 11:45 HSZ 204

η-pairing in one-dimensional Mott insulators — •Satoshi Ejima[1], Tatsuya Kaneko[2], Florian Lange[1], Seiji Yunoki[3,4,5], and Holger Fehske[1] — [1]Institute of Physics, University Greifswald, Greifswald, Germany — [2]Department of Physics, Columbia University, New York NY, USA — [3]RIKEN Cluster for Pioneering Research, Wako, Japan — [4]RIKEN Center for Emergent Matter Science, Wako, Japan — [5]RIKEN Center for Computational Science, Kobe, Japan

Very recently, it was theoretically demonstrated that unconventional superconductivity correlation can be induced by pulse irradiation in the simple Mott insulator of the half-filled Hubbard model [1]. This superconducting-like state stems from the so-called η-pairing mechanism, characterized by staggered pair-density-wave oscillations of the off-diagonal correlations.

In this study, we first explore precisely under which conditions the η-pairing state appears most pronouncedly at zero temperature by means of the time-dependent density-matrix renormalization group (DMRG) method in the matrix-product-state representation. Carrying out temperature-dependent DMRG in combination with the purification technique, we furthermore prove whether this state can survive at finite temperatures, in order to check the possible experimental observation of the pairing state, e.g., in optical lattices.

[1] T. Kaneko, T. Shirakawa, S. Sorella and S. Yunoki, Phys. Rev. Lett. **122**, 077002 (2019).

DY 19.10 Tue 12:00 HSZ 204

Effect of dimensionality on the dynamics of optically excited Mott-Hubbard clusters — •Junichi Okamoto — Institute of Physics, University of Freiburg, Freiburg, Germany

Development of intense light sources and of various time-resolved spectroscopies has opened up a new avenue in condensed matter physics. In particular, optically excited nonequilibrium states of strongly correlated systems show nontrivial and intriguing phenomena such as light-induced superconductivity or ultrafast structural switching. An important step to understand these phenomena is to investigate the excitation spectrum of a system. To this end, we use an exact diagonalization method to study the effect of dimensionality on the dynamics of optically excited states in Mott-Hubbard clusters. We compare the excitation spectrum in one and two dimensions, and demonstrate the different transient dynamics induced by short optical pulses.

DY 19.11 Tue 12:15 HSZ 204

Disentangling sources of quantum entanglement in quench dynamics — •Lorenzo Pastori[1], Markus Heyl[2], and Jan Carl Budich[1] — [1]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

Quantum entanglement may have various origins ranging from solely interaction-driven quantum correlations to single-particle effects. Here, we explore the dependence of entanglement on time-dependent single-particle basis transformations in fermionic quantum many-body systems, thus aiming at isolating single-particle sources of entanglement growth in quench dynamics. Using exact diagonalization methods, for paradigmatic nonintegrable models we compare to the standard real-space cut various physically motivated bipartitions. Moreover, we search for a minimal entanglement basis using local optimization algorithms, which at short to intermediate postquench times yields a significant reduction of entanglement beyond a dynamical Hartree-Fock solution. In the long-time limit, we identify an asymptotic universality of entanglement for weakly interacting systems, as well as a crossover from dominant real-space to momentum-space entanglement in Hubbard models undergoing an interaction quench. Finally, we discuss the relevance of our findings for the development of tensor-network based algorithms for quantum dynamics.

DY 19.12 Tue 12:30 HSZ 204

Statistical localization: from strong fragmentation to strong edge modes — •Tibor Rakovszky[1], Pablo Sala[1], Ruben Verresen[2], Michael Knap[1], and Frank Pollmann[1] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

Certain disorder-free Hamiltonians can be non-ergodic due to a strong fragmentation of the Hilbert space into disconnected sectors. Here, we characterize such systems by introducing the notion of "statistically localized integrals of motion" (SLIOM), whose eigenvalues label the connected components of the Hilbert space. SLIOMs are not spatially

localized in the operator sense, but appear localized to sub-extensive regions when their expectation value is taken in typical states with a finite density of particles. We illustrate this general concept on several Hamiltonians, both with and without dipole conservation. Furthermore, we demonstrate that there exist perturbations which destroy these integrals of motion in the bulk of the system, while keeping them on the boundary. This results in statistically localized strong zero modes, leading to infinitely long-lived edge magnetizations along with a thermalizing bulk, constituting the first example of such strong edge modes in a non-integrable model. We also show that in a particular example, these edge modes lead to the appearance of topological string order in a certain subset of highly excited eigenstates. Some of our suggested models can be realized in Rydberg quantum simulators.

DY 19.13 Tue 12:45 HSZ 204

Matrix product state investigations of time-dependent spectral functions after a photoexcitation — •Constantin Meyer and Salvatore R. Manmana — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We study the time-dependent dynamical structure factor after a photoexcitation of a variant of the 1d Hubbard model with a background staggered magnetic field using matrix product state (MPS) techniques. In particular, we use the time-dependent variational principle (TDVP) to investigate the time evolution of the band population, which is a quantity accessible to time-resolved ARPES experiments. Different scenarios for the photoexcitations are discussed, e.g., Peierls-substitution or direct excitation in k-space. Using MPS, we can study in detail the effect of the electron-electron interaction on the redistribution of the band populations in the various photoexcitation setups. An outlook to the relevance of electron-electron interactions on light-harvesting mechanisms in correlated materials is given.

We acknowledge financial support by SFB/CRC 1073 (project B03) of the DFG.

DY 20: Data analytics for dynamical systems I (Focus Session joint with DY and BP) (joint session SOE/DY/CPP/BP)

Data analytics is often focussed on (generalized) regression to create models of the structure of complex systems. Here we focus on data-driven approaches of data analytics for complex systems that take into account their intrinsic nonlinear dynamics. Applications to natural and human-made systems, from cardiac dynamics to human mobility, illustrate recent progress and current methodological challenges. (Session organized by Marc Timme)

Time: Tuesday 9:30–13:15 Location: GÖR 226

Topical Talk DY 20.1 Tue 9:30 GÖR 226

One model to rule them all — •Jens Timmer — Institute of Physics, University of Freiburg, Germany

A major goal in systems biology is to reveal potential drug targets for cancer therapy. A common property of cancer cells is the alteration of signaling pathways triggering cell-fate decisions resulting in uncontrolled proliferation and tumor growth. However, addressing cancer-specific alterations experimentally by investigating each node in the signaling network one after the other is difficult or even not possible at all. Here, we use quantitative time-resolved data from different cell lines for non-linear modeling under L1 regularization, which is capable of detecting cell-type specific parameters. To adapt the least-squares numerical optimization routine to L1 regularization, subgradient strategies as well as truncation of proposed optimization steps were implemented. Likelihood-ratio tests were used to determine the optimal penalization strength resulting in a sparse solution in terms of a minimal number of cell-type specific parameters that is in agreement with the data. The uniqueness of the solution is investigated using the profile likelihood. Based on the minimal set of cell-type specific parameters experiments were designed for improving identifiability and to validate the model. The approach constitutes a general method to infer an overarching model with a minimum number of individual parameters for the particular models.

DY 20.2 Tue 10:00 GÖR 226

Volatility and Fractionality in Power-Grid Frequency — •Leonardo Rydin Gorjão[1,2], Anton Yurchenko-Tytarenko[3], and Dirk Witthaut[1,2] — [1]Forschungszentrum Jülich, Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE), 52428 Jülich, Germany — [2]Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany — [3]Department of Mathematics, University of Oslo, P.O. Box 1053 Blindern, N-0316 Oslo

Power-grid frequency is a key indicator of stability in power grids. The trajectory of power-grid frequency embodies several processes of different natures: the control systems enforcing stability, the trade markets, production and demand, and the correlations between these. In this article, we study power-grid frequency from Central Europe, the United Kingdom, and Scandinavia under the umbrella of fractional stochastic processes. We introduce an estimator of the Hurst index for fractional Ornstein–Uhlenbeck processes. We show that power-grid frequency exhibits time-dependent volatility, driven by daily human activity and yearly seasonal cycles. Seasonality is consistently observable in smaller power grids, affecting the correlations in the stochastic noise. The United Kingdom displays daily rhythms of varying volatility, where the noise amplitude consistently doubles its intensity, and displays bi- and tri-modal distributions. Both the Scandinavian and United Kingdom power-grids exhibit varying Hurst indices over yearly scales. All the power grids display highly persistent noise, with Hurst indices above $H > 0.5$.

Topical Talk DY 20.3 Tue 10:15 GÖR 226

Gaming the system - Analyzing Uber price data reveals anomalous supply shortages — •Malte Schröder[1], David Storch[1], Philip Marszal[1], and Marc Timme[1,2] — [1]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden — [2]Lakeside Labs, Klagenfurt

Dynamic pricing schemes are ubiquitously employed across industries to balance demand and supply. One well-known example is the ride-hailing platform Uber and their *surge pricing* intended to incentivize drivers to offer their service during times of high demand. However, recent reports [WJLA, Uber, Lyft drivers manipulate fares at Reagan National causing artificial price surges (2019)][Möhlmann and Zalmanson, ICIS 2017 Seoul (2017)] indicate that this surge pricing may instead cause demand-supply imbalances by incentivizing drivers to switch off their app to increase their revenue. Analyzing price estimate time series for trips from 137 locations in 59 urban areas across six continents, we identify locations with strong, repeated price surges. Correlations with demand patterns demonstrate that the observed price surges are indeed driven by supply anomalies instead of demand fluctuations. Moreover, we capture the minimal incentives driving the supply dynamics in a simple game-theoretic model, illustrating that such incentives constitute generic consequences of dynamic pricing schemes.

DY 20.4 Tue 10:45 GÖR 226

Estimation of Langevin equations with correlated noise for signals of complex systems — •Clemens Willers and Oliver Kamps — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Germany

Over the last years, the estimation of stochastic evolution equations of complex systems has been applied in many scientific fields ranging from physics to biology and finance. Especially, Langevin models with delta-correlated noise terms, which realize a Markovian dynamic, have been used successfully in this context [1]. However, many real world data sets exhibit correlated noise and a non-Markovian dynamic, for example data sets from turbulence [2].

To tackle this problem, we use Langevin models containing an added

hidden component which realizes a driving correlated noise. We develop two methods for the systematic estimation of the drift- and diffusion functions, parameterized through spline functions. The first method is based on a likelihood function which is constructed by a short-time propagator for the measured values of the visible component. For the second method, we use a comparison of transition probabilities via Jensen-Shannon divergence. Both methods are demonstrated using real world data sets as the turbulent air flow of a free jet [3], stock market prices [4] and wind energy production [5].

[1] Friedrich et al., Phys. Rep. 506, 87 (2011) [2] Friedrich et al., Phys. Rev. Lett. 78, 863 (1997) [3] Renner et al., J. Fluid Mech. 433, 383 (2001) [4] Nawroth et al., Eur. Phys. J. B 50, 147 (2006) [5] Kamps, in Wind Energy-Impact of Turbulence, Springer 2014, p. 67.

DY 20.5 Tue 11:00 GÖR 226

Hyper-Parameter Optimization for Identification of Dynamical Systems — •Tobias Wand[1], Alina Steinberg[1], Tim Kroll[2], and Oliver Kamps[2] — [1]Institut für Theoretische Physik, Universität Münster, Deutschland — [2]Center for Nonlinear Science, Universität Münster, Deutschland

In recent years, methods to identify dynamical systems from experimental or numerical data have been developed [1,2]. In this context, the construction of sparse models of dynamical systems has been in the focus of interest and has been applied to different problems. These data analysis methods work with hyper-parameters that have to be adjusted to improve the results of the identification procedure. If more than one hyper-parameter has to be fine-tuned, simple methods like grid search are computationally expensive and due to this, sometimes not feasible. In this talk, we will introduce different approaches to optimally select the hyper-parameters for the identification of sparse dynamical systems.

[1] Brunton et al. Proceedings of the National Academy of Sciences, 2016, 113, 3932-3937
[2] Mangan et al. Proceedings of the Royal Society A, 2017, 473, 20170009

Topical Talk DY 20.6 Tue 11:15 GÖR 226

Data driven modelling of spatio-temporal chaos in extended dynamical systems — •Ulrich Parlitz[1,2], Sebastian Herzog[1,3], Florentin Wörgötter[3], Roland S. Zimmermann[1,2], Jonas Isensee[1,2], and George Datseris[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institut für Dynamik komplexer Systeme, Georg-August-Universität Göttingen, Germany — [3]Drittes Physikalische Institut, Georg-August-Universität Göttingen, Germany

Many spatially extended nonlinear systems, an example being excitable media, exhibit complex spatio-temporal dynamics. We shall present machine learning methods to predict the temporal evolution of these systems or estimate their full state from limited observations. The applied techniques include Reservoir Computing [1] and a combination of a Convolutional Autoencoder with a Conditional Random Field [2,3], whose perfomance will be compared to Nearest Neighbours Prediction based on dimension reduced local states [4]. Examples for demonstrating and evaluating the methods employed include the Lorenz-96 model, the Kuramoto-Sivashinsky equation, the Barkley model, and the Bueno-Orovio-Cherry-Fenton model, describing cardiac (arrhythmia) dynamics.

[1] R. S. Zimmermann and U. Parlitz, Chaos 28, 043118 (2018)
[2] S. Herzog et al., Front. Appl. Math. Stat. 4, 60 (2018)
[3] S. Herzog et al., Chaos (to appear) (2019)
[4] J. Isensee, G. Datseris, U. Parlitz, J. of Nonlinear Sci. (2019)

DY 20.7 Tue 11:45 GÖR 226

Predicting Spatio-Temporal Time Series Using Dimension Reduced Local States — •Jonas Isensee[1,2], George Datseris[1,2], and Ulrich Parlitz[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institut für Dynamik komplexer Systeme, Georg-August Universität Göttingen, Germany

Understanding dynamics in spatially extended systems is central to describing many physical and biological systems that exhibit behaviour such as turbulence and wave propagation. Correctly predicting dynamics is advantageous in experimental settings and data-driven approaches are useful, particularly when no adequate mathematical models are available. We present an approach to iterated time series prediction of spatio-temporal dynamics based on local delay coordinate states and local modeling using nearest neighbour methods [1]. A crucial step in this process is to find predictive yet low-dimensional descriptions of the local dynamics . We discuss how imposing symmetries on the dynamics can be used to increase the predictiveness of our approach. The efficacy of this approach is shown for (noisy) data from a cubic Barkley model, the Bueno-Orovio-Cherry-Fenton model.

[1] J. Isensee, G. Datseris, U. Parlitz, J. of Nonlinear Sci. (2019)

Topical Talk DY 20.8 Tue 12:00 GÖR 226

Limits to predictability of complex systems dynamics — Jonathan Brisch and •Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Motivated by the challenges of weather forecasting and the well known fact that atmospheric dynamics takes place on many temporal and spatial scales, we discuss the possibility of scale dependent error growth and its consequences for predictions. In case that the growth rate of small errors depends on the error magnitude as an inverse power law, we can explain why forecasts of macroscopic observables can be successful on time scales which are orders of magnitude longer than the (estimated) Lyapunov time, and at the same time we find a strictly finite prediction horizon even for arbitrary accuracy of the initial condition. We propose a hierarchical model class, which is able to generate such an error growth behaviour, and finally we re-analyze published data of error-growth in a numerical weather forecast system to present evidence that the error growth rate there is indeed consistent with a power law with diverging growth rate for infinitesimal errors. It is plausible that the same mechanism is active in other complex phenomena which live on a variety of spatial and temporal scales.

DY 20.9 Tue 12:30 GÖR 226

Network inference from event sequences: Disentangling synchrony from serial dependency — •Reik Donner[1,2], Forough Hassanibesheli[2,3], Frederik Wolf[2,3], and Adrian Odenweller[4,5] — [1]Magdeburg-Stendal University of Applied Sciences, Magdeburg — [2]Potsdam Institute for Climate Impact Research — [3]Department of Physics, Humboldt University, Berlin — [4]Center for Earth System Research and Sustainability, University of Hamburg — [5]Max Planck Institute for Meteorology, Hamburg

Inferring coupling among interacting units or quantifying their synchronization based on the timing of discrete events has vast applications in neuroscience, climate, or economics. Here, we focus on two prominent concepts that have been widely used in the past - event synchronization (ES) and event coincidence analysis (ECA). Numerical performance studies for two different types of spreading processes on paradigmatic network architectures reveal that both methods are generally suitable for correctly identifying the unknown links. By further applying both concepts to spatiotemporal climate datasets, we demonstrate that unlike ECA, ES systematically underestimates linkages in the presence of temporal event clustering, which needs to be accounted for in network reconstruction from data. In turn, for spike train data from multi-channel EEG recordings (with relatively narrow inter-event time distributions), the obtained results are practically indistinguishable. Our findings allow deriving practical recommendations for suitable data preprocessing in the context of network inference and synchronization assessment from event data.

DY 20.10 Tue 12:45 GÖR 226

Reconstruction of nonlinear correlations and dynamical laws — Mirko Rossini, Konstantin Schmitz, and •Jürgen Stockburger — ICQ, Ulm University, Germany

Time series taken from a stationary process may feature dependencies far more subtle than linear correlations. We introduce a method based on non-linear feature extraction which can uncover and quantify such dependencies. Its utility is demonstrated using both synthetic and real-world data.

DY 20.11 Tue 13:00 GÖR 226

Collective Response of Reservoir Networks — •Arash Akrami, Fabio Schittler Neves, Xiaozhu Zhang, Malte Schröder, and Marc Timme — Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden

Reservoir Computing constitutes a paradigm of bio-inspired machine learning relying on dynamical systems theory, that exploits high dimensionality of a large network of processing units (reservoir). However, as the collective dynamics of artificial neural networks is far from understood, their learning outcome is hardly predictable or transparent.

In Reservoir Computing systems, learning occurs exclusively in a read-out layer, with the intrinsic reservoir dynamics freely evolving.

Here we study reservoirs of processing units with linear activation functions, i.e., linear reservoirs and analytically predict the dynamic responses of all network units as a function of general, distributed and time-dependent input signals. These insights may help identifying nodes especially suitable for receiving input signals, and finding minimal reservoirs capable of performing a given task.

DY 21: Invited Talk

Time: Tuesday 9:30–10:00 Location: HÜL 186

Invited Talk DY 21.1 Tue 9:30 HÜL 186

From Non-normalizable Boltzmann-Gibbs statistics to infinite-ergodic theory — •Eli Barkai — Physics Department, Bar-Ilan University, Ramat-Gan, Israel

We consider a single particle coupled to a a thermal heat bath, when the system approaches in the long time limit a non-normalised Boltzmann state. This could be a particle interacting with a wall, the force field falling off faster than one over the particle-wall distance. We show how infinite ergodic theory is a useful tool, the infinite invariant measure (the non-normalised state) is given by Boltzmann-Gibbs theory. Time averages of integrable observables are described by the Aaronson-Darling-Kac theorem. We derive our main results using an entropy maximum principle, and discuss the virial theorem when Boltzmann-Gibbs measure is non-normalisable.

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

Time: Tuesday 9:30–13:00 Location: HÜL 386

DY 22.1 Tue 9:30 HÜL 386

Sedimentation and Convection of Bottom-Heavy Squirmers — •Felix Rühle, Jan-Timm Kuhr, and Holger Stark — TU Berlin, Institut für Theoretische Physik, Berlin, Germany

Active particles form appealing patterns, in particular, when hydrodynamic interactions are present [1-3]. A fascinating example known from biology is bioconvection of microswimmers under gravity [4]. In order to study such systems, we simulate bottom-heavy squirmers (neutral squirmers, pushers, and pullers) under different gravitational forces and torques. The relevant parameters are the ratio of swimming to bulk sedimentation velocity and the normalized torque.

In the state diagram of these parameters, for neutral squirmers we observe sedimentation at strong gravitational forces and inverted sedimentation at finite torques, when activity dominates. In between, we identify plumes of collectively sinking squirmers that feed convective rolls of circling squirmers at the bottom of the simulation cell. At velocity ratios slightly above one and large torques squirmers form a spawning cluster, which floats above the bottom wall and from which squirmers occasionally escape. For strong pushers and pullers, we find that the dipolar flow fields weaken the formation of plumes and convective rolls.

[1] M. Hennes, *et al.*, PRL **112**, 238104 (2014)
[2] J.-T. Kuhr, *et al.*, Soft Matter **13**, 7548 (2017).
[3] H. Jeckel, *et al.*, PNAS **116**, 1489 (2019).
[4] T.J. Pedley, and J.O. Kessler, Annu. Rev. Fluid Mech. **24**, 313 (1992).

DY 22.2 Tue 9:45 HÜL 386

Sculpting vesicles with active particles — Masoud Hoore[1], Clara Abaurrea-Velasco[1], Hanumantha Rao Vutukuri[2], Thorsten Auth[1], Jan Vermant[2], Gerhard Gompper[1], and •Dmitry Fedosov[1] — [1]Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Materials, ETH Zürich, 8093 Zürich, Switzerland

Biological cells are able to generate intricate structures and respond to external stimuli, sculpting their membrane from inside. Simplified biomimetic systems can aid in understanding the principles which govern these shape changes and elucidate the response of the cell membrane under strong deformations. We employ a combined simulation and experimental approach to investigate different non-equilibrium shapes and active shape fluctuations of vesicles enclosing self-propelled particles. Interestingly, the most pronounced shape changes are observed at relatively low particle loadings, starting with the formation of tether-like protrusions to highly branched, dendritic structures. At high volume fractions, globally deformed vesicle shapes are observed. The obtained state diagram of vesicles sculpted by active particles predicts the conditions under which local internal forces can generate dramatic cell shape changes, such as branched structures in neurons.

DY 22.3 Tue 10:00 HÜL 386

Diffusing Activity: Active Particles in Evolving Environments — •Nima H. Siboni, S. Mohsen J. Khadem, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

We study the dynamics of a single active Brownian particle (ABP) and the collective behavior of interacting ABPs in a heterogeneous medium. We apply the idea of the diffusing diffusivity model [1] to mimic the environmental heterogeneity in the equation of motion of the ABPs via a time-dependent activity and diffusivities. In our model, the fluctuations of the environment affect simultaneously and similarly the motility and diffusion coefficients. We obtain analytically the probability distribution function of the particle displacement and its moments and support our results via particle-based simulations. We finally investigate the impact of the introduced fluctuations on the collective behavior of ABPs. We obtain the phase diagram of motility-induced phase separation [2,3] for a wide range of noise strength and compare our results with that for the conventional ABPs [4].

[1] M. V. Chubynsky and G. W. Slater, Phys. Rev. Lett. **113**, 098302 (2014).
[2] I. Buttinoni, J. Bialké, F. Kümmel, H. Löwen, C. Bechinger, and T. Speck, Phys. Rev. L. **110**, 238301 (2013).
[3] J. Stenhammar, A. Tiribocchi, R. J. Allen, D. Marenduzzo, and M. E. Cates, Phys. Rev. L. **111**, 145702 (2013).
[4] S. M. J. Khadem, N. H. Siboni, and S. H. L. Klapp, in preparation.

DY 22.4 Tue 10:15 HÜL 386

Phoretic interactions of two chemically-active particles — •Babak Nasouri[1] and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Catalytically-coated active particles in a viscous medium interact with one another by altering the chemical and hydrodynamic fields in their surroundings. Such phoretic interactions may drive particles in motion and are strongly dependent on the physico-chemical properties of the system, namely: the response of the particles to the interaction fields, and geometric factors such as inter-particle distances and particle sizes. In this work, we discuss an analytical approach which can accurately capture the dynamical behaviour of two phoretic spherical particles, for any given configuration.

DY 22.5 Tue 10:30 HÜL 386

Axisymmetric spheroidal squirmers and self-diffusiophoretic particles — Ruben Poehnl[1], •Mihail Popescu[2], and William Uspal[1] — [1]Dept. of Mech. Eng., Univ. of Hawai'i at Manoa, 2540 Dole St., Honolulu, HI 96822, USA — [2]Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany

By using previously published analytical solutions for Stokes flow around a spheroid, here we investigate the motion of a spheroidal, axisymmetric squirmer in an unbounded fluid and the low Reynolds

number hydrodynamic flow induced by the squirmer.

In contrast to the case of a spherical squirmer, for the spheroidal squirmer each slip mode either contributes to the velocity, or contributes to the stresslet. Additionally, and also distinct from the case of a spherical squirmer, each slip mode excites either all of the fore-aft symmetric or fore-aft asymmetric components of the flow field, respectively. Accordingly, with small modifications of the squirming pattern, a microrganism could maintain its velocity unchanged but dramatically alter the topology of the flow around it. This raises the interesting speculative question as whether the spheroidal shape is providing an evolutionary advantage, i.e., a spheroidal squirmer possesses simple means – not available to a spherical one – for acting in hydrodynamic disguise, which can be advantageous as either predator or prey.

The results are straightforwardly extended to the self-phoresis of axisymmetric, spheroidal, chemically active particles with phoretic slip.

DY 22.6 Tue 10:45 HÜL 386

Active particle penetration through a planar elastic membrane — •Abdallah Daddi-Moussa-Ider[1], Benno Liebchen[1,2], Andreas M Menzel[1], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Theorie Weicher Materie, Fachbereich Physik, Technische Universität Darmstadt, Germany

Active penetration of nanoparticles through cell membranes is an important phenomenon which has various biomedical and clinical applications. Using particle-based computer simulations and theory, we study the penetration mechanism of an active or externally driven particle through a planar elastic membrane. We model the membrane as a self-assembled sheet of particles embedded in a viscous fluid. We introduce a coarse-grained model to describe the mutual interactions between the membrane particles. We identify three distinct scenarios, including trapping of the active particle, penetration through the membrane with subsequent self-healing, in addition to penetration with permanent disruption of the membrane. The latter scenario may be accompanied by a partial fragmentation of the membrane into bunches of isolated or clustered particles. Our approach might be helpful for the prediction of the transition threshold between the trapping and penetration states in real-space experiments involving motile swimming bacteria or artificial self-propelling active particles. Reference: Daddi-Moussa-Ider *et al.*, Theory of active particle penetration through a planar elastic membrane, *New J. Phys.* **21**, 083014 (2019).

30 min. coffee break

Invited Talk DY 22.7 Tue 11:30 HÜL 386

Physics of Growth: Another Form of Active Matter — •Jens Elgeti — Foschungszentrum Jülich, Germany Theoretical Soft Matter and Biophysics

Active matter is matter, driven out of equilibrium by its microscopic constituents. Growing mater is also active matter, but activity does not enter via the stress, but in material conservation. The material generates itself – think cells dividing or a tumor growing. Growth implies a change in volume. In physical terms, the conjugate force to volume is pressure. Thus, in order to grow, cells must exert mechanical pressure. In turn, pressure influences growth. This yields to interesting novel phenomena like infinite compressibility, self contracting materials and steady tread-milling states.

We use particle based simulations to study mechanical properties and effects in growing matter. These simulations have been helpful in understanding, interpreting and designing experiments. I will present an overview of the simulation technique, and several examples of how this model helped to gain insight in mechanical processes underlying tissue growth, ranging from growth of cancer spheroids under pressure [1], to *in silico* competition experiments [2-5] and tumor evolution [6].

[1] Montel et al., PRL **107**, 188102 (2011)
[2] Podewitz et al., EPL **109**, 58005 (2016)
[3] Basan et al., Phys. Biol. **8**, 026014 (2011)
[4] Podewitz et al., New J. Physics **18**, 083020 (2016)
[5] Ganai et al., New J. Phys. **21** 063017 (2019)
[6] Büscher et al., arxiv:1910.03263 (2019)

DY 22.8 Tue 12:00 HÜL 386

The effect of hydrodynamic interactions on self-propulsion of multiple swimmers — •Sebastian Ziegler[1], Maxime Hubert[1], Thomas Scheel[2], Jens Harting[2], and Ana-Sunčana Smith[1,3] — [1]PULS Group, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Germany — [3]Division of Physical Chemistry, Ruder Bošković Institute Zagreb, Croatia

A common theoretical approach to model systems of microswimmers is to prescribe the swimming stroke of each individual. If the system consists of more than one device, such models, however, underestimate the impact of one swimmer's stroke on the stroke of all others, reducing the problem of hydrodynamic interactions to a purely geometric one. Furthermore, a number of experimental systems are associated with imposing the forces driving each of the devices. This situation is, from a theoretical point of view, significantly more demanding and has not been investigated so far for multiple swimmers. This issue is addressed in this presentation where we employ a recently developed perturbative calculation and numerical modeling to study the effects of nearby swimmers on the stroke, swimming speed and direction. Notably, we find that for two swimmers, a significant fraction of the parameter space results in both swimmers experiencing a boost from one another. We identify the key characteristics that yield this effect.

DY 22.9 Tue 12:15 HÜL 386

Active particle scattering in structured and random environments — •Theresa Jakuszeit[1], Samuel Bell[2], and Ottavio A. Croze[1] — [1]Cavendish Laboratory, JJ Thomson Avenue, CB3 0HE, Cambridge, United Kingdom — [2]Laboratoire Physico Chimie Curie, Institut Curie,PSL Research University, CNRS UMR168, 75005 Paris, France

Active propulsion as performed by bacteria and Janus particles, in combination with hydrodynamic interaction at boundaries, can lead to the breaking of time reversibility. One typical example of this is the accumulation of bacteria on a flat wall. However, in microfluidic devices with pillars of sufficiently small radius, self-propelled particles can slide along the surface of a pillar without becoming trapped over long times. Using simulations and theory, we study the impact of different modes of obstacle interaction on the diffusive transport of active particles in a lattice of such obstacles. We find that sliding along obstacles can result in large diffusivities even at high obstacle density, unlike particles that undergo classical specular reflection, as in the Lorentz gas. We introduce a microscopically derived run-and-tumble model, which describes the macroscopic transport for different scattering rules very well, and test it in microfluidic channels for E.coli. Finally, we discuss the role of tumbling in structured and random environments.

DY 22.10 Tue 12:30 HÜL 386

Swimming behavior of squirmer dumbbells and polymers — •Judit Clopés Llahí, Gerhard Gompper, and Roland G. Winkler — Theoretical Soft Matter and Biophysics, Institute for Advanced Sim- ulation and Institute of Complex Systems, Forschungszentrum Jülich, D-52425 Jülich, Germany

Nature provides a plethora of microswimmers, which can be rather elongated, filament- or polymer-like. Examples are bacteria swarmer cells or marine phytoplankton dinoflagellates assembling in a linear fashion. In order to address the relevance of hydrodynamic interactions for the collective behavior of such organisms, we study the swimming properties of linear polymer-like assemblies by mesoscale hydrodynamic simulations, where an active unit (monomer) is described by a spherical squirmer -which can be a pusher, a neutral swimmer, or a puller. We find that the monomer hydrodynamic flow field leads to correlations in the relative orientation of adjacent monomers, and consequently the swimming efficiency differs from that of active Brownian linear assemblies. In particular, puller chains show a pronounced increase in the rotational diffusion coefficient compared to pushers, while for neutral squirmers, the rotational diffusion coefficient is similar to that of active Brownian particles. Hence, the large-scale conformational and dynamical properties depend on the specific propulsion mechanism. Refs.: [1] J. Elgeti, R. G. Winkler, G. Gompper, Rep. Prog. Phys. 78, (2015). [2] R. G. Winkler, J. Elgeti, G. Gompper, J. Phys. Soc. Jpn. 86, (2017). [3] A. Martin-Gomez, T. Eisenstecken, G. Gompper, R. G. Winkler, Soft Matter 15, (2018).

DY 22.11 Tue 12:45 HÜL 386

The step-wise induction of transcription drives morphological changes in aggregates of RNA polymerase II — Agnieszka Pancholi[1], Roshan Prizak[1], Tim Klingberg[2], Weichun Zhang[1], Amra Noa[1], Gerd Ulrich Nienhaus[1,3], Vasily Zaburdaev[2], and •Lennart Hilbert[1] — [1]Karlsruhe Institute of Technology — [2]Friedrich-Alexander University Erlangen-Nuremberg — [3]University of Illinois at Urbana-Champaign

In eukaryotic cells, a main control point of transcription is the transient pausing of engaged RNA polymerase II (Pol II) just before transcript elongation. Paused Pol II forms transient polymeric aggregates that exhibit diverse morphologies. Here, we use super-resolution microscopy in embryonic zebrafish cells to show how entry into and exit from Pol II pausing determines these aggregate morphologies. Instant structured illumination microscopy (iSIM) in live embryos revealed that aggregates initially are morphology complex, round up as they grow, and unfold again when actual transcript elongation begins. Using transcription inhibitors, we confirm that Pol II pausing indeed drives aggregate rounding. Further resolving aggregates by STimulated Emission Double Depletion (STEDD) microscopy, we found a granular fine-structure that suggests clustering aggregation rather than liquid-liquid compartmentalization. We currently develop a theoretical model to explain what underlying macro-molecular interactions could result in the observed morphologies.

DY 23: Invited Talk

Time: Tuesday 9:30–10:00 Location: ZEU 118

Invited Talk DY 23.1 Tue 9:30 ZEU 118

Collective dynamics of cell-fate decision in the early embryo — •Jordi Garcia-Ojalvo — Universitat Pompeu Fabra, Barcelona, Spain

Mammalian organisms exhibit an astonishing ability to self-organize in a highly regulated manner during development from a fertilized egg, even in the presence of perturbations that can affect the early embryo. In this talk I will describe our recent work combining theoretical modeling and experiments on mouse embryos, which has led us to establish a minimal model of cell-fate decision that relies on cell-cell communication, making this problem one of collective decision making with robust dynamics.

DY 24: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Tuesday 9:30–13:00 Location: ZEU 160

DY 24.1 Tue 9:30 ZEU 160

Topological states of hard rods in extreme annular confinement — •René Wittmann[1], Louis Cortes[2], Dirk Aarts[2], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Department of Chemistry, University of Oxford, UK

Hard particles are a standard model for colloidal systems and can be effectively studied within classical density functional theory (DFT). Fundamental mixed measure theory (FMMT) allows to predict the phase behavior of a hard-body fluid solely from the shape of individual particles. Recent experimental advances allow for the synthesis of colloids with a nearly hard interaction that can be analyzed on the single-particle level. Slices of a system of such silica rods confined in a three-dimensional chamber under gravity can be considered a quasi-two-dimensional fluid that exhibits typical liquid-crystal behavior in confinement.

Applying FMMT to hard discorectangles in two dimensions, we map out a full phase diagram. Then we focus on a smectic fluid in extreme complex confinement, where the optimal bulk layer spacing competes with the extrinsic geometric and topological constraints. As a result, we characterize a variety of topologically different states in an annular geometry, also observed in particle-resolved experiments with silica rods. By further comparing the free energy of the different states, naturally provided by our DFT, we map out a topological phase diagram, indicating the stable topology depending on the details of the annular geometry.

DY 24.2 Tue 9:45 ZEU 160

Phase Field Crystal Model of patchy colloids in two dimensions — Robert Weigel and •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Motivated by our recent simulation studies of quasicrystals that occur in systems of patchy colloids [1,2], we develop a Phase Field Crystal Model for such particles. We consider two-dimensional patchy colloids with symmetrically placed attractive sites on their surface, such that they interact with preferred binding angles. We construct a free energy functional that is similar to the free energy used for liquid crystals [3], but obeys the symmetry of the patchy colloids. The functional depends on both a density field and an orientation field. Free numerical minimization of the free energy yields a rich phase behavior of complex structures.

[1] Gemeinhardt et al., Eur. Phys. J. E 41, 126 (2018).
[2] Gemeinhardt et al., EPL 126, 38001 (2019).
[3] Achim et al., Phys. Rev. E 83, 061712 (2011).

DY 24.3 Tue 10:00 ZEU 160

Relations between angular and Cartesian orientational expansions* — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

Orientational expansions, which are widely used in the natural sciences, exist in angular and Cartesian form. Although these expansions are orderwise equivalent, it is difficult to relate them in practice. Moreover, the standard expansion has to be modified for particles with asymmetric shape, where a description in terms of spherical harmonics or symmetric traceless tensors is not sufficient. We discuss various methods for orientational expansions and their application for the definition of orientational order parameters in liquid crystal physics. In particular, we explain how conversion tables between angular and Cartesian expansions can be constructed, which we have done up to third order. This is important, e.g., for the comparison of theoretical and experimental results in liquid crystal physics.

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

DY 24.4 Tue 10:15 ZEU 160

Dynamic wrinkling of thin liquid crystal films — •Dominik Mnich, Torsten Trittel, Kirsten Harth, Christoph Klopp, and Ralf Stannarius — Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany

We demonstrate spontaneous wrinkling as a dynamical pattern in freely floating liquid-crystalline films. These films behave liquid-like with respect to flow within the film plane. The adjustment of the film shape to quick changes often requires the formation of additional layers. Centimeter-sized freely floating smectic bubbles are studied during the excitation with acoustic waves. We show that such films develop an undulation instability under acoustic excitation. The results of parabolic flight and ground lab experiments are presented. The observed "wrinkles" show charactistic wavelengths in the submillimeter range. We introduce a basic model of the wavelength selection mechanism.

DY 24.5 Tue 10:30 ZEU 160

Thermally driven material transport in thin freestanding films — •Torsten Trittel, Christoph Klopp, Kirsten Harth, and Ralf Stannarius — Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany

In addition to their important role in display applications, liquid crystals are attractive in the field of fundamental physics. Smectics can form thin free-standing films with aspect ratios exceeding one million to one (width/thickness). These homogeneously thin films serve as an ideal model system for the study of two-dimensional hydrodynamics. We investigate thermally driven material transport within the film plane under microgravity conditions. Temperature differences in the film lead to thermocapillary (Marangoni) flow. In materials

with a normal (negative) temperature coefficient of the surface tension $d\sigma/dT < 0$, temperature inhomogeneities lead to material transport from the warm to the cold film edge. In materials with $d\sigma/dT > 0$, flow is reversed. We present a quantitative model, which predicts that the temperature difference between the hot and cold film edge is the relevant parameter, not the gradient as in conventional thermoconvection.

[1] Trittel et al., Marangoni Flow in Freely Suspended Liquid Films, Phys. Rev. Lett., 122 (2019)

DY 24.6 Tue 10:45 ZEU 160

Defect annihilation 2D using free-standing smetic films — •Kirsten Harth[1], Amine Missaoui[1], Peter Salamon[2], and Ralf Stannarius[1] — [1]Institut für Physik, Otto-von-Guericke Universität Magdeburg — [2]Department of Complex Fluids, Wigner Research Center, Budapest, Hungary

Interacting defects in quasi-2D geometries occur in manifold systems, from strings in cosmology over spin systems in Bose-Einstein condensates or thin magnetic films to liquid crystals. Free-standing smecti C films (smC FSF) represent a quite simple sytem for studying fluid mechanics and pattern formation in 2D. They are particularly easy to handle and orientational patterns are directly observable using polarizing microscopy, but few experiments exist so far. Theory is either fully numerical or focuses on very simplified situations. Orientational problems among the defects and with the far director field were only recently noticed.

With a special method, we are able to prepare isolated pairs of +1 and -1 defects in homogeneous smC FSF, and we study their annihilation. Aligned defect pairs qualitatively follow expectations from theory and approach on straight paths. Misoriented defects pairs display curved trajectories, and their dynamics quantitatively disagrees with theoretical predictions[1]. We discuss experimental findings and possible explanations for the discrepancies.

[1] X. Tang and J. V. Selinger, Soft Matter 13, 5481 (2017)

[2] A. Missaoui, K. Harth, P. Salamon, R. Stannarius, arXiv:1911.05224

15 min. break.

DY 24.7 Tue 11:15 ZEU 160

Static properties of modulated hard-spheres liquid. — •Michele Caraglio, Charlotte F. Petersen, and Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria

The structure of a liquid can be manipulated with externally applied fields. This can be achieved experimentally with interfering lasers and has been implemented with colloidal particles [1, 2]. This possibility also paves the way to a better understanding of confined liquids [3], which are prevalent in nature and necessary in many industrial applications.

We investigate static properties in a hard-sphere liquid with modulated density profile obtained by applying an external periodic field. In this system we will control three dimensionless parameters: the packing fraction, the amplitude of the potential relative to temperature and its wavelength relative to particle diameter. For this purpose, the Ornstein-Zernike integral equation using Percus-Yevick closure relation is solved numerically. The theory requires the density profile as input, which can be obtained from density functional theory. Similar to a liquid confined in a slit, a non-monotonic evolution of the static structure factor peak and the pressure is observed upon variation of the potential wavelength.

[1] C. Bechinger, M. Brunner and P, Leiderer, PRL 86, 2001. [2] F. Evers, et al., PRE 88, 2013. [3] S. Saw and C. Dasgupta, J. Chem. Phys. 145, 2016.

DY 24.8 Tue 11:30 ZEU 160

Analytical classical density functionals from an equation learning network — •Shang-Chun Lin[1], Georg Martius[2], and Martin Oettel[1] — [1]Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, 72076 Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems Tübingen, 72076 Tübingen, Germany

We explore the feasibility of using machine learning methods to obtain an analytic form of the classical free energy functional for two model fluids, hard rods and Lennard*Jones, in one dimension. The Equation Learning Network proposed in Ref.[1] is suitably modified to construct free energy densities which are functions of a set of weighted densities and which are built from a small number of basis functions with flexible combination rules. This setup considerably enlarges the functional space used in the machine learning optimization. As a result in Ref [2], we find a good approximation for the exact hard rod functional. For the Lennard–Jones fluid, we let the network learn the full excess free energy functional and the excess free energy functional related to interparticle attractions. Both functionals show a good agreement with simulated density profiles inside and outside the training region. If time allow, we will show the result that forgo the idea gas contribution.

[1]G. Martius and C. H. Lampert, arXiv:1610.02995 (2016).

[2]S.-C. Lin, G. Martius and M. Oettel, arXiv:1910.12752 (2019).

DY 24.9 Tue 11:45 ZEU 160

First order phase transitions: From bifurcation diagrams to the thermodynamic limit — •Uwe Thiele[1], Tobias Frohoff-Hülsmann[1], Sebastian Engelnkemper[1], Edgar Knobloch[2], and Andrew J. Archer[3] — [1]Institut für Theoretische Physik and Center of Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK

We consider simple mean field continuum models for first order liquid-liquid demixing and solid-liquid phase transitions and show how the Maxwell construction at phase coexistence emerges on going from finite-size closed systems to the thermodynamic limit [1]. The theories considered are the Cahn-Hilliard model of phase separation, which is also a model for the liquid-gas transition, and the phase field crystal model of the solid-liquid transition. Our results show that states comprising the Maxwell line depend strongly on the mean density with spatially localized structures playing a key role in the approach to the thermodynamic limit. [1] U. Thiele et al., New J. Phys., at press (2019), doi: 10.1088/1367-2630/ab5caf.

DY 24.10 Tue 12:00 ZEU 160

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

Controlling the flow patterns of viscoelastic fluids is extremely challenging due to their inherent non-linear and time-dependent properties. These complex fluids exhibit transitions from laminar to turbulent flows, which is useful for heat and mass transport in liquids at the micron scale [1], whereas in Newtonian fluids transport is dominated by diffusion. Turbulent viscoelastic flows show similar properties as their counterparts in Newtonian fluids[1,2] and consequently the observed flow pattern is called *elastic turbulence* [1]. It occurs in shear flow for increasing Weissenberg number Wi, the product of polymer relaxation time and shear rate.

Numerically solving the Oldroyd-B model in a two-dimensional Taylor-Couette geometry, we have identified and described the supercritical transition to turbulent flow at a critical Weissenberg number [2]. Here, we demonstrate that elastic turbulence can be controlled by a time-modulated shear rate. The order parameter measuring the strength of turbulence continuously goes to zero with increasing modulation frequency or Deborah number De. It ultimately vanishes via a supercritical transition, where flow then becomes laminar. Moving closer to the critical Weissenberg number, smaller modulation frequencies are sufficient to induce laminar flow.

[1] A. Groisman and V. Steinberg, Nature **405**, 53 (2000).

[2] R. Buel, C. Schaaf, H. Stark, Europhys. Lett. **124**, 14001 (2018).

DY 24.11 Tue 12:15 ZEU 160

Universal properties of creep flow — •Marko Popović[1], Tom de Geus[1], Wencheng Ji[1], Alberto Rosso[2], and Matthieu Wyart[1] — [1]Institue of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]LPTMS, CNRS, Univ.Paris-Sud, Universite Paris-Saclay, 91405 Orsay, France

Amorphous solids, such as atomic glasses, colloidal suspensions, granular matter or foams, begin to deform plastically when exposed to external stress Σ. Steady state flow of these materials in absence of thermal fluctuations is usually described as $\dot{\epsilon} \sim (\Sigma - \Sigma_c)^\beta$ for stresses above critical stress Σ_c and vanishes below it, while in presence of thermal fluctuations flow persists below Σ_c but is exponentially suppressed. The transient plastic deformation, called creep flow, is much

less understood despite its importance in practical applications. Creep flow often displays a power-law decay in time $\dot{\epsilon} \sim t^{-\mu}$ after which it can either arrest or eventually yield at fluidisation time τ_f. In recent years various numerical values and/or laws have been suggested for the exponent μ and time τ_f in particular experimental or numerical studies. We propose that mechanism underlying creep flow is the same as that of the steady state flow, which allows us to predicts parameters μ and τ_f of creep flow in terms of the steady state flow parameters, both in athermal and thermally activated systems. We successfully tested all our predictions using different mesoscopic elasto-plastic models of amorphous solids and found them to be consistent with published experimental results.

DY 24.12 Tue 12:30 ZEU 160

Formation of networks from attractive particles under shear — •Sebastian Bindgen[1], Dieter Diels[1], Pierre de Buyl[2], Joost de Graaf[3], and Erin Koos[1] — [1]Department of Chemical Engineering, KU Leuven, Celestijnenlaan 200f - box 2424, 3001 Leuven, Belgium — [2]Institute for Theoretical Physics, KU Leuven, Celestijnenlaan 200d - box 2415, 3001 Leuven, Belgium — [3]Institute for Theoretical Physics, Utrecht University, Princetonplein 5, 3584 CC Utrecht, The Netherlands

Simulations give access to physical quantities at the particle-level, which are not readily accessible via experimental techniques. Lees-Edwards boundary conditions replicate in-vitro conditions and have seen significant use in the polymer community. We have implemented and tested a version of this algorithm in the MD simulation package ESPResSo. The implementation, which is based on pair-wise thermostating using the dissipative particle dynamics technique, can also mimic non-linear effects such as shear banding. We demonstrate that our implementation captures the enhanced diffusion of particles coupled to the fluid. Furthermore, we use our implementation to study the dynamic properties of depletion gels including their formation and breakup under shear flow. Recent investigations have shown that hydrodynamics affects the time scales on which these gels form under quiescence, while leaving the final structure unaltered. We aim to show these processes under dynamic conditions. Our study is of clear interest for industrial systems such as ink or pastes as they can experience various complex flow fields during processing and application.

DY 24.13 Tue 12:45 ZEU 160

Tactoids, membranes and fribrils – finite assemblies of rod-like particles — •Anja Kuhnhold, Nils Göth, Nadja Helmer, Victor Tänzel, and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Systems composed of rod-like particles and spherical depleting agents show a variety of self-assembled shapes and structures. We discuss a few of them and present corresponding Monte Carlo simulation results. The model system ingredients are hard spherocylinders as rod-like component and implicit Asakura-Oosawa spheres as depletants. In addition we study the effect of a chiral pair interaction between the rods.

This work got inspired by experiments using viruses as rod-like particles and polymer coils as depleting agents, see e.g. [1,2]. The monodispersity of viruses makes them a nice model system to compare simulations to. Beyond the comparison simulation results can be used to direct the self-assembly for specific structure-function relationships, e.g. templating or sensing.

[1] T. Gibaud, J. Phys.: Condens. Matter **29**, 493003 (2017).
[2] B. Sung et al., Soft Matter **15**, 9520 (2019).

DY 25: Interfaces and Thin Films II (joint session CPP/O/DY)

Time: Tuesday 9:30–13:00 Location: ZEU 260

Invited Talk DY 25.1 Tue 9:30 ZEU 260

Phospholipid membranes as model systems for fundamental soft matter research — •Sebastian Jaksch — Forschungszentrum Jülich GmbH Jülich Centre for Neutron Science, Garching, Germany

Phospholipid membranes play an important role as interfaces in virtually all biological systems. By their interplay between structure and dynamics they provide the basic functions necessary to support living organisms, such as stability for the cells and trans-membrane transport for nutrients and drugs. Using SoyPC as an example, this presentation will give an overview of grazing incidence neutron techniques for structure and dynamics measurements of phospholipid membranes.[1] We investigated the structure with grazing incidence small-angle neutron scattering (GISANS) at extremely low background conditions [2] and correlated that data with grazing incidence neutron spin-echo spectroscopy [3] (GINSES). These investigations revealed thermally excited modes in the plane of the membrane and its corresponding structures. This modes could be frozen in at temperatures below room temperature and reappeared after reheating to physiological temperatures.

[1] Jaksch, S., Gutberlet, T., Müller-Buschbaum, P. (2019). Grazing Incidence Scattering - Status and Perspectives in Soft Matter and Biophysics. Current Opinion in Colloid & Interface Science.

[2] Jaksch, S., et al. (2019). Long-range excitations in phospholipid membranes. Chemistry and physics of lipids, 225, 104788.

[3] Jaksch, S., et al. (2017). Nanoscale rheology at solid-complex fluid interfaces. Scientific reports, 7(1), 4417.

DY 25.2 Tue 10:00 ZEU 260

Brownian motion in near-surface pressure driven flows with 3D-nanometric spatial resolution — •Joshua McGraw[1], Alexandre Vilquin[1,2], Pierre Soulard[1], Vincent Bertin[1], Gabriel Guyard[1,2], David Lacoste[1], Elie Raphael[1], Frederic Restagno[2], and Thomas Salez[3] — [1]ESPCI Paris — [2]Université Paris Sud — [3]Université de Bordeaux

In near-surface flows, interfaces play a major role by imposing (typically) no-slip boundary conditions, greatly reducing the fluid velocity compared to the central part of a channel. With total internal reflection fluorescence (TIRF), a flow is illuminated with an evanescent field decaying over a few hundred nanometers into the channel; this decay allowing a determination of nanoparticle altitudes. Combined with particle tracking, experimental determination of the velocity profile and local velocity distributions in three dimensions are possible. Here we present a detailed look at the statistics of near-surface particle motions in pressure-driven water for which diffusion is important compared to advection. The distribution of displacements in the invariant flow direction is Gaussian as for normal diffusion. Significant anomalies are however observed for both of the other spatial dimensions. Combining experiments and simulations, we disentangle contributions from so-called Taylor-Aris dispersion, nanoparticle polydispersity and the optical measurement system. This description of TIRF allows for the study of many Brownian motion problems, such as near-surface polymer solution dynamics or particle motion near soft boundaries.

DY 25.3 Tue 10:15 ZEU 260

Relation between stability and interfacial structure of polyelectrolyte containing foam films — •Larissa Braun and Regine von Klitzing — TU Darmstadt, Darmstadt, Germany

For many industrial applications foams of oppositely charged polyelectrolyte/surfactant-mixtures are of high impact, as they form surface active complexes.

Extensive research on such mixtures was already performed[1,2] but the influence of the ionic strength is still unclear.

This work focuses on the influence of added LiBr on foam films of mixtures of the anionic polyelectrolyte $sPSO_2$-220 (similar to PSS but stiffer) with the cationic surfactant $C_{14}TAB$. Therefore, disjoining pressure isotherms were measured with a fixed $C_{14}TAB$ concentration and a variable polyelectrolyte concentration.

Different stability regimes were identified. Already a low salt concentration of 10^{-4} M leads to a considerably less stable foam films regarding the maximum disjoining pressure. An unexpected formation of an unstable Newton Black Film was found at this low salt concentration. Higher salt concentrations will also be considered. These findings will be correlated with the surface excesses of both compounds which can be separated from each other by neutron reflectometry measurements.

[1] N. Kristen, A. Vüllings, A. Laschewsky, R. Miller, R. v. Klitzing, Langmuir, 2010, 12, 9321-9327. [2] M. Uhlig, R. Miller, R. v. Klitzing, Phys. Chem. Chem. Phys., 2016, 18, 18414-18423

DY 25.4 Tue 10:30 ZEU 260

Near-surface dynamics of semidilute polymer solutions: dif-

fusion, nonlinear rheology, and the hydrodynamic boundary condition — •Gabriel Guyard[1,2], Alexandre Vilquin[1,2], Frederic Restagno[2], and Joshua McGraw[1] — [1]ESPCI Paris — [2]Université Paris Sud

The near-surface dynamics of polymer solutions challenge both experimental and theoretical efforts – especially in the case of semi-dilute solutions for which chains overlap – yet evanescent wave microscopy allows for the characterization of such interfacial flows. Here we report molecular-size-resolution particle motions in microfluidic channels for pressure-driven flows of semidilute polymer solutions. The results using polymer-free water are in good agreement with Stokes-flow hydrodynamic and diffusive theory. Experiments using polyacrylamide at different volume fractions close to and above the overlap concentration are done in the same chips as for the water experiments. In contrast to Newtonian fluid behaviour, the shear-rate/pressure drop relation is non-linear for the polymer solution flows, suggesting nanometrically-resolved, shear-thinning effects, accompanied with a non-trivial hydrodynamic boundary condition. The diffusive motion of the tracer particles is also distinguished from that of the water experiments, and such motions detailed here. These results set the basis for a study of near-wall hydrodynamic flow and diffusion in complex fluids, notably including semidilute polymer solutions.

DY 25.5 Tue 10:45 ZEU 260

AFM Force-Distance-Curves on Different Lubricants — •Sebastian Friedrich and Brunero Cappella — Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, D-12205 Berlin

AFM force-distance-curves have been recorded on thin films of nine different lubricant liquids. Those lubricants wet the AFM-tip, which causes a capillary force. This force depends on the tip shape, as well as on liquid properties like surface tension, contact angle, and viscosity. Those liquid properties have been measured independently with other methods, so their influence on the shape of the force-distance-curves can be discussed. This study provides a tool for the characterization of thin lubricant films and contributes to the understanding of tribology on the nanoscale.

DY 25.6 Tue 11:00 ZEU 260

Revealing the formation of sputter deposited copper nanolayers on functional polymer thin films for lithium-ion batteries — •Simon J. Schaper[1], Franziska C. Löhrer[1], Senlin Xia[1], Matthias Schwartzkopf[2], Pallavi Pandit[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2,4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, Photon Science, 22607 Hamburg — [3]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel — [4]KTH, Department of Fibre and Polymer Technology, 100 44 Stockholm, Sweden

Understanding the interface between metals, commonly used as current collectors, and ion-conducting polymers used in polymer lithium-ion batteries (LIBs) is crucial to develop highly reproducible, low-cost and reliable devices. To address these issues, sputter deposition is the technique of choice to fabricate scalable, reproducible and controllable nanometer and sub-nanometer metal layers on polymer thin films. The sputter deposition process, being well understood and controlled, offers advantages over chemical methods to tailor metal thin-film morphologies on the nanoscale and offers a superior adhesion of the deposited material. We use in-situ grazing incidence small angle X-ray scattering (GISAXS) to investigate the formation, growth and, self-assembled structuring of copper on polymer thin films and composites used in LIBs. The growth of copper on polymer thin films is described based on a model approach.

15 min. break

DY 25.7 Tue 11:30 ZEU 260

Insight into ion transport across polypyrrole-electrolyte interfaces by in situ X-ray reflectivity and electrochemistry — •Pirmin H. Lakner[1,2], Manuel Brinker[3], Christoph Seitz[1], Sergey Volkov[1], Patrick Huber[3], and Thomas F. Keller[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Physics Department, Universität Hamburg, Germany — [3]Institute of Materials Physics and Technology, Technische Universität Hamburg-Harburg, Germany

Polypyrrole (PPy) is a conducting polymer with actuatoric and pseudocapacitive properties due to potential-induced ion incorporation/expulsion. Electrical potentials were applied to a perchlorate-doped PPy thin film ($\sim$ 30 nm) in an aqueous perchloric acid electrolyte and the associated changes in thickness and electron density were recorded by X-ray reflectivity (XRR). Assuming a sole perchlorate anion transfer carrying 50 electrons, a ratio of 50:1 is expected between electrons crossing the PPy-substrate interface and electrons crossing the electrolyte-PPy interface. By correlating the XRR data and the electrochemical data, a ratio of 10:1 was obtained, which indicates that water movement takes place as an anion counter-flow. The recorded low strain-charge coefficient supports this assumption. One explanation is the high stability and the low porosity of the PPy film due to its fast potentiodynamic deposition method. The properties of the analyzed PPy film make it a suitable choice for supercapacitor applications.

DY 25.8 Tue 11:45 ZEU 260

Revealing Lithium Transport Processes in Lithium-Ion Battery Anodes Using Neutron Depth Profiling — •Markus Trunk[1,2], Fabian Linsenmann[3], Philip Rapp[3], Jamie Weaver[4], Lukas Werner[1], Roman Gernhäuser[1], Ralph Gilles[2], Bastian Märkisch[1], Zsolt Revay[2], and Hubert Gasteiger[3] — [1]TUM, Physik-Department, Garching — [2]TUM, Heinz Maier-Leibnitz Zentrum, Garching — [3]TUM, Lehrstuhl für Technische Elektrochemie, Chemie Department, Garching — [4]Material Measurement Laboratory, NIST, Gaithersburg, Maryland

Neutron Depth Profiling (NDP) is a non-destructive, isotope-specific, high-resolution nuclear analytical technique, which is often used to probe lithium or boron concentration profiles in different thin substrates. NDP provides depth sensitivities up to a few ten nanometers and the maximum viewing depth is limited to tens of micrometers. The non-destructive nature of the measurement is of special interest for lithium-ion batteries, where the lithium transport processes can be studied during operation. However, due to the limited viewing depth a special battery cell design is required, which is transparent for the charged particles while ensuring an undisturbed battery performance even at low ambient pressures. We present NDP measurements on lithium-ion batteries performed using a newly developed cell design and discuss insights into the lithium transport processes occurring in the anode material during battery operation.

DY 25.9 Tue 12:00 ZEU 260

Comparison of the effects of solvent additives on the morphology development of printed PPDT2FBT:PC71BM films — •Dan Yang[1], Sebastian Grott[1], Xinyu Jiang[1], Kerstin S. Wienhold[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1,3] — [1]TU München,Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Lichtenbergstr. 1, 85748 Garching, Germany

The morphology and crystallinity of bulk heterojunction (BHJ) films have profound effects on the performance of organic photovoltaics. Currently, most morphological studies on BHJ films are based on spin-coating as deposition technique. However, to commercialize organic photovoltaic products, large-scale fabrication processes such as printing must be taken into consideration. In the present study, the effects of solvent additives on the morphology formation and polymer crystallinity growth of printed BHJ films are investigated by in-situ grazing incidence small/wide-angle X-ray scattering (GISAXS/GIWAXS). The results show that the solvent additives with different boiling points lead to different film drying behaviors, and the phase demixing is changing in the forming BHJ film along with solvent evaporation. These findings provide valuable insights into the film morphology and crystallinity developments of printed BHJ films, which determines the future design of BHJ film printing for large-scale fabrication.

DY 25.10 Tue 12:15 ZEU 260

Functionalization of Metalloxid surfaces with Porphyrins — •Klaus Götz[1,2], Annemarie Prihoda[1,2], and Tobias Unruh[1,2] — [1]Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, Staudtstr. 3, 91058 — [2]Interdisziplinäres Zentrum für Nanostrukturierte Filme, Cauerstr. 3, 91058 Erlangen

Porphyrins are widely studied for their use as catalysts and in dye sensitized solar cells. In these systems the porphyrins are bound to metal oxide surfaces as a functionalizing layer.

We study the binding mechanism in the porphyrin - metal oxide interface on TiO_2 and Co_3O_4. Special emphasis of our work is focused on the exchange process of organic stabilizing molecules with porphyrins. This process is studied using a variation of different scattering techniques. The talk will focus on the characterization of the exchange reaction on the surface of nanoparticles.

Therefore, the combination of small angle x-ray and neutron scattering (SAXS and SANS) experiments will be a key element. These measurements are well suited to study core/shell systems. X-rays interact mainly with electrons and therefore SAXS yields information about the inorganic core of the nanoparticles. Neutrons on the other hand are very sensitive to hydrogen and therefore SANS is well suited to get information about the organic stabilizer shell.

The talk will focus on SAXS/SANS measurements and give an overview over complimentary technique. Furthermore, their usage in the characterization of the morphology of the produced particles and the ligand exchange to porphyrins will be presented.

DY 25.11 Tue 12:30 ZEU 260

Atomistic modelling of confined molecules between atomically flat surfaces — •Jose D. Cojal Gonzalez and Jürgen P. Rabe — Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

The contact interface created between an atomically flat cleavage plane of a layered crystal and a 2D material forms a flexible slit or nano pore which can be occupided by (macro)molecules. This arrangement offers a versatile platform for the study of structural, vibrational, elastic and electrical properties of those highly confined molecules. Using molecular dynamics simulations of a graphene-mica slit pore filled with small solvent molecules such as water and ethanol, we provide an instructive model to establish structure and dynamics, i.e. nature and interactions of the molecular layers, mica and graphene. Furthermore, it provides the first step towards the incorporation of larger molecules, such as Rhodamine 6G and dendronized polymers (denpols) in order to complement and better understand the results obtained from Raman spectroscopy and scanning force microscopy measurements.

DY 25.12 Tue 12:45 ZEU 260

Exploring the Resistive Switching Properties of HfO2 Nanoparticle Assemblies — •Sonam Maiti[1], Chen Liu[1], Thorsten Ohlerth[2], Ulrich Simon[2], and Silvia Karthäuser[1] — [1]Peter Grünberg Institut (PGI-7), Forschungszentrum Jülich GmbH, Germany — [2]Institute of Inorganic Chemistry (IAC), RWTH Aachen University, Germany

Hafnium oxide nanocrystals (NCs) can be considered as possible candidates for further miniaturization of future resistive random access memories. The switching properties of NC assemblies remain underexplored due to difficulties in fabricating ordered structures. Here, we use a facile, low-cost method to prepare highly ordered assemblies of 6 nm HfO2 NCs capped with TOPO via evaporation based self-assembly. X-ray photoelectron spectroscopy is applied to investigate the oxidation state of near surface HfOx under various conditions. Electrical transport measurements were performed on devices with micrometer and nanometer sized gaps to determine the resistive switching character of NCs arrays. They enable the observation of cyclic voltammograms with redox reaction peaks when used with micrometer sized gaps. We discuss the electronic properties of these devices in the light of varying contributions of electronic vs ionic transport and highlight the effect on the device stability. We especially focus on the resistive switching behaviour of the NP assemblies which is dependent on the oxygen vacancy formation under the influence of the capping ligand.

DY 26: Brownian Motion, Transport and Anomalous Diffusion

Time: Tuesday 10:00–13:15 Location: HÜL 186

DY 26.1 Tue 10:00 HÜL 186

Topological solitons driven through grain boundaries — •Xin Cao[1], Emanuele Panizon[1,2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy

Topological solitons, or kinks, widely exists in materials and at interfaces. They play important roles in the elastic deformation of metals and alloys and in the mobility of nano contacts. Here, by driving such solitons through grain boundaries in colloidal crystals, we study the influence of such boundaries to the dynamics of solitons. We show that when small solitons are travelling through the grain boundaries, their motion is delayed at the grain boundary with the delay time depending on the driving force. In contrast large extended solitons are splitted upon approaching grain boundaries. Afterwards they split into several smaller solitons due to variations in the delay times at different regions of the grain boundary. At small driving forces, solitons are not able to cross grain boundaries which leads to their accumulation (pile up) at these locations. In addition to the time delay, splitting and pile up of solitons, we also found that the grain boundary can reflect incoming solitons when driving forces are parallel to the grain boundary. Such reflections strongly depend on the mismatch of lattice orientations at the grain boundary and can be used for the controlled guiding of solitons.

DY 26.2 Tue 10:15 HÜL 186

Transport and Constrictivity in Porous Media — •Johannes Hauskrecht and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

Geometric quantities such as porosity and physical quantities such as permeability determine transport in porous media. The constrictivity, on the other hand, which is intended to describe the influence of cross-sectional variations of the pore space on transport, is a less-used quantity. It is therefore an interesting question whether transport in porous media can be characterized additionally with the help of this quantity.

Existing definitions of constrictivity from the literature and their relation to the macroscopic transport coefficients have been investigated. In general, they can be divided into physical and geometrical definitions. The physical definitions directly relate the constrictivity to the transport coefficients, the geometrical definitions, on the other hand, calculate the constrictivity directly from the pore structure. However, most of the geometrical definitions are only defined for simplified models of the pore space and are ill defined for general pore spaces. In addition, it is shown for homogeneous and isotropic media that the existing geometrical definitions of constrictivity can be expressed as a variation of porosity.

DY 26.3 Tue 10:30 HÜL 186

Heterogeneous diffusion with(out) stochastic resetting — •Trifce Sandev[1,2,3], Viktor Domazetoski[1], Aleksei Chechkin[2,4], Ljupco Kocarev[1,3], and Ralf Metzler[2] — [1]Macedonian Academy of Sciences and Arts — [2]University of Potsdam — [3]Ss. Cyril and Methodius University in Skopje — [4]Akhiezer Institute for Theoretical Physics, Kharkov

We analyze diffusion processes with finite propagation speed in heterogeneous media in terms of the telegrapher's or Cattaneo equation with position-dependent diffusion coefficient. In the diffusion limit of infinite-velocity propagation we recover the results for diffusion equations with position-dependent diffusivity. We observe various diffusive regimes including hyperdiffusion, ballistic motion, superdiffusion, normal diffusion and subdiffusion. We further consider heterogeneous diffusion process under stochastic resetting. We find exact results for the mean squared displacement and the probability density function for three different stochastic interpretations of the multiplicative process. The stationary distributions reached in the long time limit are derived as well. The obtained results are verified by numerical simulations employing the Langevin equation with position dependent diffusivity in different stochastic calculi.

DY 26.4 Tue 10:45 HÜL 186

Cooperatively enhanced reactivity and stabilitaxis of dissociating oligomeric proteins — •Jaime Agudo-Canalejo[1], Pierre Illien[2], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), D-37077 Göttingen, Germany — [2]Sorbonne Université, CNRS, Laboratoire PHENIX, UMR CNRS 8234, 75005 Paris, France — [3]Rudolf Peierls Centre for Theo-

retical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Many functional units in biology, such as enzymes or molecular motors, are composed of several subunits that can reversibly assemble and disassemble. This includes oligomeric proteins composed of several smaller monomers, as well as protein complexes assembled from a few proteins. By studying the generic spatial transport properties of such proteins, we investigate here whether their ability to reversibly associate and dissociate may confer them a functional advantage with respect to nondissociating proteins. In uniform environments with position-independent association-dissociation, we find that enhanced diffusion in the monomeric state coupled to reassociation into the functional oligomeric form leads to enhanced reactivity with distant targets. In non-uniform environments with position-dependent association-dissociation, caused e.g. by spatial gradients of an inhibiting chemical, we find that dissociating proteins generically tend to accumulate in regions where they are most stable, a process that we term 'stabilitaxis'.

DY 26.5 Tue 11:00 HÜL 186

Influence of fractional hydrodynamic memory on superdiffusion and supertransport in tilted washboard potentials — •Igor Goychuk — Friedrich-Alexander Universität Erlangen-Nürnberg — Universität Augsburg, Germany

Diffusion in tilted washboard potentials can paradoxically exceed free normal diffusion [1]. The effect becomes much stronger in the underdamped case due to inertial effects [2]. What happens upon inclusion of usually neglected fractional hydrodynamics memory effects (Basset-Boussinesq frictional force), which result in a heavy algebraic tail of the velocity autocorrelation function of the potential-free diffusion making it transiently superdiffusive? Will a giant enhancement of diffusion become even stronger, and the transient superdiffusion last even longer? These are the basic questions which we answer [3] based on an accurate numerical investigation. We show that a resonance-like enhancement of normal diffusion becomes indeed much stronger and sharper. Moreover, a long-lasting transient regime of superdiffusion, including Richardson-like diffusion, $\langle \delta x^2(t) \rangle \propto t^3$ and ballistic supertransport, $\langle \delta x(t) \rangle \propto t^2$, is revealed.
[1] P. Reimann, C. Van den Broeck, H. Linke, P. Hänggi, J. M. Rubi, and A. Perez-Madrid, Phys. Rev. Lett. **87**, 010602 (2001).
[2] I. G. Marchenko and I. I. Marchenko, EPL **100**, 50005 (2012); B. Lindner and I. M. Sokolov, Phys. Rev. E **93**, 042106 (2016).
[3] I. Goychuk, Phys. Rev. Lett. **123**, 180603 (2019), Editors' Suggestion.

DY 26.6 Tue 11:15 HÜL 186

Hydrodynamics of Active Levy Matter — Andrea Cairoli and •Chiu Fan Lee — Imperial College, London, U.K.

Collective motion emerges spontaneously in many biological systems such as bird flocks, insect swarms and tissue under dynamic reorganization. This phenomenon is often modeled within the framework of active fluids, where the constituent active particles, when interactions with other particles are switched off, perform normal diffusion at long times. However, single-particle superdiffusion and fat-tailed displacement statistics are also widespread in biology. The collective properties of interacting systems exhibiting such anomalous diffusive dynamics – which we call active Levy matter – cannot be captured by current active fluid theories. Here, we formulate a hydrodynamic theory of active Levy matter by coarse-graining a microscopic model of aligning polar active particles performing superdiffusive Levy flights. We then perform a linear stability analysis at the onset of collective motion and find that in contrast to its conventional counterpart, the order-disorder transition can become critical. We further support our analytical predictions with simulation results. This work not only highlights the need for more realistic models of active matter integrating both anomalous diffusive motility and inter-particle interactions, but also potentially enriches the universal properties of active systems.

15 min. break.

DY 26.7 Tue 11:45 HÜL 186

Subdiffusion in the Anderson model on random regular graph — •Giuseppe De Tomasi[1], Soumya Bera[2], Antonello Scardicchio[3], and Ivan Khaymovich[4] — [1]TUM Munich/Cambridge University — [2]IIT Bombay — [3]ICTP Trieste — [4]MPIPKS Dresden

We study the finite-time dynamics of an initially localized wave-packet in the Anderson model on the random regular graph (RRG) and show the presence of a subdiffusion phase coexisting both with ergodic and putative non-ergodic phase. The full probability distribution $\Pi(x,t)$ of a particle to be at some distance x from the initial state at time t, is shown to spread subdiffusively over a range of disorder strengths. The comparison of this result with the dynamics of the Anderson model on Z^d lattices, $d > 2$, which is subdiffusive only at the critical point implies that the limit $d \to \infty$ is highly singular in terms of the dynamics. A detailed analysis of the propagation of $\Pi(x,t)$ in space-time (x,t) domain identifies four different regimes determined by the position of a wave-front $X_{\mathrm{front}}(t)$, which moves subdiffusively to the most distant sites $X_{\mathrm{front}}(t) \sim t^{\beta}$ with an exponent $\beta < 1$.

DY 26.8 Tue 12:00 HÜL 186

Entropic contribution to surface diffusion barriers of oligophenyls — •Mila Miletic[1], Karol Palczynski[1,2], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, Freiburg, Germany

Surface diffusion is usually described by Arrhenius laws, with a diffusion energy barrier in the exponent and a prefactor. The prefactor contains not only the jump length and attempt frequency but also contributions of the system's entropy to the diffusion. However, the decomposition into these three contributions is often unclear, which hampers the interpretation of the prefactor. We successfully perform such a decomposition for single oligophenyl molecules of different length on an amorphous silica surface using atomistic molecular dynamics simulations, and find meaningful values for the jump length, attempt frequency and entropy of the adsorbates. We systematically increase the molecular length, from a single phenyl ring, up to six phenyl rings and study the influence of the increase in length on surface diffusion and binding. First, we find a substantial difference in entropy of about one order of magnitude between the shortest and longest adsorbates and entropy contributions to the diffusion barrier of about 20-30%. Second, as for the binding to the surface, we find that longer molecules display higher binding free energies with substantial entropic contributions coming from the increase in internal degrees of freedom with the molecular length. Our results demonstrate that it is essential for investigations of surface diffusion to consider entropic effects.

DY 26.9 Tue 12:15 HÜL 186

A finite-radius stochastic action — •Julian Kappler and Ronojoy Adhikari — Department of Applied Mathematics and Theoretical Physics, Cambridge University, Cambridge, United Kingdom

A fundamental question associated with Langevin dynamics is to quantify the (relative) probability of individual trajectories. Due to the singular nature of an individual stochastic trajectory, quantifying its probability is both technically challenging, and the result is not directly related to any physical observable. We regularize the singular concept of an individual trajectory by considering the tubular ensemble, which consists of all stochastic trajectories that remain within a ball of small but finite radius, and with moving center given by a smooth reference path. We derive the finite-radius generalization of the Onsager-Machlup stochastic action, characterize explicitly the stochastic dynamics within the tubular ensemble, and generalize the well-known single-trajectory entropy to the tubular ensemble. Our work thus establishes the finite-radius tubular ensemble as a useful extension of a single stochastic trajectory. In particular, introducing a finite threshold distance in the discussion of path probabilities, and relating experimental observables to the Onsager-Machlup action, brings the latter within reach of direct measurement.

DY 26.10 Tue 12:30 HÜL 186

Infinite-densities and the Moses, Noah and Joseph effects in Levy walks — •Erez Aghion[1], Vidushi Adlakha[2], Kevin Bassler[2], Holger Kantz[1], and Philipp Meyer[1] — [1]mpiPKS, Dresden, Germany — [2]U. Huston, Dep. of Physics, USA

When one is presented with an ensemble of data sets, each obtained as a time series, for example in an experiment, which anomalous diffusion, it is often not possible to know exactly the details of the underlying dynamics that produced it. The braking of the CLT can be decomposed into three root causes: temporal correlations in the process, statistical aging, and power-law distributions, known respectivley as the Joseph, Moses and Noah effects. These effects, are quantified individually, and measured individually from the time series.

We study this decomposition using numerical simulations, which are compared with analytical results, for a coupled Levy walk model,

where the particle's velocity v at each step is decays nonlinearly with the step-duration Tau. The step durations are independent, identically distributed random variables, taken from the fat tailed distribution where the mean <Tau> is divergent. Here, recently it was shown [Akimoto et al., 2019] that the velocity distribution of the particles converges to a non-normalizable infinite-invariant density, when t approaches infinity. This scenario is tantamount to a sort-of "temporal equilibrium", when we rescale the probability density properly with time. We study how this leads to a different manifestation of the three effects, depending on whether infinite-ergodic theory describes the time-average of |v| or v^2.

DY 26.11 Tue 12:45 HÜL 186

Hydrodynamic resistance matrices of colloidal particles with various shapes* — Johannes Voss and •Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

The hydrodynamic resistance matrix encodes the shape- and size-dependent hydrodynamic properties of a colloidal particle that is suspended in a liquid. It determines the particle's diffusion tensor and is typically needed when modeling the motion of purely Brownian, externally driven, or self-propelled colloidal particles or the behavior of dilute suspensions of such particles on the basis of Langevin equations, Smoluchowski equations, dynamical density functional theory, or other appropriate methods. So far, however, the hydrodynamic resistance matrix is available only for selected particle shapes. In this talk, we present and compare the hydrodynamic resistance matrices for various additional particle shapes that are relevant for current research, including apolar and polar as well as convex and partially concave shapes. The elements of the hydrodynamic resistance matrices are given as functions of shape parameters like the aspect ratio of the corresponding particle so that the results apply to continuous sets of particle shapes. This opens up new possibilities for studying the dynamics of colloidal particles with anisometric and even variable shapes. **Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

DY 26.12 Tue 13:00 HÜL 186

Hot Brownian Motion in the Ballistic Timescale — •Xiaoya Su[1], Alexander Fischer[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 times. Yet, the ballistic 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 5ns. We show how the mean squared displacement of the particle from the nanoseconds to the seconds 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 27: Statistical Physics II

Time: Tuesday 10:00–11:30 Location: ZEU 118

DY 27.1 Tue 10:00 ZEU 118

Fractional Diffusion Equation - Derivation and Numerical Approach — •Philipp Roth and Igor M. Sokolov — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, D-12489 Berlin

We consider the continuous limit of a lattice continuous time random walk (CTRW) scheme with power-law waiting-time probability density function (WTD) with position-dependent parameters leading to a variable-order time-fractional diffusion equation. Two different situations are discussed, the ones corresponding to abrupt and to continuous changes of the parameters of the WTD. In the first case we derive the matching conditions for the solutions on the border of two subdiffusive media. In the second case we provide the solution for the case of linearly changing exponent in the WTD. We moreover present a numerical method for the solution of such equations based on the Laplace representation and the Laplace inversion using the Gaver-Stehfest algorithm, and compare our analytical solution with numerical results.

DY 27.2 Tue 10:15 ZEU 118

Kinetic proofreading of epigenetic patterns — •Bahareh Kiani[1], Fabrizio Olmeda[2], and Steffen Rulands[3] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

During early development, the assignment of cellular identities is closely associated with the acquisition of epigenetic marks on the DNA (DNA methylation). Aberrations in the spatial arrangement of these patterns along the sequence of the DNA lead to the death of the embryo and, in adulthood, are one of the hallmarks of cancer. How, despite the limits imposed by thermodynamics, epigenetic information is precisely encoded along the DNA sequence remains to be understood. Here, we show that the paradoxical co-expression of antagonistic players in the DNA methylation machinery provides an ATP-dependent kinetic proof-reading mechanism which enhances specificity and sensitivity of these patterns by orders of magnitude. We characterise the range of possible behaviours and define optimality conditions of such a mechanism. Finally, by drawing on single-cell sequencing experiments we establish the biological significance of proofreading. Our work highlights the importance of collective, non-equilibrium processes in the establishment of epigenetic marks and sheds new lights on the epigenetic regulation of cell fate decisions in early development.

DY 27.3 Tue 10:30 ZEU 118

Interfaces: A step beyond the elastic approximation — •Nirvana Caballero and Thierry Giamarchi — University of Geneva

Diverse systems including ferroic domain walls, cell fronts, or contact lines have been usually described as disordered elastic systems, even when critical hypotheses of the theory are not satisfied. Solving domain walls dynamics and statics beyond the elastic approximation is still a largely open theoretical/analytical problem. In this work, we propose to address it by analyzing a Ginzburg-Landau model, which describes the main dynamics of driven systems and where interfaces with bubbles and overhangs can be studied. We show the connection between the two-dimensional Ginzburg-Landau model and the one-dimensional elastic description for disordered systems and probe the validity of the elastic theory as a function of "defects". We examine observables such as the interface roughness and the structure factor, both numerically and analytically. Our simulations and calculations, in addition to making contact with experiments, allow to test and provide insight to develop new analytical approaches to this problem.

DY 27.4 Tue 10:45 ZEU 118

General solution to the one-dimensional connectivity problem — Fabian Coupette, •Andreas Härtel, and Tanja Schilling — Institut of Physics, University of Freiburg, Germany

We present a general method to obtain the connectivity properties of an arbitrary one-dimensional pairwise interacting n-body system in thermal equilibrium. As input, solely the pair density distribution associated to the equilibrium state is required. Accordingly, if exact analytic results exist for the pair density distribution, the pair connectivity can be determined equally exactly. This is illustrated for fully penetrable and impenetrable rods as well as a repulsive 1/r^2

nearest-neighbor interaction potential. We also discuss implications of our work for long-ranged interactions, systems in external fields and higher dimensions.

DY 27.5 Tue 11:00 ZEU 118

Universality of photon counting below a bifurcation threshold — •Lisa Arndt and Fabian Hassler — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

At a bifurcation point, a small change of a system's parameter causes a qualitative change in the dynamics of the system. This behavior can, for example, be observed in a parametrically driven system or in a laser. In both systems, the driving strength needs to exceed a threshold before classical radiation is produced. We study the photon counting statistics below the instability threshold, where quantum fluctuations enable the emission of photons. Close to the bifurcation point, these fluctuations are determined by the instability threshold. Here, we focus on one-dimensional bifurcations and provide deeper insight into the universal behavior of the photon counting statistics in different physical systems.

DY 27.6 Tue 11:15 ZEU 118

Pearl-Necklace-Like Local Ordering Drives Polypeptide Collapse — •Suman Majumder[1], Ulrich H.E. Hansmann[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany — [2]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma 73019, USA

The collapse of the polypeptide backbone is an integral part of protein folding. Using polyglycine as a probe, we explore the nonequilibrium pathways of protein collapse in water. We find that the collapse depends on the competition between hydration effects and intrapeptide interactions. Once intrapeptide van der Waal interactions dominate, the chain collapses along a nonequilibrium pathway characterized by formation of pearl-necklace-like local clusters as intermediates that eventually coagulate into a single globule. By describing this coarsening through the contact probability as a function of distance along the chain, we extract a time-dependent length scale that grows in a linear fashion. The collapse dynamics is characterized by a dynamical critical exponent $z \approx 0.5$ that is much smaller than the values of $z = 1 - 2$ reported for nonbiological polymers. This difference in the exponents is explained by the instantaneous formation of intrachain hydrogen bonds and local ordering that may be correlated with the observed fast folding times of proteins.

DY 28: Pattern Formation and Reaction-Diffusion Systems

Time: Tuesday 10:00–12:30 Location: ZEU 147

DY 28.1 Tue 10:00 ZEU 147

Calculating Coexistence in a two-field Phase-Field-Crystal model — •Max Philipp Holl[1] and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 9, D-48149 Münster, Germany — [2]Center for Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Corrensstr. 2, D-48149 Münster, Germany

We show that well-established numerical continuation methods can be employed to calculate the fully nonlinear phase behaviour in a range of thermodynamic systems. This method is illustrated by applying it to a two-field Phase-Field-Crystal model describing the crystallisation of a mixture of two types of colloidal particles. We compare the resulting phase diagrams containing different liquid and crystalline phases to those obtained from a one-mode approximation.

DY 28.2 Tue 10:15 ZEU 147

Oscillatory active phase separation in two-species chemotactic systems — •Andre Förtsch and Walter Zimmermann — Theoretische Physik I, Unversität Bayreuth

Two chemically interacting particle species are modelled, which are either attracted or repelled by chemicals produced by them. We show by analytical calculations and simulations, that this two-species model with a conserved particle dynamics exhibits in a wide parameter range time-dependent density modulations. This two-species system belongs to a new class of non-equilibrium phase transitions. It shows a coarsening behavior, which is fundamentally different form coarsening in common (active) phase separation. Moreover, the basic properties of these oscillatory density modulations can be described by a non-reciprocal coupling of two Cahn-Hilliard models.

DY 28.3 Tue 10:30 ZEU 147

Phase separation and time-periodic behaviour in coupled Cahn-Hilliard models — •Tobias Frohoff-Hülsmann[1], Jana Wrembel[1], and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster — [2]Center of Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Corrensstr. 2, 48149 Münster

The Cahn-Hilliard equation is the paradigmatic mean-field model describing phase separation in a system characterized by a single order parameter field, e.g., the concentration for binary alloys. Decreasing the underlying free energy while preserving the total mass, this equation corresponds to a conserved gradient dynamics. Two coupled Cahn-Hilliard equations are able to represent ternary systems with two conserved quantities and are the subject of our study. Using coupling terms that either preserve or break the gradient structure, we investigate how the coupling alters the system behaviour. Employing numerical path continuation we present the fully nonlinear bifurcation behaviour and trace the transitions from the uncoupled equations to the coupled model of gradient dynamics form and further to the coupled model without overall gradient dynamics form. Selected results are illustrated by exemplary time simulations.

DY 28.4 Tue 10:45 ZEU 147

Nonlinear patterns shaping the domain on which they live — •Mirko Ruppert and Walter Zimmermann — Universität Bayreuth, Bayreuth, Deutschland

Nonlinear stripe patterns in two spatial dimensions break the rotational symmetry and generically show a preferred orientation near domain boundaries, as described by the famous Newell-Whitehead-Segel (NWS) equation. We first demonstrate that, as a consequence, stripes favour rectangular over quadratic domains. We then investigate the effects of patterns "living" in deformable domains by introducing a model coupling a generalized Swift-Hohenberg model to a generic phase field model describing the domain boundaries. If either the control parameter inside the domain (and therefore the pattern amplitude) or the coupling strength ("anchoring energy" at the boundary) are increased, the stripe pattern self-organizes the domain on which it "lives" into anisotropic shapes. For smooth phase field variations at the domain boundaries, we simultaneously find a selection of the domain shape and the wave number of the stripe pattern. This selection shows further interesting dynamical behavior for rather steep variations of the phase field across the domain boundaries. The here-discovered feedback between the anisotropy of a pattern and its orientation at boundaries is relevant e.g. for shaken drops or biological pattern formation during development.

DY 28.5 Tue 11:00 ZEU 147

Phase transition in a biased reaction-diffusion system — •Pratik Mullick[1,2] and Parongama Sen[2] — [1]Department of Physics and Astronomy 'Galileo Galilei', University of Padova, Via Francesco Marzolo 8, 35131 Padova, Italy — [2]Department of Physics, University of Calcutta, 92 APC Road, Kolkata 70009, India

Reaction diffusion systems being a prototype model for pattern formation have shown diverse applications in several complex systems. Different categories of reaction diffusion systems depends on the number and types of the reactants. The simplest is the single species reaction diffusion system generally described as as $kA \to lA$. We consider a two dimesnional lattice, on which the particles A are biased to move towards their nearest neighbours and annihilate when they arrive at the same site; $A+A \to \emptyset$. Several systems with interacting entities e.g. bacteria and antibiotics, predators and preys, individuals in a society can be studied using reaction diffusion models with a bias, which can be either positive or negative. Any nonzero bias is seen to drastically affect the behaviour of the system compared to the unbiased (diffusive)

case. For positive bias, the system shows formation of dimers, which are isolated pairs of particles located in nearest neighbouring positions with no other particles around, while for negative bias a finite density of particles are seen to survive in the system. Both the quantities vanish in a power-law manner close to the diffusive limit with different exponents. The results indicate the presence of a continuous phase transition at the diffusive point.

Journal reference: Phys. Rev. E **99**, 052123 (2019).

15 min. break

DY 28.6 Tue 11:30 ZEU 147

Pattern selection in reaction diffusion systems — Srikanth Subramanian and •Sean Murray — Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

Turing's theory of pattern formation has been used to describe self-organisation in many biological, chemical and physical systems. However, while conditions sufficient for the existence of patterns are known, the nonlinear mechanisms responsible for pattern selection are not. Here, we show the physical principle of mass flow through the system has a critical role in pattern determination. In particular, mass flow, rather than growing Fourier modes, underlies the regular positioning of peaks within a pattern and is responsible for a competition instability that leads to a reduction in the number of peaks. These results also explain the coarsening and lack of peak movement observed in the limit of no mass flow, namely, in mass-conserved systems.

DY 28.7 Tue 11:45 ZEU 147

Pattern formation in confined magnetizable granular matter — •Eric Opsomer[1], Simon Merminod[2], Julien Schockmel[1], Nicolas Vandewalle[1], Michael Berhanu[3], and Eric Falcon[3] — [1]University of Liège, Liège, Belgium — [2]Brandeis University, Waltham, USA (MA) — [3]CNRS, Université Paris Diderot, Paris, France

Magnetizable granular materials can be used as model systems for the study of phase transitions, crystallization and pattern formation. Indeed, in addition to granular gases and crystalline arrangements, labyrinthine structures have been reported in confined vibrated systems were agitation is competing with magnetic repulsion between particles.

Here, we present DEM simulations of vibrated magnetizable spheres in a Hele-Shaw cell and study the impact of the gap size on the observed structures. By tuning the confinement, we recreate established experimental data and generate new structures displaying herringbone patterns.

DY 28.8 Tue 12:00 ZEU 147

Salt polygons are caused by convection — •Lucas Goehring[1], Jana Lasser[2], Marcel Ernst[2], and Joanna Nield[3] — [1]Nottingham Trent University — [2]Max Planck Institute for Dynamics and Self-Organisation — [3]University of Southampton

From fairy circles to patterned ground and columnar joints, natural patterns spontaneously appear in many complex geophysical settings. Here, we shed light on the origins of polygonally patterned crusts of salt playa and salt pans. These beautifully regular features, approximately a meter in diameter, are found worldwide and are fundamentally important to the transport of salt and dust in arid regions. We show that they are consistent with the surface expression of buoyancy-driven convection in the porous soil beneath a salt crust. By combining quantitative results from direct field observations, analogue experiments, linear stability theory, and numerical simulations, we further determine the conditions under which salt polygons should form, as well as how their characteristic size emerges.

DY 28.9 Tue 12:15 ZEU 147

Periodic patterns emerge beyond active phase separation — •Frederik J. Thomsen, Lisa Rapp, Fabian Bergmann, and Walter Zimmermann — Theoretische Physik, Universität Bayreuth

A generic model for a conserved order-parameter field is suggested and investigated that shows a primary transition to large-scale active phase separation. It is a first example of a nonlinear conserved system that shows a secondary bifurcation to spatially periodic patterns. The transition is hysteretic. This spatially periodic patterns show multistability, i. e. we find wavenumber bands of stable periodic patterns as in classial pattern forming systems with unconserved order parameter fields. In a certain parameter subrange this model follows a gradient dynamics. In this range and in its neighborhood homogeneous phase separated states coexist with spatially periodic patterns.

DY 29: Nonequilibrium Quantum Many-Body Systems 2 (joint session TT/DY)

Time: Tuesday 14:00–16:00 Location: HSZ 204

DY 29.1 Tue 14:00 HSZ 204

Robust and ultrafast state preparation by ramping artificial gauge potentials — •Botao Wang, Xiaoyu Dong, F. Nur Ünal, and André Eckardt — Max-Planck-Institut für Physik komplexer Systeme Nöthnitzer Str. 38, D-01387 Dresden, Germany

The implementation of static artificial magnetic fields in ultracold atomic systems has been established as a powerful tool, e.g. for simulating quantum-Hall physics with charge-neutral atoms. Taking an interacting bosonic flux ladder as a minimal model, we investigate protocols for adiabatic state preparation based on ramping up the vector potential (in the form of Peierls phases), which is engineered to give rise to the desired magnetic flux. We find that the time required for adiabatic state preparation dramatically depends on the spatial pattern of Peierls phases used to create the flux. This is explained by the fact that, while different patterns (i.e. vector potentials) just correspond to different gauges for static fluxes, they induce different electric fields during the ramp. Remarkably, we find that for an optimal choice, it allows for preparing the ground state almost instantaneously. This provides a novel concept for shortcuts to adiabaticity and may open up a new way for robust state preparation.

DY 29.2 Tue 14:15 HSZ 204

Non-equilibrium steady state solutions of time-periodic driven Luttinger liquids — •Serena Fazzini[1], Piotr Chudinski[2], Chirstoph Dauer[1], Imke Schneider[1], and Sebastian Eggert[1] — [1]Physik und OPTIMAS, Technische Universität Kaiserslautern — [2]School of Mathematics and Physics, Queens Univ. Belfast

The recent development of Floquet engineering has made periodic driving a versatile tool for achieving new phases not accessible in static equilibrium systems. We now study the exact Floquet steady states of the periodically driven Tomonaga-Luttinger liquid without resorting to any high frequency approximations. We show that the time-dependent Schrödinger equation can be solved analytically for a large class of driven interacting 1D systems, which give the resulting non-equilibrium steady states. Remarkably, we observe regions of instabilities as a function of total momentum where the solution is not of Floquet form, which implies a loss of time translational invariance and therefore heating of excitations. For small driving amplitudes the instabilities are close to the naively expected resonance condition $n\omega = 2vq$, but for stronger driving the heating regions separate a rich structure of bands of steady state solutions. Physical consequences are discussed.

DY 29.3 Tue 14:30 HSZ 204

Periodically Driven Manybody System: a Density Matrix Renormalization Group Study — •Imke Schneider[1], Shaon Sahoo[2], and Sebastian Eggert[1] — [1]Department of Physics and Research Center Optimas, Technical University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Department of Physics, Indian Institute of Technology Tirupati, Tirupati 517506, India

Driving a quantum system periodically in time can profoundly alter its long-time dynamics and trigger exotic quantum states of matter. We propose a new DMRG method which directly deals with the Fourier components of the eigenstates of a periodically driven system using Floquet theory. With this new method we can go beyond effective Hamiltonians and take into account higher Floquet modes. Numerical results are presented for the isotropic Heisenberg antiferromagnetic spin-1/2 chain under both local (edge) and global driving for energies, spin-spin correlation and temporal fluctuations. As the frequency is lowered, the spin system enters into a Floquet regime with coherent

excitations of a large number of Floquet modes, which shows characteristic quantum correlations that cannot be described by any effective static model.

DY 29.4 Tue 14:45 HSZ 204

Suppression of the horizon effect in pairing correlation functions of t-J chains after a quantum quench — Ansgar Kühn, Lorenzo Cevolani, and •Salvatore R. Manmana — Institut für Theoretische Physik, U. Göttingen

We investigate the time evolution of density, spin, and pairing correlation functions in one-dimensional t-J models following a quantum quench using the time-dependent density matrix renormalization group. While density and spin correlation functions show the typical light-cone behavior over a wide range of parameters, in pairing correlation functions it is strongly suppressed. This is supported by time-dependent BCS theory, where the light cone in the pairing correlation functions is found to be at least two orders of magnitude weaker than in the density correlator. These findings indicate that in global quantum quenches not all observables are affected equally by the excitations induced by the quench.
We acknowledge financial support by SFB/CRC 1073 (project B03) of the DFG.
[1] Phys. Rev. A **98**, 013616 (2018).

DY 29.5 Tue 15:00 HSZ 204

Iterative path integral summations for nonequilibrium quantum transport — •Stephan Weiss, Simon Mundinar, and Jürgen König — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

We have developed a numerically exact scheme, the **I**terative **S**ummation of **P**ath-**I**ntegrals (ISPI), to calculate observable of interest in quantum transport setups out of equilibrium [1,2]. Our main focus aims at small interacting quantum dot systems which are coupled to ferromagnetic [2] as well as superconducting leads in a nonequilibrium environment. We take into account small to intermediate Coulomb interactions, finite lead polarizations as well as finite superconducting gap parameters and finite temperature for the respective setups. Our method treats spin-dependent resonant-tunnelling processes in a natural manner. Examples of the tunnelling current are presented for different setups.
[1] S. Weiss, R. Hützen, D. Becker, J. Eckel, R. Egger, and M. Thorwart, Phys. Stat. Sol. B 250, 2298 (2013).
[2] S. Mundinar, Ph. Stegmann, J. König, and S. Weiss, Phys. Rev. B 99, 195457 (2019).

DY 29.6 Tue 15:15 HSZ 204

Mobility of the Fermi polaron for strong couplings — •Stefan Wittlinger[1], Lode Pollet[1], and Andrey Mishchenko[2] — [1]LMU Munich, Munich, Germany — [2]RIKEN, Wako, Japan

We present an algorithmic scheme to calculate the mobility of the Fermi polaron, an impurity immersed into a Fermi bath, for strong couplings. In general, Monte Carlo simulations of the Fermi polaron problem suffer from the fermionic sign problem. For our scheme, we find a wide parameter range with a tractable sign problem. The perturbative expansion of the interaction is sampled using the diagrammatic determinantal quantum Monte Carlo algorithm. The sampling is done in imaginary time, which requires analytical continuation. Most theoretical treatments of the Fermi polaron problem only consider s-wave interactions or rely on the heavy particle approximation. Our scheme allows for the study of more realistic potentials by also considering higher order scattering terms. It also allows for the study of the problem without the heavy particle approximation. I will present results for a repulsive potential well for a wide range of masses and varying interaction ranges. Possible connections to the Anderson orthogonality catastrophe of the infinite mass case will also be discussed.

DY 29.7 Tue 15:30 HSZ 204

Chiral kinetic theory avoiding anomalies — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics - UFRN, Campus Universitário Lagoa nova, 59078-970 Natal, Brazil

The anomalous term $\sim \vec{E}\vec{B}$ in the balance of the chiral density can be rewritten as quantum current in the classical balance of density. This term is derived from the quantum kinetic equations for systems with SU(2) structure within a completely conserving approach and it is suggested that the term is of kinetic origin instead of anomaly. Regularization-free density and pseudospin currents are calculated in Graphene and Weyl-systems realized as the infinite-mass limit of electrons with quadratic dispersion and a proper spin-orbit coupling. The intraband and interband conductivities are discussed. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to the Zeeman field. [Eur. Phys. J. B 92 (2019) 176, Phys. Lett. A 383 (2019) 1362, Phys. Rev. B 94 (2016) 165415, Phys. Rev. B 92 (2015) 245425 errata: Phys. Rev. B93 (2016) 239904(E), Phys. Rev. B 92 (2015) 245426

DY 29.8 Tue 15:45 HSZ 204

Optical excitation of magnons in an easy-plane antiferromagnet: Application to Sr_2IrO_4 — •Urban F. P. Seifert[1,2] and Leon Balents[2,3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA — [3]Canadian Institute for Advanced Research, Toronto, Ontario, Canada M5G 1M1

Recent experiments show that ultrafast radiation at energies below the optical gap can create coherent magnetic excitations in Mott insulating antiferromagnets. In this talk, we introduce a quantum theory for the interaction of a (classical) light field with the magnetic degrees of freedom in the paradigmatic two-dimensional antiferromagnet Sr_2IrO_4. The reduced space group symmetry of the crystal allows for several channels for spin-operator bilinears to couple to the electric field. Integrating out high-energy degrees of freedom in a Keldysh framework, we derive induced effective fields which enter the equations of motion of the low-energy mode of in-plane rotations which couple to the out-of-plane magnetization. Considering a pump-probe protocol, these induced fields excite magnetization oscillations which can subsequently probed, e.g. using Kerr rotation. We discuss how the induced fields depend on polarization and frequency of the driving light, and our study applies to both resonant and non-resonant regimes. Crucially, the induced fields depend on the two-magnon density of states, thus allowing for further insight into properties of the magnetic excitation spectrum.

DY 30: Active Matter III (joint session DY/BP/CPP)

Time: Tuesday 14:00–16:00 Location: ZEU 160

DY 30.1 Tue 14:00 ZEU 160

Uncovering novel phase transitions in dense dry polar active fluids using a lattice Boltzmann method — David Nesbitt, Gunnar Pruessner, and •Chiu Fan Lee — Imperial College, London, U.K.

The dynamics of dry active matter have implications for a diverse collection of biological phenomena spanning a range of length and time scales, such as animal flocking, cell tissue dynamics, and swarming of inserts and bacteria. Uniting these systems are a common set of symmetries and conservation laws, defining dry active fluids as a class of physical system. Many interesting behaviors have been observed at high densities, which remain difficult to simulate due to the computational demand. Here, we devise a new method to study dry active fluids in a dense regime using a simple modification of the lattice Boltzmann method. We apply our method to an active model with contact inhibition of locomotion, which has relevance to collective cell migration, and uncover multiple novel phase transitions: two first-order and one potentially critical. We further support our simulation results with an analytical treatment of the hydrodynamic equations.

Reference: D Nesbitt, G Pruessner, and CF Lee. Preprint: arXiv:1902.00530.

DY 30.2 Tue 14:15 ZEU 160

Irreversibility in Active Matter Systems: Fluctuation Theorem and Mutual Information — Lennart Dabelow[2], •Stefano Bo[1], and Ralf Eichhorn[3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Universität Bielefeld — [3]Nordita, Royal In-

stitute of Technology and Stockholm University

We consider a Brownian particle, which, in addition to being in contact with a thermal bath, is driven by active fluctuations. These active fluctuations do not fulfill a fluctuation-dissipation relation and therefore play the role of a non-equilibrium environment. Using an Ornstein-Uhlenbeck process as a model for the active fluctuations, we derive the path probability of the Brownian particle subject to both, thermal and active noise. From the case of passive Brownian motion, it is well-known that the log-ratio of path probabilities for observing a certain particle trajectory forward in time versus observing its time-reserved twin trajectory quantifies the entropy production in the thermal environment. We calculate this path probability ratio for active Brownian motion and derive a generalized "entropy production", which fulfills an integral fluctuation theorem. We show that those parts of this "entropy production", which are different from the usual dissipation of heat in the thermal environment, can be associated with the mutual information between the particle trajectory and the history of the non-equilibrium environment.

DY 30.3 Tue 14:30 ZEU 160

Rheotaxis of active drops in confinements — •Ranabir Dey[1], Carola M. Buness[1,2], Chenyu Jin[1], and Corinna C. Maass[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Goettingen — [2]Institute for the Dynamics of Complex Systems, Georg August Universitaet Goettingen

Biological microswimmers commonly navigate confinements having liquid flows, e.g. locomotions of spermatozoa through the reproductive tract and bacteria in the gut or in blood vessels. The directed motion of the microorganisms in response to the gradients in external flow velocity is classically called 'rheotaxis'. Recently, rigorous efforts have been made to understand the rheotaxis of microorganims, specifically bacteria. In contrast, there is very little quantitative understanding of rheotaxis of artificial microswimmers. It must be noted that artificial microswimmers, e.g. those designed for drug delivery, are often required to navigate confinements having external flows. Here, we elucidate the swimming dynamics of a common type of artificial microswimmer, i.e. active drops, in micro-confinements having Poiseuille flow. We experimentally quantify the rheotaxis of these droplet microswimmers, intrinsically undergoing Marangoni stress dominated 'self-propulsion', in response to velocity gradients of varying strength. We try to understand the observed rheotaxis of the active drops in confinements in the context of a hydrodynamic model– the active Jeffery-Bretherton model. We strongly feel that detailed understanding of artificial active matter rheotaxis will make significant contributions towards better design optimization for practical applications.

DY 30.4 Tue 14:45 ZEU 160

Multiple Particle Correlation Analysis of Many-Particle Systems: Formalism and Application to Active Matter — •Rüdiger Kürsten[1], Sven Stroteich[1], Martín Zumaya Hérnandez[2], and Thomas Ihle[1] — [1]Universität Greifswald, Institut für Physik, Felix-Hausdorff-Str.6 — [2]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Apartado Postal 48-3, Código Postal 62251, Cuernavaca, Morelos, México

We introduce a fast spatial point pattern analysis technique which is suitable for systems of many identical particles giving rise to multi-particle correlations up to arbitrary order. The obtained correlation parameters allow to quantify the quality of mean field assumptions or theories that incorporate correlations of limited order. We study the Vicsek model [1] of self-propelled particles and create a correlation map marking the required correlation order for each point in phase space incorporating up to ten-particle correlations. We find that multi-particle correlations are important even in a large part of the disordered phase. Furthermore, the two-particle correlation parameter serves as an excellent order parameter to locate both phase transitions of the system, whereas two different order parameters were required before [2].

[1] Phys. Rev. Lett. 75, 1226 (1995). [2] Phys. Rev. Lett. 92, 025702 (2004); Phys. Rev. E 77, 046113 (2008).

DY 30.5 Tue 15:00 ZEU 160

Nonuniversality in scalar active matter with diffusivity edge under periodic confinement — •Benoît Mahault[1] and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Germany — [2]University of Oxford, United Kingdom

Scalar active matter is often described at the mean field level by nonlinear Fokker-Planck equations with density-dependent diffusion coefficients integrating fast degrees of freedom, as well as various equilibrium and/or nonequilibrium processes. A generic class, characterized by a diffusivity vanishing above some threshold density, was recently introduced [Golestanian, Phys. Rev. E 100, 010601(R)]. In presence of harmonic confinement, such 'diffusivity edge' was shown to lead to condensation in the ground state, with the associated transition exhibiting formal similarities with Bose-Einstein condensation (BEC).

Many active systems, such as self-propelled Janus particles, can however self-assemble into finite-size coexisting clusters. To account for such feature in the diffusivity edge framework, a periodic egg-crate confinement, that provides multiple sites for condensation, is considered in arbitrary dimensions. While for high barriers separating two minima the system essentially behaves as in the single harmonic trap case, for shallow potentials the transition is qualitatively different as the exponent associated to the scaling of the condensate fraction with an effective temperature is found to be nonuniversal. We nevertheless show from a generalized thermodynamic description that the overall phenomenology of BEC, such as the divergence of the isothermal compressibility at the transition, holds in both cases.

DY 30.6 Tue 15:15 ZEU 160

Anomalous fluctuations accompany dynamical arrest in a cluster of chemically active colloids — •Supropriya Saha, Prathyusha K R, and Ramin Golestanian — Max Planck Institute for Dynamics and Self Organisation

Recent years have seen enormous scientific activity exploring the ability of catalytic colloids to collectively form patterns and clusters. However, fluctuations of individual colloids within a cluster remains unstudied, and is the focus of our work. Using the simplest example of active colloids, hard spheres that generate an isotropic chemical field, we find that an interplay of non-local interactions and finite system size results in the formation of a core and a surface layer in the cluster, both of which exhibit dynamics distinct from one another. The simplicity of our model suggests that aspects of the fluctuations revealed here are generic to matter driven phoretically, including enzymes.

DY 30.7 Tue 15:30 ZEU 160

Transport coefficients of active particles: Reverse perturbations and response theory — •Thomas Ihle[1], Arash Nikoubashman[2], Alexander Unruh[1], Sven Stroteich[1], and Rüdiger Kürsten[1] — [1]Institute for Physics, Greifswald University — [2]Institute of Physics, Johannes-Gutenberg-University Mainz

Müller-Plathe's reverse perturbation method [Phys. Rev. E 59, 4894 (1999)] for shearing simple liquids is extended to the Vicsek model (VM) of self-propelled particles. It is shown how the shear viscosity ν and the momentum amplification coefficient λ, can be extracted from simulations by fitting to an analytical solution of the hydrodynamic equations for the VM. The viscosity consists of two parts, a kinetic and a collisional contribution. While analytical predictions already exist for the former [T. Ihle, J. Stat. Mech. 2016, 083205], a novel expression for the collisional part is derived by an Enskog-like kinetic theory [A. Nikoubahsman, T. Ihle, Phys. Rev. E 100, 042603 (2019)]. Using several methods to measure transport coefficients such as reverse perturbations, Green-Kubo relations and transverse current correlations, we find excellent agreement between the different methods and good agreement with theory. We introduce a novel kind of response theory that allows us to not only verify the analytical predictions of kinetic theory but also to efficiently obtain expressions for non-local (wavevector dependent) transport coefficients of active systems, avoiding tedious multiple-scale methods like the Chapman-Enskog expansion. The method is applied to the VM with metric and topological interactions as well as to a model with continuous time dynamics.

DY 30.8 Tue 15:45 ZEU 160

Effect of Vicsek-like Activity on the collapse of a Flexible Polymer — •Subhajit Paul[1], Suman Majumder[1], Subir K Das[2], and Wolfhard Janke[1] — [1]Institüt für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [2]JNCASR, Jakkur P.O., Bangalore- 560064, India.

Dynamics of various biological filaments can be understood within the framework of active polymer models. In this context, we construct a bead-spring model for a flexible polymer chain in which the activity or self-propulsion of the beads has been defined in the Vicsek-like manner. Following a quench from a high-temperature coil phase to the low-temperature state we have studied the nonequilibrium dynamics of this model by solving the Langevin equation via molecular dynamics (MD) simulations. The low-T equilibrium state for the passive poly-

mer in which the interaction among the beads modeled via standard LJ potential, is a compact globular one. Results from our MD simulations reveal that the globular state is also likely to be the final equilibrium in the active case also, the nonequilibrium dynamics is quite different than the passive case. We observe that the deviation from the intermediate 'pearl-necklace' arrangement and the formation of elongated structures for the polymer increases with activity. Also, it appears that whether smaller values of the activity makes the coarsening faster, activity beyond a certain value makes it slower. On this nonequilibrium front we also compare various results with that of the passive case, viz., scaling laws related to collapse time, cluster coarsening, etc.

DY 31: Many-body Systems: Equilibration, Chaos and Localization II (joint session DY/TT)

Time: Wednesday 9:30–13:00 Location: HÜL 186

DY 31.1 Wed 9:30 HÜL 186

Many-body dynamical localization in the kicked Bose-Hubbard chain — Michele Fava[1], Rosario Fazio[2,3], and •Angelo Russomanno[4] — [1]Rudolf Peierls Centre for Theoretical Physics, Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, UK — [2]Abdus Salam ICTP, Strada Costiera 11, I-34151 Trieste, Italy — [3]Dipartimento di Fisica, Universit\'a di Napoli "Federico II", Monte S. Angelo, I-80126 Napoli, Italy — [4]Max-Planck-Institut f\"ur Physik Komplexer Systeme, N\"othnitzer Strasse 38, D-01187, Dresden, Germany

We show that a clean kicked Bose-Hubbard model exhibits a many-body dynamically localized phase. This phase shows ergodicity breaking and we can argue that this property persists in the large-size limit: the Floquet states violate eigenstate thermalization and then the asymptotic value of local observables depends on the initial state and is not thermal. This implies that the system does not generically heat up to infinite temperature, for almost all the initial states. Differently from many-body localization here the entanglement entropy linearly increases in time. This increase corresponds to space-delocalized Floquet states which are nevertheless localized across specific subsectors of the Hilbert space: In this way the system is prevented from randomly exploring all the Hilbert space and does not thermalize.

DY 31.2 Wed 9:45 HÜL 186

Entanglement clusters in many-body localized systems — •Kevin Hemery, Adam Smith, and Frank Pollmann — Department of Physics, T42, Technische Universität München, James-Franck-Strasse 1, D-85748 Garching, Germany

A complete understanding of the many body localized (MBL)-ergodic transition is still missing. We investigate this phenomenon by analysing the entanglement structure of the eigenstates of the Heisenberg chain in presence of a disordered field. Our method is based on a combination of the two-site mutual information and a graph theory clustering algorithm.

First we test our approach by recovering the scaling behaviour of the number of entangled clusters across the phase transition, which has previously been extracted using the full density matrix. On the MBL side, we access large systems by using the so-called "DMRG-X" algorithm, a variational matrix-product-states based method. We compare our results to predictions drawn from renormalisation group based theories of the thermalisation avalanche.

DY 31.3 Wed 10:00 HÜL 186

Emergent localization in euclidean random matrices without small parameter — •Anton Kutlin and Ivan Khaymovich — Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

We study the wave functions localization properties for the isotropic euclidean random matrix (ERM) model in arbitrary dimension. Due to its generality, this model arises naturally in various physical contexts such as studies of vibrational modes [1,2], artificial atomic systems [3,4], liquids and glasses [5-7], ultracold gases and photon localization phenomena [8,9]. We generalize the known[10,11] renormalization group (RG) approach, formulate universal sufficient conditions for localization in ERM models and inspect a striking duality of the wave function spatial structure between ERMs and translation-invariant (TI) models with a diagonal disorder[12]. Finally, we discuss possible extensions of the approach to anisotropic models.

[1] B. Ash et al., PRE 98, 042134 (2018) [2] A. Amir et al., PRX 3, 021017 (2013) [3] A. de Paz et al., PRL 111, 185305 (2013) [4] P. I. Karpov et al., PRE 97, 062157 (2018) [6] J .Rehn et al., Phil. Trans. R. Soc. A 374: 20160093 (2016) [7] J. Rehn et al., PRB 92, 085144 (2015) [8] T. Scholak et al., PRA 90, 063415 (2014) [9] A. Gero et al., PRA 88, 023839 (2013) [10] A. L. Burin et al., Pis'ma Zh. Eksp. Teor. Piz. 50, No. 6, 304-306 (1989). [11] L. S. Levitov, PRL 64, 547 (1990). [12] X. Deng et al., PRL 120, 110602 (2018).

DY 31.4 Wed 10:15 HÜL 186

Ergodization times and dynamical glass in classical Josephson junction chains — •Carlo Danieli[1], Mithun Thudiyangal[2], Yagmur Kati[3], and Sergej Flach[4] — [1]Max Planck Institute for the Physics of Complex Physics, Noethnitzer Str. 38, 01187 Dresden, Germany — [2]Department of Mathematics and Statistics, University of Massachusetts, Amherst MA 01003-4515, USA — [3]Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon, Korea — [4]Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon, Korea

Models of classical Josephson junction chains turn integrable in the limit of large energy densities or small Joseph- son coupling strength. Close to these limits, the Josephson coupling between superconducting grains induces a short range network. We compute distributions of finite-time averages of grain charges and extract the ergodization time TE which controls their convergence to ergodic delta distributions. We relate TE to the statistics of the fluctuations in time of the grain charges, which are dominated by fat tails. The ergodization time TE grows anomalously fast upon approaching the integrable limit as compared to the Lyapunov time TΛ - the inverse largest Lyapunov expo- nent. The microscopic reason for the observed behavior - which we labeled dynamical glass - is rooted in a growing number of grains evolving over long time in a regular fashion due to low probability of resonant interactions with the neighboring ones. We conjecture that the observed dynamical glass is Josephson junction networks irrespective of their dimensionality. Ref: Phys.Rev.Lett. 122 054102 (2019).

DY 31.5 Wed 10:30 HÜL 186

Real-time dynamics of string breaking in quantum spin chains — •Roberto Verdel[1], Fangli Liu[2], Seth Whitsitt[2], Alexey V. Gorshkov[2,3], and Markus Heyl[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187-Dresden, Germany — [2]Joint Quantum Institute, NIST/University of Maryland, College Park, MD 20742, USA — [3]Joint Center for Quantum Information and Computer Science, NIST/University of Maryland, College Park, MD 20742, USA

String breaking is a central dynamical process in theories featuring confinement, where a string connecting two charges decays at the expense of the creation of new particle-antiparticle pairs. In this talk, we show that this process can also be observed in quantum Ising chains [1], where domain walls get confined either by a symmetry-breaking field or by long-range interactions. Our main finding is that string breaking occurs, in general, as a two-stage process: First, the initial charges remain static and stable; yet, the connecting string can undergo complex dynamics. In the second stage, which can be severely delayed due to dynamical constraints happening in the previous phase, the string finally breaks. We analyse the constrained many-body dynamics of the first stage and its consequences for the final string breaking or the suppression of it.

References: [1] R. Verdel, F. Liu, S. Whitsitt, A. V. Gorshkov, and M. Heyl, (2019), arXiv:1911.11382 [cond-mat.stat-mech].

DY 31.6 Wed 10:45 HÜL 186

Dynamics of strongly interacting systems: From Fock-space fragmentation to Many-Body Localization — •Giuseppe De Tomasi[1], Daniel Hetterich[2], Pablo Sala[3], and Frank Pollmann[4] — [1]TUM Munich/Cambridge University — [2]TUM Munich — [3]TUM Munich — [4]TUM Munich

We study the t-V disordered spinless fermionic chain in the strong coupling regime, t/V –> 0. Strong interactions highly hinder the dy-

namics of the model, fragmenting its Hilbert space into exponentially many blocks in system size. Macroscopically, these blocks can be characterized by the number of new degrees of freedom, which we refer to as movers. We focus on two limiting cases: Blocks with only one mover and the ones with a finite density of movers. The former many-particle block can be exactly mapped to a single-particle Anderson model with correlated disorder in one dimension. As a result, these eigenstates are always localized for any finite amount of disorder. The blocks with a finite density of movers, on the other side, show an MBL transition that is tuned by the disorder strength. Moreover, we provide numerical evidence that its ergodic phase is diffusive at weak disorder. Approaching the MBL transition, we observe sub-diffusive dynamics at finite time scales and find indications that this might be only a transient behavior before crossing over to diffusion.

15 min. break

DY 31.7 Wed 11:15 HÜL 186

Impact of pertubations on expectation value dynamics — •Robin Heveling, Lars Knipschild, and Jochen Gemmer — University of Osnabrueck, Osnabrueck, Germany

Recently it was advocated by several groups that a variety of pertubations in condensed matter type systems may have "generic" effects on the dynamics of expectation values [1,2,3]. We investigate this approach numerically and to some extend analytically, scrutinizing various ways of modelling said generic effects.

[1] L. Dabelow, P. Reimann, Perturbed relaxation of quantum many-body systems, arXiv:1903.11881
[2] J. Richter et al., Exponential damping induced by random and realistic pertubations, arXiv:1906.09268
[3] L. Knipschild, J. Gemmer, Stability of quantum dynamics under constant Hamiltonian pertubations, arXiv:1811.00381

DY 31.8 Wed 11:30 HÜL 186

Influence of drive smoothness on the Floquet MBL transition — •Tobias Gulden[1,2], Asaf Diringer[2], and Netanel Lindner[2] — [1]IST Austria — [2]Technion - Israel Institute of Technology

We investigate how the critical driving amplitude at the Floquet MBL-to-ergodic phase transition changes between smooth and non-smooth driving over a large range of frequencies. To this end we study numerically a disordered spin-1/2 chain which is periodically driven by a sine or a square-wave drive, respectively. In both cases the critical driving amplitude increases monotonically with the frequency, and at large frequencies it is identical for the two drives. However, at low and intermediate frequencies the critical amplitude of the square-wave drive depends strongly on frequency, while the one of the cosine drive is almost constant in a wide frequency range. By analyzing the density of drive-induced resonances we conclude that this difference is due to resonances induced by higher harmonics in the Fourier spectrum which are present (absent) in the spectrum of the square-wave (sine) drive.

DY 31.9 Wed 11:45 HÜL 186

Periodic projections in quantum spin chains — •S. Harshini Tekur[1], Arnd Bäcker[2,1], and David J. Luitz[1] — [1]MPI für Physik komplexer Systeme, Dresden — [2]TU Dresden, Institut für Theoretische Physik

We investigate a new class of systems where a driven, disordered spin chain is opened by the addition of a periodic projection at one end of the chain, in analogy with classical or quantum maps with escape. The evolution operator over one period then becomes sub-unitary with a complex spectrum inside the unit circle. This class of systems exhibits several interesting properties, which we demonstrate by studying its level statistics, entanglement dynamics and spectral features like exceptional points which are unique to non-normal matrices. These may also be experimentally realized in a set-up where certain configurations of the spin chain are post-selected after a measurement.

DY 31.10 Wed 12:00 HÜL 186

Long-lived coherence in driven spin systems: from two- to infinite spatial dimensions — •Walter Hahn and V. V. Dobrovitski — QuTech, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands

We study dipolar-coupled quantum many-spin systems with local disorder, subject to periodic pulse driving, in different spatial dimensions: from two-dimensional to (effectively) infinite-dimensional systems. Using direct numerical simulations, we show that these systems exhibit long-lived magnetization response for all dimensions, despite strong fluctuations in the spin-spin couplings, and corresponding strong singularities in the spin dynamics. We observe the long-lived magnetization response for the initial polarization being either along the driving pulses, or along the axis conserved by the internal Hamiltonian. For longer time delays, the magnetization echoes exhibit an even-odd asymmetry, i.e. the system's response is modulated at the period which is twice the period of the driving. The above results are corroborated by a Floquet-operator analysis.

This work was supported by Dutch Research Council (NWO) and by DARPA DRINQS program.

DY 31.11 Wed 12:15 HÜL 186

Disorder-free localization in an interacting two-dimensional lattice gauge theory — •Petr Karpov[1,2], Roberto Verdel[1], Yi-Ping Huang[1,3], Markus Schmitt[1,4], and Markus Heyl[1] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, Dresden 01187, Germany — [2]National University of Science and Technology "MISiS", Moscow, Russia — [3]The Paul Scherrer Institute, Forschungsstrasse 111, 5232 Villigen, Switzerland — [4]University of California, Berkeley, California 94720, USA

Recently, disorder-free localization has been introduced as a new mechanism for ergodicity breaking in homogeneous systems caused by local constraints imposed by gauge invariance [1,2]. Here, we show that disorder-free localization can occur in genuinely interacting systems in two spatial dimensions. Specifically, we show that the quantum link model can become nonergodic by providing a strict bound on the localization-delocalization transition through an unconventional classical percolation problem. We investigate the quantum dynamics in this system by means of an improved classical network description [3] endowed with a time-dependent variational principle.

[1] A. Smith, J. Knolle, D.L. Kovrizhin, and R. Moessner, Phys. Rev. Lett. **118**, 266601 (2017).
[2] M. Brenes, M. Dalmonte, M. Heyl, and A. Scardicchio, Phys. Rev. Lett. **120**, 030601 (2018).
[3] M. Schmitt and M. Heyl, SciPost Phys. **4**, 013 (2018).

DY 31.12 Wed 12:30 HÜL 186

Learning many-body localization indicators directly from the Hamiltonian — •Alexander Gresch, Lennart Bittel, and Martin Kliesch — Heinrich-Heine University, Düsseldorf, Germany

Many-body localization (MBL) captures the phenomenon that the propagation of correlations in disordered quantum systems can be strongly suppressed due to interference effects. Quantum systems undergoing MBL do practically not equilibrate but instead preserve local signatures of their initial conditions for arbitrarily long times. This property makes such systems potential candidates for storage devices in quantum computation. However, a full analytical understanding has not been achieved and numerical approaches have to deal with the exponential growth of the Hilbert space dimension. Hence, approximate methods have been proposed. A recent approach uses artificial neural networks for distinguishing MBL states from non-localized ones, which allows to calculate the phase diagram of the transition. The already proposed deep learning schemes require an expensive preprocessing, e.g. the eigenstates of the Hamiltonian or their entanglement spectrum, as inputs.

In this work, we investigate the Heisenberg spin chain with random local magnetic field. We demonstrate that an MBL-prediction is possible from the given disorder parameters alone without any preprocessing. We guide the learning process via several different indicators for MBL that have previously served as a basis for numerical studies. Here, we provide new insights in their predictive capabilities from a machine learning perspective.

DY 31.13 Wed 12:45 HÜL 186

Anderson Localization in a Rydberg Composite — •Matthew Eiles, Alexander Eisfeld, and Jan-Michael Rost — Max Planck Institute for the Physics of Complex Systems, 38 Noethnitzer Str. Dresden 01187

We demonstrate the localization of a Rydberg electron in a Rydberg composite, a system containing a Rydberg atom coupled to a structured environment of neutral ground state atoms. This localization is caused by weak disorder in the arrangement of the atoms and increases with the number of atoms M and principal quantum number ν. We develop a mapping between the electronic Hamiltonian in the basis of degenerate Rydberg states and a tight-binding Hamiltonian in

the so-called "trilobite" basis, and then use this concept to pursue a rigorous limiting procedure to reach the thermodynamic limit in this system, taken as both M and ν become infinite, in order to show that Anderson localization takes place. This system provides avenues to study aspects of Anderson localization under a variety of conditions, e.g. for a wide range of interactions or with correlated/uncorrelated disorder.

DY 32: Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)

Time: Wednesday 9:30–12:30 Location: ZEU 114

DY 32.1 Wed 9:30 ZEU 114

Graphical Magnetogranulometry — •Ingo Rehberg, Reinhard Richter, and Stefan Hartung — Bayreuth University

The dipole strength of magnetic particles in a colloidal suspension can be obtained by a graphical rectification of the magnetization curves based on the inverse Langevin function. The method [1] yields the arithmetic and the harmonic mean of the particle distribution. It has an advantage compared to the fitting of magnetization curves to some appropriate mathematical model: It does not rely on assuming a particular distribution function of the particles.

[1] Measuring magnetic moments of polydisperse ferrofluids utilizing the inverse Langevin function, Ingo Rehberg, Reinhard Richter, Stefan Hartung, and Niklas Lucht, Birgit Hankiewicz, and Thomas Friedrich, Phys. Rev. B 100, 134425 (2019).

DY 32.2 Wed 9:45 ZEU 114

Phase Behavior of Charged Magnetic Nanoplatelets — •Margaret Rosenberg[1] and Sofia Kantorovich[1,2] — [1]Department of Physics, University of Vienna, Austria — [2]2Department of Mathematical Physics, Ural Federal University, Russia

Recent decades have seen the emergence of a new branch of science, magnetic soft matter, fueled by the advances in synthesis techniques, which have also made a wide variety of anisotropic magnetic colloidal nanoparticles available. Colloidal anisometry can be used as an effective control parameter to tune both self-assembly scenarios and thermodynamic, rheological and phase behavior of dipolar (magnetic) soft matter. For instance, magnetic nanoplatelets can form macroscopic ferromagnetic phases at room temperature. Although the phase behavior of a system hard-core platelets is well known, the influence of the magnetic dipole moment and electrostatic repulsion on suspensions of magnetic platelets is not yet fully understood. We use MD simulations to recreate such a system. The colloidal particles are modelled by charged soft spheres, with a central dipole possessing a magnetic moment of a constant length, permanently oriented perpendicular to the platelet surface. In order to investigate the self-assembly and structural properties of the platelets, we vary the amplitude of an applied magnetic field and the magnetic dipole. We analyze at which electrostatic conditions the system exhibits self-assembly or/and field alignment, based on RDFs, structure factors parallel and perpendicular to the field and extensive cluster analysis.

DY 32.3 Wed 10:00 ZEU 114

Construction of 1D hollow cube chains as a platform for synthesis of nanoscopic magnetic filaments. — •Deniz Mostarac[1], Yan Xiong[3], Pedro A. Sanchez[2], Oleg Gang[3,4], and Sofia Kantorovich[1,2] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]Columbia University, New York, USA — [4]Brookhaven National Laboratories, New York, USA

Construction of smart materials with sophisticated magnetic response by incorporating magnetic nanoparticles (MNPs) within permanently cross-linked structures, opens up the possibility for synthesis of complex, highly magneto-responsive systems. Assembly using DNA origami frames where the structure building instructions are encoded via DNA sequencing, provides a new perspective on construction of filaments with MNPs. Using programable DNA origami assembly, one can create scaffolds that serve as a blueprints for chain-like conformations of MNPs. Challenge is to produce a DNA based backbone that can be populated with MNPs, which when not subjected to an external magnetic field would in its polymeric properties resemble a real polymer. We present synthesis approach and results of 1D hollow cube chain scaffolds, together with preliminary results of AFM, TEM and SAXS measurements. We present computational models with both explicit and implicit DNA linker modeling, demonstrating the utility of such systems and exploring the influence of the number of DNA linkers between the hollow cubes, and their length, on the polymeric properties of the chained assemblies.

DY 32.4 Wed 10:15 ZEU 114

Dynamic Self-assembly of Magnetic Janus Particles — •Sofia Kantorovich[1,2], Pedro Sanchez[1,2], Maximilian Neumann[3], Sibylle Gemming[3,4], and Artur Erbe[3] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]Helmholtz-Zentrum Dresden-Rossendorf, Rosendorf, Germany — [4]Technische Universität Chemnitz, Chemnitz, Germany

In this contribution we explain how the interplay between hydrodynamics, magnetic interactions and the frequency of an applied magnetic field affect the structure and the size of clusters formed by magnetic Janus particles. We study silica particles (radius of 2.27μm) with a magnetic thin film coating (of a multilayer stack of Ta(3.0 nm)/Pd(3.0 nm)/[Co(0.28 nm)/Pd(0.9 nm)]8/Pd (1.1 nm)) on one hemisphere. Such a layer exhibits perpendicular magnetic anisotropy, i.e., the magnetic flux points out of the film plane [1]. Our previous combined experimental-simulation study showed that if the monolayer of such Janus particles is exposed to a low-frequency magnetic field, one can efficiently control self-assembly letting branched clusters of staggered chains, compact clusters, linear chains, and dispersed single particles to form and reconvert reversibly [2]. In the present contribution, we extend our investigation to high frequency out-of-equilibrium transformations.

[1] M. Albrecht et al., Nat. Mater. 4, 203 (2005). [2] Steinbach et al., PRE 100, 012608 (2019).

DY 32.5 Wed 10:30 ZEU 114

Magnetically Functionalized Star Polymers in Equilibrium and under Shear — •Gerhard Kahl[1], David Toneian[1], and Christos N. Likos[2] — [1]Institut für Theoretische Physik, TU Wien — [2]Fakultät für Physik, Universität Wien

Star polymers are macromolecules consisting of a central site, attached to which are a number f of linear polymer chains, called arms. Depending on the chemical composition of the arms, the polymer stars exhibit intriguing features, both in isolation and in concentrated solution.

We present star polymers with magnetically functionalized end groups as a novel polymeric system whose morphology, self-aggregation and orientation can easily be tuned by exposing these macromolecules simultaneously to an external magnetic field and to shear forces within a channel. Our investigations are based on a specialized simulation technique which faithfully takes into account the hydrodynamic interactions of the surrounding, Newtonian solvent. We find that the combination of magnetic field (including both strength and direction) and shear rate controls the mean number of magnetic clusters, which in turn is largely responsible for the static and dynamic behavior. While some properties are similar to comparable non-magnetic star polymers, others exhibit novel phenomena; examples of the latter include the breakup and reorganization of the clusters beyond a critical shear rate and a strong dependence of the efficiency with which shear rate is translated into whole-body rotations on the direction of the magnetic field.

DY 32.6 Wed 10:45 ZEU 114

A biaxial nematic liquid crystal composed of matchbox-symmetric molecules — •Robert A. Skutnik[1], Immanuel S. Geier[1], and Martin Schoen[1,2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische UniversitätBerlin, Straße des 17. Juni 115, 10623 Berlin, Germany — [2]Department of ChemicalEngineering, Imperial College London, South Kensington Campus, London SW7 2AZ,United Kingdom

By means of Monte Carlo simulations in the isothermal-isobaric ensemble we investigate the structure and phase behaviour of a ther-

motropic liquid crystal composed of matchbox-symmetric (or board-like) molecules. Besides the isotropic phase the liquid crystal exhibits also uniaxial and biaxial nematic phases. We analyse the orientation distribution function which allows us to distinguish between intrinsic and extrinsic biaxiality. In addition, we study the orientation-dependent correlation functions. In the limit of large intermolecular separations the value of the orientation correlation function corresponds to the uniaxial and biaxial order parameters which are coupled in a complex fashion.

DY 32.7 Wed 11:00 ZEU 114

Lyotropic liquid crystals in microfluidic environments — •Anshul Sharma and Anupam Sengupta — Physics of Living Matter Group, University of Luxembourg, Luxembourg City, Luxembourg

Recent progress in liquid crystal microfluidics has demonstrated how hydrodynamics, in combination with confinement and surface anchoring, can be harnessed to generate tunable flow and topological structures [1, 2]. Lyotropic liquid crystals (LLCs), solutions of disc-shaped amphiphilic mesogens with aromatic core, form linear stacks that aggregate to show nematic or columnar LC phases as a function of temperature or mesogen concentration. LLCs have long been studied for their role in drug and dye manufacturing, and more recently in rapid detection of pathogens. Yet, we lack a fundamental understanding of the response of LLC to micro-scale flows a universal parameter in medical, cellular and industrial settings. With aqueous solution of disodium cromoglycate as our model LLC, we study its behavior under different concentrations and micro-scale flow regimes. Static and flow-induced textures characterized using polarizing microscopy, conoscopy and particle tracking techniques, show emergence of distinctly oriented micro-domains in the flowing LLC. Our results indicate that, for a given surface anchoring, the domain size and lifetime vary with channel geometry and flow speed. Such spontaneous orientational domains could be harnessed to generate locally distinct transport properties within a globally advected material. [1] Sengupta et al., Liquid Crystals Reviews 2, 2014. [2] Giomi et al., PNAS 114, 2017. [3] Sharma et al. (in prep.)

15 min. break

DY 32.8 Wed 11:30 ZEU 114

Light driven passive and active motion of colloidal particles — •Pooja Arya, David Feldmann, and Svetlana Santer — University of Potsdam, Potsdam, Germany

We report on how one can manipulate an ensemble of colloidal particles trapped at a solid/liquid interface during irradiation with light of different wavelengths. The colloids are dispersed in an aqueous solution of photosensitive azobenzene containing cationic surfactant, which can photo-isomerize from trans to cis state under irradiation with light of appropriate wavelength. When focused light is applied, light-driven diffusioosmotic (LDDO) flow1 is generated at the solid/liquid interface resulting in a passive motion of particles within this flow. Utilizing the same LDDO mechanism one can also induce active motion of porous particles. Here the radially directed flow is generated by and around a single porous colloid when it is irradiated with either UV or blue light. This results in either mutual long-range diffusioosmotic repulsion of the particles or in even self-propelled motion when the colloids are turned into a Janus-like shape. Here, we discuss how to extend of passive and active motion of colloidal particles depends on the irradiation conditions such as wavelengths and intensities of light.

1.*Feldmann, D.; Maduar S.R.; Santer, M.; Lomadze, N.; Vinogradova O.I.; Santer, S., 6 (2016) 36443

DY 32.9 Wed 11:45 ZEU 114

Charge regulation radically modifies electrostatics in membrane stacks — •Arghya Majee[1], Markus Bier[1,2], Ralf Blossey[3], and Rudolf Podgornik[4] — [1]MPI for Intelligent Systems, Stuttgart & University of Stuttgart, Germany — [2]University of Applied Sciences, Würzburg-Schweinfurt, Germany — [3]University of Lille, CNRS, UMR8576 UGSF, France — [4]CAS & KAVLI Institute of Theoretical Sciences, Beijing

Motivated by biological membrane-containing organelles in plants and photosynthetic bacteria, we study charge regulation in a model membrane stack [1]. Considering (de)protonation as the simplest mechanism of charge equilibration between the membranes and with the bathing environment [2], we uncover a symmetry-broken charge state in the stack with a quasiperiodic effective charge sequence. In the case of a monovalent bathing salt solution, our model predicts complex, inhomogeneous charge equilibria depending on the strength of the (de)protonation reaction, salt concentration, and membrane size. Our results shed light on the basic reorganization mechanism of thylakoid membrane stacks.

References:

[1] A. Majee, M. Bier, R. Blossey, and R. Podgornik, Phys. Rev. E **100**, 050601(R) (2019).

[2] A. Majee, M. Bier, and R. Podgornik, Soft Matter **14**, 985 (2018).

DY 32.10 Wed 12:00 ZEU 114

Polymer Micelles with Crystalline Cores: self-assembly, molecular exchange kinetics and confinement effects — Nico König[1], Lutz Willner[2], and •Reidar Lund[1] — [1]Department of Chemistry, University of Oslo, Norway — [2]Institute for Complex Systems ICS, Forschungszentrum Jülich, Germany

Partially crystalline, self-assembling systems with multiple components are omnipresent in nature with living cells as a prominent example. Here we study micelles formed by self-assembly of a series of well-defined n-alkyl-(polyethylene oxide) (Cn-PEO) polymers in aqueous solutions . By using small-angle X-ray scattering (SAXS), densiometry and differential scanning calorimetry (DSC), we show that the n-alkane exhibit a first-order phase transition, but with reduced melting points compared to bulk. Correlating the structural and thermodynamic data, we found that the melting depression can be accurately described by the Gibbs-Thomson equation. The effect of core crystallinity on the molecular exchange kinetics is investigated using time-resolved small-angle neutron scattering (TR-SANS). We show that the melting transition is cooperative in the confined micellar core, whereas the exchange process is widely decoupled and unimeric in nature. Upon crossing the melting point, a discrete change in the activation energy is found. This suggests that a "local, single-chain melting process" preludes the molecular diffusion out of the micelle during chain exchange

DY 32.11 Wed 12:15 ZEU 114

Emulsion destabilisation by squeeze flow — •Riande Dekker, Antoine Deblais, and Daniel Bonn — Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

There is a large debate on the destabilisation mechanism of emulsions. We present a simple technique using mechanical compression to destabilise oil-in-water emulsions while at the same time confocal microscopy allows to visualise the mechanism directly. Upon compression of the emulsion, the continuous aqueous phase is squeezed out, while the dispersed oil phase progressively deforms from spherical to honeycomb-like shapes. The liquid films that separate the oil droplets are observed to thin and break at a critical oil/water ratio, leading to coalescence events that destabilise the emulsion. The destabilisation occurs like an avalanche propagating through the system. Local rearrangements occur after the fist destabilisation due to the fist coalescence event. The films participating in the cascade are the finest ones.

DY 33: Granular Matter and Granular Dynamics I

Time: Wednesday 9:30–12:45 Location: ZEU 118

Invited Talk DY 33.1 Wed 9:30 ZEU 118

Statistical Mechanics of Granular Clogging — •Douglas Durian — University of Pennsylvania, Philadelphia PA, USA

The gravity-driven flow of grains from a hole in a hopper is an iconic granular phenomenon. It's different from a fluid in that the rate is constant also in that it can suddenly and unexpectedly clog. How does the susceptibility to clogging decrease with increasing hole size, and is there a well-defined clogging transition above which the system never clogs? This problem is distinct from jamming due to the presence of boundaries and gradients. We show how the fraction F of flow con-

figurations that cause a clog may be deduced from the average mass discharged between clogs. We construct a simple model to account for the observation that F decays exponentially in hole width to the power of dimensionality. Thus the clogging transition is not sharp but rather is defined by observation limits, similar to the glass transition. When the system is immersed in water, F barely changes. Therefore, grain momenta play only a secondary role in destabilizing weak incipient arches and the crucial microscopic variables are likely the grain positions. Work is now in progress to distinguish free-flowing versus clog-causing position microstates using machine learning.

DY 33.2 Wed 10:00 ZEU 118

Tuning Mechanical Properties of Granular Matter Via Confinement — •Rishab Handa, Jorge Fiscina, and Christian Wagner — Department of Experimental Physics, Saarland University, Saarbruecken, Germany

We compare the high energy dissipation dynamics of dry and wet granular matter subjected to several degrees of confinement under large amplitude oscillatory shear (LAOS). Under confinement, the energy dissipated by dry grains was more pronounced than wet grains, at increasing strain rate. Scaling the elastic modulus of dry grains as a function of shear stress revealed a power law behavior, which we relate to the formation of filament-like force-chain networks. Contrarily, for wet granular matter, linear dependence of elastic modulus indicated the process of breaking and regeneration of capillary bridges, seemingly caused by non-affine motions of grains associated with the noise temperature. Therefore, we show that the degree of confinement can be used as a controlling parameter to adjust the mechanical properties of granular matter.

DY 33.3 Wed 10:15 ZEU 118

Machine Learning aided tracking of rod-like particles in 3D microgravity experiments on granular gases — •Dmitry Puzyrev, Kirsten Harth, Torsten Trittel, and Ralf Stannarius — Institute for Experimental Physics, Otto von Guericke University, Magdeburg, Germany

Granular gases are nonlinear systems which exhibit fascinating dynamical behavior far from equilibrium, including unusual cooling properties, clustering and violation of energy equipartition. Our investigation is focused on 3D microgravity experiments with dilute ensembles of rod-like particles, where the mean free path is substantially reduced as compared to gases of spherical grains of identical volume fraction [1]. Moreover, elongated particles provide the possibility to efficiently study the energy transfer between the translational and rotational degrees of freedom.

One particular problem is the reliable detection and tracking of the rods in 3D, especially at volume fractions beyond the very dilute limit. We have developed a Machine Learning aided approach to the experimental data analysis which allows to recognize and track individual particles in ensemble.

[1] K. Harth et al., Free cooling of a granular gas of rodlike particles in microgravity, Phys. Rev. Lett., 120 (2018), 214301

DY 33.4 Wed 10:30 ZEU 118

Influence of high temperature exposure on adhesive forces in chondritic material — •Cynthia Pillich[1,2], Tabea Bogdan[1], Joachim Landers[1,2], Gerhard Wurm[1], and Heiko Wende[1,2] — [1]Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

The growth of planetesimals at the so called „bouncing barrier“ is still not fully understood. Compositional and concomitant structural changes of protoplanetary dust induced by high temperatures in the vicinity of the young star might explain improved sticking at the mm-range. As meteorites contain primordial phases representing the material in our young solar system, they offer an insight into the mechanics of planetary formation. A fragment of the iron rich meteorite „Sayh al Uhaymir“ was ground and subsequently heated in vacuum at temperatures up to 1400 K and adhesive forces were determined by Brazilian tests after cooling down to room temperature. We present an altered behaviour of adhesive forces in meteoritic matter upon exposure to high temperatures accompanied by a compositional and structural change, which was investigated by ^{57}Fe Mössbauer spectroscopy probing the abundance of iron bearing phases.

Funding by the DFG (project WE 2623/19-1 and WU 321/18-1) is gratefully acknowledged.

DY 33.5 Wed 10:45 ZEU 118

Pauling Structures in Tribocharged Granular Media — •Philip Born, Jan Haeberle, and Matthias Sperl — Institut für Materialphysik im Weltraum, DLR e.V., Linder Höhe, 51147 Köln

Ordered, non-densest packings of granular particles are rarely observed. The hard core and the frictional contacts of the particles impose disordered packings, or, under suitable conditions like mobilization and small size dispersity of the particles, ordered densest packings with hexagonal symmetry. However, we could show that binary packings of granular particles with strong tribocharging take BCC-like packing structures under suitable conditions [1]. The observed packing behavior is to large extent in agreement with the prediction of Pauling's rules for ionic crystals, i.e., equilibrium structures of thermal ions. Here we want to discuss the observation that the Pauling structure is only observed in an incommensurate container, which may give a hint on the rules how granular media take equilibrium structures with suitable mobilization.

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

DY 33.6 Wed 11:00 ZEU 118

Particle shape-dependence of the stability properties of granular piles — •Steffen Richters-Finger and Stefan J. Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Germany

It is well known that the shape of particles has a major influence on the behavior of densely packed granular matter making it an important subject of interest for various applications. Multiple schemes for the numerical simulation of non-spherical particles have previously been proposed in the literature [1].

Applying a discrete function representation (DFR) approach for collision detection, we investigate the shape-dependence of the stability properties (e.g. critical angle of stability) of a granular pile in a two-dimensional discrete element model for a wide range of polar geometries generated by the so-called superformula [2].

[1] G. Lu, J.R. Third, C.R. Müller, Chem. Eng. Sci. 127, 425 (2015).
[2] J. Gielis, Am. J. Bot. 90, 333 (2003).

DY 33.7 Wed 11:15 ZEU 118

Using machine learning to identify variables of a granular theory — •Ansgar Kühn and Matthias Schröter — Max-Planck Institute for Dynamics and Self-organization (MPIDS), Göttingen, Germany

The prediction of contact numbers in granular packings using the local package fraction is described by a theory from [1]. In order to find higher order corrections to that theory, a more detailed descriptions of the local geometry is given by the Minkowski tensors of the Voronoi cell. With this data, machine learning provides a more accurate prediction of contact numbers than [1]. Thus, it can be used to identify new variables relevant for the prediction in order to expand the theory.

[1] Song, C., Wang, P., & Makse, H. A. (2008). Nature, 453, 629.

15 min. break.

DY 33.8 Wed 11:45 ZEU 118

Triboelectric charges in granular materials, from their measurement to their effects — •Geoffroy Lumay and Nicolas Vandewalle — GRASP Laboratory, CESAM Research Unit, University of Liège, Belgium

It is well known in industrial applications involving powders and granular materials that the presence of electrostatic charges influences drastically the material properties. The apparition of electrostatic charges is due to the triboelectric effect at the contacts between the grains and also at the contacts between the grains and the container. This triboelectric effect in granular materials is drastically influenced by humidity and is still poorly understood from a fundamental point of view. Moreover, reproducible electrostatic measurements are difficult to perform. A few years ago, we developed an experimental device dedicated to the measurement of powder triboelectric properties. This device is now commercialized under the name GranuCharge by the company GranuTools and measures the ability of a powder to charge electrostatically during a flow in contact with a selected material. In this presentation, we will analyse the link between powder electrostatic properties, hygrometry and powder macroscopic properties (packing fraction, cohesiveness, flow, ...) from a fundamental point of view. Afterward, we will show how flow aid agents can be used to decrease the

cohesiveness of industrial powders by playing a role on both capillary and electrostatic forces.

This study was conducted in the framework of the PowderReg project, funded by the European programme Interreg VA GR

DY 33.9 Wed 12:00 ZEU 118

Collective abrasion of pebbles — •János Török[1,2], András Sipos[1,3], and Gábor Domokos[1,2] — [1]MTA-BME Morphodynamics Research Group, Budapest University of Technology and Economics — [2]Department of Theoretical Physics, Budapest University of Technology and Economics — [3]Department of Mechanics, Materials and Structures, Budapest University of Technology and Economics

Fragments of rocks start their life after removal from their original position. Natural elements take over the formation of the resulting pebbles. Much is known about the evolution of the shapes of the pebbles depending on the size of the object they collide with. However the abrasion of these fragments never happens in a solitary manner rather it is a collective phenomenon.

We investigate the collective equations driving the particle size probability distribution functions and identify the stationary distributions. We examine the possible physical processes and derive the corresponding partial differential equations for the collective process. These physical models have to take into account the actual particle size distribution the collision probability, the relative velocities of the particles and the collision energy.

We analyze the resulting models using both stochastic simulation and direct simulations of the Fokker-Planck equations. We analytically identify the cases where unimodal or bimodal particle size distribution can be obtained in the stationary state.

DY 33.10 Wed 12:15 ZEU 118

Superballistic propagation of density correlations in quenched granular media — •Thomas Schindler[1], Christian M. Rohwer[2], and Sebastian C. Kapfer[1] — [1]Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — [2]Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany

We investigate granular particles in a shaken quasi two dimensional box in molecular dynamics computer simulations. After suddenly changing the shaking amplitude, transient density correlations are observed, that go beyond the steady state correlation length scale. Propagation of the correlations is faster than ballistic for increasing as well as decreasing amplitude, which is in contrast to recently investigated quenches of Brownian particles that show diffusive propagation. [1,2] When performing simulations with side walls, we find finite size effects for the wall pressure in steady state simulations and an additional transient pressure contribution when changing the shaking amplitude. We treat the question if the observed effects with and without side walls originate from the same mechanisms.

[1] Christian M Rohwer, Mehran Kardar, and Matthias Krüger. Transient Casimir Forces from Quenches in Thermal and Active Matter. Physical Review Letters, **118** (2017), 015702

[2] Christian M Rohwer, Alexandre Solon, Mehran Kardar, and Matthias Krüger. Nonequilibrium forces following quenches in active and thermal matter. Physical Review E, **97** (2018),032125

DY 33.11 Wed 12:30 ZEU 118

Flow study for transparent model system of concrete and cement paste — •Himanshu P Patel[1] and Günter K Auernhammer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Straße 6, D-01069 Dresden, Germany — [2]Max Planck Institute for Polymer Research, Ackermannweg 10 - D-55128 Mainz, Germany

The study of internal dynamics in a complex granular suspension, such as flowing concrete, poses couple of scientific challenges. Concrete, being opaque, restricts the possibility of optical observations. Non-optical techniques such as Ultrasonic and slipper test provides limited understanding.

We here demonstrate the development of highly transparent model system for concrete. The system is an optically transparent dense granular suspension (42% to 48% by volume) that mimics rheology behavior of concrete on the parameters of shear stress and viscosity. Further, we analyze the flow in continuous phase using specific experimental setup. The setup allows vertical and horizontal flow analysis, to understand shear and plug flow in addition to insight about lubrication layer formation. The study is part of understating flow induced particle migration for dense granular suspensions.

The flow profile of model concrete is observed using high-speed camera and tracer particles are used to undertake the study.

DY 34: Invited Talk

Time: Wednesday 9:30–10:00 Location: ZEU 160

Invited Talk DY 34.1 Wed 9:30 ZEU 160

Brownian systems with time-delay: non-equilibrium thermodynamics and connection to active systems — •Sabine H.L. Klapp and Sarah A.M. Loos — Institut für Theoretische Physik, TU Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Recently, the dynamics of stochastic systems involving time-delay has become a focus of growing interest. Time delay may originate, e.g., from a feedback control protocol, but it is also inherent in many living and active systems. The corresponding theoretical description is challenging due to the non-Markovian nature of the underlying Langevin equations [1]. Here we discuss such systems in terms of stochastic thermodynamics. Considering first a colloidal particle in a double-well potential and a time-delayed trap, we provide a novel analytical expression and numerical results for the heat production [2]. We then discuss systems with discrete and distributed delay, describing them by coupled Markovian equations involving n auxiliary variables with linear, yet *non-reciprocal* coupling [3]. We provide arguments that non-reciprocity inevitably leads to non-equilibrium as reflected by a broken fluctuation-dissipation theorem and nonzero entropy production. We also discuss connections to active systems, particularly the active Ornstein-Uhlenbeck model involving coloured noise.

[1] S. A. M. Loos and S. H. L. Klapp, Phys. Rev. E **96**, 012106 (2017); J. Stat. Phys. **77**, 95 (2019)
[2] S. A. M. Loos and S. H. L. Klapp, Sci. Rep. **9**, 2491 (2019)
[3] S. A. M. Loos, S. M. Hermann, S. H. L. Klapp, arXiv 1910.08372.

DY 35: Modelling and Simulation of Soft Matter I (joint session CPP/DY)

Time: Wednesday 9:30–13:00 Location: ZEU 255

Invited Talk DY 35.1 Wed 9:30 ZEU 255

Structure and dynamics of semiflexible polymers in bulk and confinement — •Arash Nikoubashman — Institut für Physik, Johannes Gutenberg Universität Mainz, Mainz, Deutschland

Semiflexible macromolecules are important constituents of living matter and also find various applications as versatile materials, in particular due to their possible liquid crystalline order. To better understand these systems, we employed coarse-grained molecular dynamics simulations to study lyotropic solutions of semiflexible polymers in the bulk as well as in confinement over a wide range of monomer densities, persistence lengths, and contour lengths. In bulk systems, we observed an isotropic-nematic transition and a nematic-smectic transition as the persistence length and monomer density were increased. Further, we found that semiflexible polymers exhibited a much lower diffusivity and higher shear viscosity compared to their flexible counterparts. Under spherical confinement, we discovered that densely packed semiflexible polymers could not anymore exhibit uniform nematic order when their contour length became of the same order as the sphere radius. Instead, confinement led to the emergence of topological defects on the sphere

surface with competing ordering in the interior of the sphere. Each of the configuration variables including chain length, chain stiffness, packing density, and shell thickness uniquely affected the ordering, including the nature and relative orientation of the defects on the surface.

DY 35.2 Wed 10:00 ZEU 255

Thermal conductivity of commodity plastics: From conventional to smart polymers — •Debashish Mukherji — Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver Canada

Polymers are an important class of soft matter whose properties are dictated by large fluctuations. Because of this reason commodity polymers are ideal for the flexible design of advanced materials. However, applications of polymers are often hindered by their low thermal conductivity κ. While low κ values are desirable for thermoelectric materials, they create severe problems when used under the high temperature conditions. Going from the polymers dictated by weak Van der Waals to hydrogen-bonded interactions, κ varies between 0.1-0.4 W/Km. Using molecular dynamics simulations we study thermal transport and its links to the elastic response of polymers. We find that there exists a maximum attainable stiffness, thus limiting an upper bound of κ. The specific chemical details and the glass transition temperature play no role in controlling κ, especially when the microscopic interaction is hydrogen bonded. These results are consistent with the minimum thermal conductivity model and experiments.

[1] D. Mukherji, C. M. Marques, K. Kremer, Annual Review of Condensed Matter Physics 11, 271 (2020). [2] D. Bruns, T. E. de Oliveira, J. Rottler, D. Mukherji, Macromolecules 52, 5510 (2019). [3] C. Ruscher, J. Rottler, C. Boott, M. J. MacLachlan, D. Mukherji, Physical Review Materials (accepted) (2019).

DY 35.3 Wed 10:15 ZEU 255

Polymer Architectures by Chain Walking Catalysis - Theory, Simulations, and Experiments — •Ron Dockhorn[1], Laura Plüschke[1,2], Albena Lederer[1,2], Jan Merna[3], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — [3]University of Chemistry and Technology Prague, CZ-16628 Praha, Czech Republic

Recently developed chain walking catalysis is an elegant approach to synthesize branched polyethylenes (CWPE) with controllable structure and properties. The catalyst is able to walk along the polymer and to polymerize ethylene and α-olefines into complex topologies depending on pressure, temperature, and olefine concentration introducing branch-on-branch structures. Coarse-grained Monte Carlo simulations utilizing the bond fluctuation model of the CWPE are performed to investigate the influence of the walking mechanism on the polymer architecture. For slow walking rates the structure growths with linear chain extensions, whereas fast walking rates promote dendritic growth of the polymer. The crossover regime is characterized by linear global features and dendritic local substructures contrary to randomly hyperbranched systems. Indeed, the obtained CWPE systems have characteristics of dendritic bottle brushes and the degree of branching can be adjusted by the walking rate of the catalyst. These findings are aimed to understand the physical properties of the CWPE structures and to improve the synthesis of a new class of hyperbranched molecules.

DY 35.4 Wed 10:30 ZEU 255

Morphology on Reaction Mechanism Dependency for Twin Polymerization — •Janett Prehl[1], Robin Masser[1], Peter Salamon[2], and Karl Heinz Hoffmann[1] — [1]Insitut für Physik, Technische Universität Chemnitz, Chemnitz, Germany — [2]Department of Mathematics and Statistics, San Diego State University, San Diego, USA

Within this presentation we will present our latest results [1] on the 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 the 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 can identify key factors to adapt structural properties to fulfill desired requirements for possible applications. Hereby, we point out which implications theses parameter changes have on the underlying chemical structure.

[1] 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

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

DY 35.5 Wed 10:45 ZEU 255

Effect of the Backbone Chemical Composition and Monomer Sequence on Phenylene Polymer Persistence Lengths — •Nancy C. Forero-Martinez[1], Björn Baumeier[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]University of Technology, P.O. BOX 513-5600 MB, Eindhoven, The Netherlands

The study of the physical properties of phenylene polymer precursors used in the fabrication of graphene nanoribbons poses open questions whose answers will contribute to the design of more efficient synthesis protocols. Particularly, size-exclusion chromatography combined with persistence length measurements assigns both, semiflexible to semirigid structures depending on the molecular weight of the precursor. Surprisingly, these results suggest an apparent structural change upon increasing the length of the polymer. In this work, we use a generic model to build phenylene polymer chains as random walks that take into consideration the nature of the arene substitutions along the backbone. In addition to conformational changes, this model allows one to study the backbone contribution to the persistence length by modifying a small set of parameters controlling chemical content and structure. We consider the flexibility of polyphenylene precursors in a theta-like solvent in terms of chain composition by building both, chains that are purely composed by meta or para connected repeat units, and randomly mixed chains with a given composition. We find that systems with apparently the same chemistry have different persistence length due to different monomer mixing ratios and sequence along the chain.

DY 35.6 Wed 11:00 ZEU 255

Structure of bottlebrush polymers end-grafted to a planar surface — •Jaroslaw Paturej[1], Paul Jungmann[2], Jens-Uwe Sommer[3], and Torsten Kreer[2] — [1]University of Silesia, Katowice, Poland — [2]IPF, Dresden, Germany — [3]Johannes Gutenberg Universität, Mainz, Germany

Polymer brush is a hybrid material composed of a solid substrate coated with end-grafted polymers. We conducted coarse-grained molecular dynamics simulations and scaling theory of the equilibrium structure of planar brushes formed by bottlebrush polymers. Bottlebrushes are branched macromolecules consisting of densely spaced linear side chains grafted along a central (linear) backbone. We elucidate the relationship between bottlebrush architecture, surface coverage σ and polymer brush thickness H. We study the impact of three length scales on the brush height H: D_0 , the cross-section radius of bottlebrushes determined by the degree of polymerization of side chains N_{sc} , R_0 the (overall) size of bottlebrushes controlled by the degree of polymerization of backbone N_{bb} and d the distance between nearest-neighbor tethering sites. The latter quantity provides a measure of molecular coverage σ of a substrate defined as the number of bottlebrush polymers per unit surface area $\sigma \propto 1/d^2$. Our theoretical analysis identifies three conformational regimes for the height H, which gradually establish upon increasing substrate coverage and stem from interplay between relevant length scales: d, D_0 and R_0.

15 min. break

DY 35.7 Wed 11:30 ZEU 255

Modeling Depletion Interactions in Blends of Branched and Linear Polymers — •Martin Wengenmayr[1,2], Ron Dockhorn[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]TU Dresden, Germany

Effective attractive interactions in colloidal systems are well understood and described by depletion potentials. Similar effective attractions have been found for a wide range of soft matter systems like brush coated particles and dendrimers as well. For colloidal particles the depletion potentials are deduced from volume exclusion layers around the hard particles, but this is not applicable for soft particles, which are interpenetrated by the depletant. In this work we present a mean field free energy approach modeling the origin of the soft matter depletion interactions by balancing the excess free energy between the soft particle and the depletant with the elastic repulsion between particles. This approach is adopted for a model system containing dendrimers as soft particles in the melt of linear polymer chains acting as depletant. From

recent investigations [1] it is known that the dendrimers display so called crowded conformations that are compact but not fully collapsed and the dendrimers are strongly interpenetrated by linear chains. The mean field model is compared with coarse grained computer simulations applying the bond fluctuation model. This work contributes to the understanding of soft matter interactions and provides predictions for the occurrence of depletion interactions in experimental setups.

[1] Wengenmayr, Dockhorn, Sommer; *Macromolecules* **2019**, 52, 2616-2626

DY 35.8 Wed 11:45 ZEU 255

Role of preferential adsorption in cononsolvency — •Swaminath Bharadwaj and Nico van der Vegt — Technische Universität Darmstadt, Germany

Cononsolvency is the phenomenon in which a polymer chain collapses in a mixture of good solvents. The solvation forces and interactions that drive this phenomenon however remain poorly understood. An important question which arises is whether the cononsolvency mechanism is generic. In this regard, studies have proposed simple and universal mechanisms depending on preferential cosolvent adsorption [1] and solvent-cosolvent clustering [2].

We demonstrate through computer simulations that cononsolvency is not a generic phenomenon driven by a universal interaction. We show that cononsolvency can occur with and without the preferential adsorption of the cosolvent and discuss the related experimental results [3]. We also discuss preliminary results on the role of attractive polymer-solvent/cosolvent interactions in cononsolvency. Our results highlight the need to understand the role of microscopic interactions in polymer solubility. The aforementioned generic models [1,2], though not universal, can still be employed on a case-by-case basis depending on the dominant underlying interactions.

[1]Mukherji, D., Marques, C. M. & Kremer, K. Nat. Commun. 5,4882 (2014).

[2]Zhang, G. & Wu, C. J. Am. Chem. Soc. 123, 1376 (2001)

[3]Bharadwaj, S. & van der Vegt, N. F. A. Macromolecules 52, 4131 (2019)

DY 35.9 Wed 12:00 ZEU 255

Mesoscopic modeling of disordered morphologies of blends and block-copolymers for light-emitting diodes — •Jianrui Zhang, Kurt Kremer, Jasper Michels, and Kostas Daoulas — Max Planck Institute for Polymer Research, Mainz, Germany

Experiments have demonstrated [1] that the luminous efficiency of polymer light emitting diodes can be significantly increased by blending the semiconducting polymer with an insulator. However, the limited thermodynamic stability of the disordered phase in polymer blends motivates the consideration of alternatives, e.g. block-copolymers (BCPs) comprising semiconducting and insulating blocks. We choose as model systems blends and BCPs of poly(p-phenylene vinylene) (PPV) and polyacrylates. Using a hybrid mesoscopic model, disordered morphologies of these blends and BCPs are obtained with Monte Carlo simulations. We study different compositions and vary the immiscibility to mimick annealing at different temperatures. We find that disordered blends and BCPs are heterogeneous because of fluctuations and local segregation. Local segregation is stronger in BCPs than in their equivalent blends, even though the strength of immiscibility, normalized by the mean-field spinodal, is the same. Using a qualitative charge-percolation model, we link the spatial distribution of PPV with electric conductance. We predict that the annealing temperature affects the electrical percolation in disordered BCPs much stronger than in blends. The observed differences between blends and BCPs are enhanced at high contents of insulator. [1] Abbaszadeh et al., Nature Materials 2016, 15, 628.

DY 35.10 Wed 12:15 ZEU 255

Chemically-transferable structure-based coarse-grained models — •Kiran H. Kanekal and Tristan Bereau — Max Planck Institute for Polymer Physics, Mainz, Germany

An attractive feature of the popular Martini [1] coarse-grained force field is its chemical transferability. Multiple chemical fragments can be assigned to the same Martini representation based on their similar hydrophobicity, maintaining thermodynamic accuracy in the resulting simulations [2]. However, since the Martini force field was optimized in order to reproduce certain thermodynamic properties of various condensed phase systems in a top-down fashion, it does not accurately portray the internal structures of these systems when compared to results from corresponding simulations at atomistic resolutions. On the other hand, implementing bottom-up coarse-graining approaches results in highly accurate structural properties by construction, yet these methods are traditionally performed on a small set of compounds, limiting their chemical transferability. In this work, we establish a new technique for building chemically-transferable coarse-grained models with high structural accuracy by coupling bottom-up coarse-graining methods with unsupervised machine learning. We validate our results by comparing our new model to Martini and show how changing the resolution of our coarse-grained model affects these results. 1. Marrink, S. J. & Tieleman, D. P. Chem. Soc. Rev. 42, (2013). 2. Menichetti, R., Kanekal, K. H. & Bereau, T. ACS Cent. Sci. 5, (2019).

DY 35.11 Wed 12:30 ZEU 255

Consistent representation of structural and dynamical properties from coarse-grained simulation models — •Joseph Rudzinski — Max Planck Institute for Polymer Research, Mainz, Germany

"Bottom-up" coarse-grained models retain chemical specificity by targeting the reproduction of properties from a higher-resolution reference model. These models are inherently limited by the molecular representation, set of interaction potentials, and parametrization method. These limitations often result in an inaccurate description of cross-correlations between coarse-grained degrees of freedom, complicating the stabilization of hierarchical structures in soft matter systems. Perhaps more troubling, reduced molecular friction and softer interaction potentials obscure the connection to the true dynamical properties of the system. In this talk, I will discuss the relationship between these two problems and introduce methodologies for characterizing and improving the dynamical properties generated by coarse-grained simulation models.

DY 35.12 Wed 12:45 ZEU 255

Coarse graining of Bovine serum albumin (BSA) — •Frank Hirschmann[1], Hender López[2], and Martin Oettel[1] — [1]University of Tübingen — [2]Dublin Institute of Technology

The intercellular medium of living cells typically contains biomolecules (such as proteins) at high packing fractions, which directly affects diffusive and transport properties of the suspended components. Additionally, molecular shape plays a key role for interactions in crowded environments.

To treat these systems computationally, we present a coarse grained model of the globular antibody BSA, which neglects full atomistic details, but enables access to larger system sizes of hundreds to thousands of molecules. Using Brownian dynamics, we present static and dynamic properties of different implementations of our model. A particular emphasis is on the influence of molecule flexibility on diffusion coefficients. A comparison is made with an already existing coarse grained model of γ-Globulin (IgG), which is a significantly more flexible molecule.

DY 36: Stochastic Thermodynamics

Time: Wednesday 10:00–11:30 Location: ZEU 147

DY 36.1 Wed 10:00 ZEU 147

Operationally Accessible Bounds on Fluctuations and Entropy Production in Periodically Driven Systems — •Timur Koyuk and Udo Seifert — II. Institut für Theoretische Physik

For periodically driven systems, we derive a family of inequalities that relate entropy production with experimentally accessible data for the mean, its dependence on driving frequency, and the variance of a large class of observables [1]. With one of these relations, overall entropy production can be bounded by just observing the time spent in a set of states. Among further consequences, the thermodynamic efficiency both of isothermal cyclic engines like molecular motors under a periodic load and of cyclic heat engines can be bounded using experimental data without requiring knowledge of the specific interactions within

the system. We illustrate these results for a driven three-level system and for a colloidal Stirling engine.

[1] T. Koyuk and U. Seifert, Phys.Rev.Lett.122, 230601(2019).

DY 36.2 Wed 10:15 ZEU 147

Stochastic thermodynamics of processes coupled to finite reservoirs — •Jonas Fritz, Basile Nguyen, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart, Germany

Biomolecular processes are typically modeled using chemical reaction networks coupled to infinitely large chemical reservoirs. Through a chemical free energy difference between reservoirs, the system can be driven into a non-equilibrium steady state (NESS). In reality, cells are finite systems containing a finite number of molecules. In such systems, a NESS can be reached with the help of an externally driven pump. We introduce a simple model for finite-size chemical reservoirs with such a pumping mechanism. Crucial parameters then are the pumping rate and the size of the chemical reservoir. We apply this model to a simple biochemical oscillator, the Brusselator, and quantify the performance using the number of coherent oscillations. As a surprising result, we find that higher precision can be achieved with finite-size reservoirs, even though fluctuations there are larger.

DY 36.3 Wed 10:30 ZEU 147

Quantifying information for a stochastic particle in a flow-field — •Evelyn Tang[1] and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom

Quantification of information in small fluctuating systems has seen great theoretical progress recently, and been experimentally measured in a variety of systems from colloids and electrons to active and living matter. However, these questions have not been explored in flow-fields, which are ubiquitous in microfluidics, solid-state and biological systems. In the latter, such flows transport vital signalling molecules necessary for system function. We develop a general expression for the rate of change of information content in flow-fields to identify relevant contributions from both flow features and systems fluctuations. Further, we calculate the time evolution for particles in generic flow-fields, and use this to analyze the information content and residence time scale for various geometries and scenarios. For instance, this allows the identification of a mechanism for retaining a particle for longer times than diffusion. We identify the dependence of information content on various flow features and find the long time behavior of the change of information content and particle probability. Intriguingly, vorticity produces oscillations in the probability density but only enters the change of information content when there is an additional symmetric field component.

DY 36.4 Wed 10:45 ZEU 147

Stochastic thermodynamics of a sheared nanoclutch — •Sascha Gerloff and Sabine H. L. Klapp — Hardenbergstr. 36, D-10623 Berlin

Colloidal nanomachines convert optical-, electromagnetic-, acoustic- or chemical energy into *usefull* mechanical motion. Applications include colloidal microswimmers actuated by an external magnetic field [1] and sheared nanoclutches [2]. In the framework of stochastic thermodynamics, these nanomachines provide a powerful testing bed to explore this conversion of energy, which is related to the microscopic many-body dynamics of the colloids [3]. Following previous experimental studies [2], we focus on a sheared nanoclutch system, which consists of a circular, two-dimensional cluster of colloids that is confined between two rings and driven by optical- and magnetic fields. This system displays a complex non-linear mechanical response, characterized by shear-thinning, local shear-thickening and shear-banding. Performing (overdamped) Stokesian dynamics, we now turn to analyze the stochastic nature of the work and heat produced by this machine. In particular, we investigate how the many-body character of the non-equilibrium dynamics is reflected by the fluctuations of the thermodynamic quantities in the presence of hydrodynamic interactions.

[1] F. Martinez-Pedrero et al., *Phys. Rev. Lett.* **13**, 138301 (2015)
[2] A. Ortiz-Ambriz et al., *Soft Matter* **14**, 5121 (2018)
[3] S. Gerloff and S. H. L. Klapp, *Phys. Rev. E* **98**, 062619 (2018).

DY 36.5 Wed 11:00 ZEU 147

Affinity-dependent bound on the spectrum of stochastic matrices — •Matthias Uhl and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Affinity has proven to be a useful tool for quantifying the non-equilibrium character of time continuous Markov processes since it serves as a measure for the breaking of time reversal symmetry. It has recently been conjectured that the number of coherent oscillations, which is given by the ratio of imaginary and real part of the first non-trivial eigenvalue of the corresponding master matrix, is constrained by the maximum cycle affinity present in the network. In this talk, we present a conjectured bound on the whole spectrum of these master matrices that constrains all eigenvalues in a fashion similar to the well known Perron-Frobenius theorem that is valid for any stochastic matrix. As in other studies that are based on affinity-dependent bounds, the limiting process that saturates the bound is given by the asymmetric random walk. For unicyclic networks, we prove that it is not possible to violate the bound by small perturbation of the asymmetric random walk and provide numerical evidence for its validity in randomly generated networks. The results are extended to multicyclic networks, backed up by numerical evidence provided by networks with randomly constructed topology and transition rates.

DY 36.6 Wed 11:15 ZEU 147

Non-reciprocal hidden degrees of freedom: an attempt to define entropy production in non-Markovian systems — •Sarah A. M. Loos, Simon M. Hermann, and Sabine H. L. Klapp — TU Berlin, Hardenbergstr. 36, 10623 Berlin

Real-world stochastic systems are often non-Markovian. This might be due to hydrodynamic backcoupling, viscoelastic effects, persistence in active swimmers, or an external feedback control loop acting on the system. Despite the omnipresence of memory, the incorporation of non-Markovian dynamics in the framework of stochastic thermodynamics is poorly understood [1,2]. In fact, fundamental problems remain, which are associated with the acausality of the backward process in the total entropy production functional. We discuss this crucial issue focusing on the case of discrete time delay, and show the implications of different approaches. As a first example, we review the outcome of a direct calculation on the basis of the acausal path integrals, which requires redefining the definition of entropy production, and, in fact, yields a functional which by construction cannot be calculated for any nonlinear system. Furthermore, we suggest a Markovian embedding approach [3]. While this strategy allows us to employ the standard formulae and is technically much simpler, it demands the interpretation of entropy production of auxiliary variables. For the case of a feedback controller, we offer an appropriate interpretation.

[1] Munakata, Rosinberg, PRL 112, 180601 (2014).
[2] Loos, Klapp, Sci. Rep. 9, 2491 (2019).
[3] Loos, Hermann, Klapp, preprint: arXiv:1910.08371 (2019).

DY 37: Active Matter IV (joint session DY/CPP/BP)

Time: Wednesday 10:00–12:30 Location: ZEU 160

DY 37.1 Wed 10:00 ZEU 160

Quantitative Assessment of the Toner and Tu Theory of Polar Flocks — •Benoît Mahault[1,2], Francesco Ginelli[3,4], and Hugues Chaté[1,5,6] — [1]Service de Physique de l'Etat Condensé, CEA, CNRS, Université Paris-Saclay, CEA-Saclay, France — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Germany — [3]University of Aberdeen, United Kingdom — [4]Università degli Studi dell'Insubria, Italy — [5]Beijing Computational Science Research Center, China — [6]LPTMC, CNRS UMR 7600, Université Pierre et Marie Curie, France

We present a quantitative assessment of the Toner and Tu theory describing the universal scaling of space-time correlations functions in polar phases of dry active matter. Using large-scale simulations of the

Vicsek model in two and three dimensions, we find the overall phenomenology and generic algebraic scaling predicted by Toner and Tu, but our data on density correlations reveal some qualitative discrepancies. The values of the associated scaling exponents we estimate differ significantly from those conjectured in 1995. In particular, we identify a large crossover scale beyond which flocks are only weakly anisotropic. We discuss the meaning and consequences of these results.

DY 37.2 Wed 10:15 ZEU 160

Swirl formation of active colloids near criticality — •Robert C. Löffler, Tobias Bäuerle, and Clemens Bechinger — Fachbereich Physik, Universität Konstanz, Konstanz D-78464, Germany

Animal groups like flocks of birds or schools of fish normally show a high degree of order. Yet they are also responsive to external factors in order to optimize nutrition and avoid predation. Various observations of such responsiveness have let to the assumption that those systems represent a state of order close to a critical point. In our experiments, we use light-responsive active Brownian particles (ABPs) to which we can apply individual torques in a feedback controlled system to study such behavioral rules. The propulsion applied to each ABP is thereby calculated based on information about its local neighbors. Through the variation of a single parameter in our interaction model, which is related to zonal models used in theoretical biology, we observe a continuous phase transition in the collective motion of the group: The ABPs transition from a disordered swarm to a stable swirl (i.e. milling, vortex-like state). Being able to continuously change our control parameter we can also measure the susceptibility of the collective motion, peaking at a critical point within the transition. Observation of such critical behavior in simple models not only allows for more insight in complex animal behavior but also helps with designing future rules for collective tasks in robotic or other autonomous systems.

T. Bäuerle *et al., Nat. Comm.* **9**, 3232 (2018); F. A. Lavergne *et al., Science* **364**, 70-74 (2019).

DY 37.3 Wed 10:30 ZEU 160

Probing mechanical properties of rod-shaped colloidal suspensions with active particles — •N Narinder and Clemens Bechinger — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Recently self-propelled colloidal particles have been shown to provide a novel tool to probe the mechanical properties of colloidal glassy states of spherical particles [1]. Unlike conventional micro-rheology, where one studies the coupling between the translational motion of a driven probe particle to a background, here the coupling of the host medium to the rotational dynamics of the self-propelled particle contains information about the mechanical properties of the host medium. Here, we apply this method to study the mechanical properties of assemblies of rod-shaped particles with a mean aspect ratio of 15. Such anisotropic colloidal suspensions exhibit a rather rich phase behavior including a two-step glass transition at the aspect ratio considered here [2]. Our first results demonstrate a strong variation of the rotational dynamics of the active particle with increasing area fraction of the rods.

[1] C. Lozano, J.R. Gomez-Solano, & C. Bechinger Nature Materials 18, 1118-1123 (2019).

[2] Z. Zheng, F. Wang, & Y. Han PRL 107, 065702 (2011).

DY 37.4 Wed 10:45 ZEU 160

Statistical mechanical sum rules for active colloids at surfaces - a touch of equilibrium — •René Wittmann[1,2], Frank Smallenburg[3], and Joseph Brader[2] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Soft Matter Theory, Université de Fribourg, Switzerland — [3]Laboratoire de Physique des Solides, Université Paris Sud, France

We study the mechanical properties of active particles in the presence of curved walls by computer simulation of Active Brownian Particles (ABPs), Active Ornstein-Uhlenbeck Particles (AOUPs) and a passive system with effective interactions [R. Wittmann, F. Smallenburg and J. M. Brader, J. Chem. Phys. 150, 174908 (2019)]. The effective theory admits analytic results for pressure, surface tension and adsorption of an active ideal gas at a two-dimensional circular wall. It further predicts that an equilibrium sum rule also holds for active fluids, which we confirm numerically for both ABPs and AOUPs in the limit of small curvature.

More precisely, we find within each model that the slope of the pressure as a function of the curvature equals the surface tension and adsorption (up to an effective temperature scale) on a planar wall. Intriguingly, the explicit value of these coefficients is model-dependent, which can be explained by the different velocity distributions. We also discuss the influence of interactions and find that the effect of curvature on the wall pressure is reduced when increasing the density. Within numerical accuracy, the equality of the slope of the pressure and the planar surface tension appears to hold at finite density.

DY 37.5 Wed 11:00 ZEU 160

Lorentz forces induce inhomogeneity and flux in active systems — •Hidde Vuijk[1], Jens-Uwe Sommer[1,2], Holger Merlitz[1], Joseph Brader[3], and Abhinav Sharma[1,2] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Universite de Fribourg, Fribourg, Switserland

We consider the dynamics of a charged active Brownian particle in three dimensions subjected to the Lorentz force due to an external magnetic field. We show that in the presence of a field gradient, a macroscopic flux emerges from a flux-free system and the density distribution becomes inhomogeneous. The flux is induced by the gradient of the magnetic field only and does not require additional symmetry breaking such as density or potential gradients, which stands in marked contrast to similar phenomena in condensed matter such as the classical Hall effect. We further demonstrate that passive tracer particles can be used to measure the essential effects caused by the Lorentz force on the active particle bath, and we discuss under which conditions this diffusive Hall-like effect might be observed experimentally. Lastly, we show that similar effects arise in case of inhomogeneous activity in combination with a constant magnetic field.

15 min. break.

DY 37.6 Wed 11:30 ZEU 160

Interaction of Active Crystallites within the Active Phase-Field-Crystal Model — •Lukas Ophaus[1], Johannes Kirchner[2], and Uwe Thiele[1,2] — [1]Center for Nonlinear Science, Münster, Germany — [2]Institut für Theoretische Physik, Münster, Germany

We use the active phase-field-crystal (PFC) model, developed by Menzel and Löwen as a model for crystallizing self-propelled particles [1], to study the interaction of traveling crystalline patches. Within the active PFC model, these localized states exist besides periodic states, i.e., spatially extended crystals [2]. Due to the activity, crystalline states undergo a drift instability and start to travel while keeping their spatial structure. Using results for the parameter ranges where the individual states exist, we explore how two and more traveling localized states interact by performing numerical collision experiments. We show that a critical minimal free path is necessary to preserve the number of colliding localized states and that the active PFC model fails to exhibit dynamical clustering and motility induced phase separation.

[1] A.M. Menzel and H. Löwen, Phys. Rev. Lett. 110, 055702 (2013)

[2] L. Ophaus, S.V. Gurevich and U. Thiele, Phys. Rev. E 98, 022608 (2018)

DY 37.7 Wed 11:45 ZEU 160

Continuum model for bacterial suspensions with density variations — •Vasco Marius Worlitzer[1], Avraham Be'er[2], Gil Ariel[3], Markus Bär[1], Holger Stark[4], and Sebastian Heidenreich[1] — [1]Physikalisch-Technische Bundesanstalt — [2]Ben-Gurion University — [3]Bar-Ilan University — [4]Technical University of Berlin

The various dynamical states found in bacterial suspensions are a fascinating illustration of the rich dynamics exhibited by active polar fluids. A recent study explored the phase space experimentally, identifying three major states: single-cell motion, collective swarming, biofilm formation and mixtures between them [1]. While a continuum model presented in [2] has been proven to describe the statistical features of the swarming phase quite successfully, it is not applicable outside this regime as a constant density is assumed. We show that new dynamical states are accessible by relaxing this assumption. In particular a regime similar to the mixed state of swarming and biofilm formation is covered, showing the same anomalous statistics as found experimentally. The new model is inspired by work on scalar active matter [3] and consist of a generic continuity equation for the density. The density is coupled to a local polar order parameter through a density dependent self-propulsion speed and an active pressure.

[1] H Jeckel et al., PNAS 116 (5) (2019) [2] J Dunkel et al., Phys. Rev. Lett. 110 (2013) 228102. [3] J Bialké et al., EPL 103 (2013) 30008.

DY 37.8 Wed 12:00 ZEU 160

A minimal model for dynamical symmetry breaking in active matter — Matt Davison and •Patrick Pietzonka — Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK

It is well known that asymmetrically shaped passive particles immersed in active matter move in a persistent direction. Recent work provides a thermodynamic framework and design principles for engines exploiting this mechanism [1]. We build on these results and reveal that symmetric passive particles in contact with active matter perform such a persistent motion as well. Its direction is determined through spontaneous symmetry breaking and remains fixed in time in the limit of a large number of active particles. We present an analytically solvable one-dimensional model for a single passive particle interacting with many active particles, which provides a physical understanding of these effects.

[1] P. Pietzonka *et al.*, Phys Rev. X **9**, 041032 (2019)

DY 37.9 Wed 12:15 ZEU 160

Self-propelled thermophoretic colloidal swimmers — •Sergi Roca-Bonet and Marisol Ripoll — Theoretical Soft Matter and Biophysics, Institute of Complex Physics, Forschungszentrum Jülich, Germany

Self-propelled phoretic colloids have recently emerged as a promising avenue for the design of artificial microswimmers. We employ a hydrodynamic fluctuating mesoscale simulation approach to study both single and collective swimming. We investigate self-propelled colloidal multimers in which one monomer can eventually get higher temperature, and it is linked with one or more other monomers which induce the multimer motion. Single colloid swimming properties are varied by changing the number of the constituting monomers (here two or three), their spatial arrangement (rod-like or v-like) and the relative sizes of such monomers. We have investigated the effect of slid confinement in comparison to the 3d-bulk motion of these dimeric and trimeric colloids. The collective system properties are determined by the competition between hydrodynamic and phoretic interactions which vary as a function of the density, the colloid geometry, and the monomers phoretic affinity (philic or phobic). Examples of the resulting behaviour are clustering, swarming, or rotational motions.

DY 38: Partial Synchronization Patterns in Neuronal Networks I (Focus Session joint with DY / SOE / BP) (joint session SOE/DY)

Understanding the dynamics of the human brain is one of the main scientific challenges today. Synchronization is important for information transmission in the brain and also plays a central role in various neurological diseases, such as Alzheimer's disease and epilepsy, for example. It is therefore crucial to develop and analyze models of brain circuits in which various synchronization patterns appear. In this focus session we show how these patterns emerge in models of neuronal networks, with particular attention to chimera states, solitary states but also with a broader outlook on partial synchronization in general. We aim to bring together scientists from different backgrounds to share ideas, in particular on analogies between partial synchronization in model systems and physiological processes in the brain. (Session organized by Giulia Ruzzene and Iryna Omelchenko)

Time: Wednesday 15:00–17:15 Location: GÖR 226

Invited Talk DY 38.1 Wed 15:00 GÖR 226

Cross frequency coupling in next generation inhibitory neural mass models — •Simona Olmi[1], Andrea Ceni[2], David Angulo Garcia[3], and Alessandro Torcini[4] — [1]Inria Sophia Antipolis Mediterranee Research Centre, 2004 Route des Lucioles, 06902 Valbonne, France — [2]Department of Computer Science, College of Engineering, Mathematics and Physical Sciences, University of Exeter, UK — [3]Grupo de Modelado Computacional - Dinamica y Complejidad de Sistemas. Instituto de Matematicas Aplicadas, Universidad de Cartagena, Colombia — [4]Laboratoire de Physique Theorique et Modelisation, Universite de Cergy-Pontoise, 95302 Cergy-Pontoise cedex, France

Coupling among neural rhythms is one of the most important mechanisms at the basis of cognitive processes in the brain. In this study we consider a neural mass model, rigorously obtained from the microscopic dynamics of an inhibitory spiking network with exponential synapses, able to autonomously generate collective oscillations. Furthermore, we show that two inhibitory populations in a master-slave configuration with different synaptic time scales can display various collective dynamical regimes: namely, damped oscillations towards a stable focus, periodic and quasi-periodic oscillations, and chaos. Finally, when bidirectionally coupled, the two inhibitory populations can exhibit different types of θ-γ cross-frequency couplings: namely, phase-phase and phase-amplitude cross-frequency couplings.

Topical Talk DY 38.2 Wed 15:30 GÖR 226

Brain functional connectivity asymmetry — •Jaroslav Hlinka — Institute of Computer Science of the Czech Academy of Sciences, Prague, Czech Republic

The brain is one of the iconic complex systems with a very intricate structure of interconnections and interactions among its many parts. It is also commonly studied via application of graph-theoretical approaches [1], while the representative graph can be defined using the functional connectivity approach: two brain regions are considered connected to an extent given by the strength of their activity synchronization, assessed by the statistical dependence between their activity as sampled over time, typicaly by linear correlation [2]. The human brain is organized into two almost symmetrical hemispheres, with the hemispheres containing further subdivision into key subnetworks/modules. However, there is some level of asymmetry that is known to be functionally relevant; in the current contribution we provide evidence that the left hemisphere functional connectivity, experimentally observed in resting state by functional magnetic resonance imaging, has more modular structure. We further discuss the origin of this asymmetry in structure or dynamics [3], its functional relevance and robustness with respect to methodological choices.

[1] Bullmore, E. et al. Nature Reviews Neuroscience, 2009, 10, 186-198

[2] Hlinka, J. et al. NeuroImage, 2011, 54, 2218-2225

[3] Hlinka, J. & Coombes, S., European Journal of Neuroscience, 2012, 36, 2137-2145

Topical Talk DY 38.3 Wed 16:00 GÖR 226

Partial Synchronization Patterns in the Brain — •Eckehard Schöll — Institut für Theoretische Physik, Technische Universität Berlin

Partial synchronization patterns play an important role in the functioning of neuronal networks, both in pathological and in healthy states. They include chimera states, which consist of spatially coexisting domains of coherent (synchronized) and incoherent (desynchronized) dynamics. We show that partial synchronization scenarios are governed by a delicate interplay of local dynamics, network topology, and time delay. Our focus is in particular on applications of brain dynamics like unihemispheric sleep [1], epileptic seizure [2], and relay synchronization between distant areas of the brain.

[1] Ramlow, L., Sawicki, J., Zakharova, A., Hlinka, J., Claussen, J. C. and Schöll, E., Partial synchronization in empirical brain networks as a model for unihemispheric sleep, EPL 126, 50007 (2019), highlighted in phys.org https://phys.org/news/2019-07-unihemispheric-humans.html and Europhys. News 50 no.5-6 (2019).

[2] Chouzouris, T., Omelchenko, I., Zakharova, A., Hlinka, J., Jiruska, P. and Schöll, E., Chimera states in brain networks: empirical

neural vs. modular fractal connectivity, Chaos 28, 045112 (2018).

DY 38.4 Wed 16:30 GÖR 226

Coexistence of fast and slow gamma oscillations in one population of inhibitory spiking neurons — Hongjie Bi, Marco Segneri, Matteo di Volo, and •Alessandro Torcini — Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, CNRS, UMR 8089, Cergy-Pontoise, France

Oscillations are a hallmark of neural population activity in various brain regions with a spectrum covering a wide range of frequencies. Within this spectrum gamma oscillations have received particular attention due to their ubiquitous nature and to their correlation with higher brain functions. Recently, it has been reported that gamma oscillations in the hippocampus of behaving rodents are segregated in two distinct frequency bands: slow and fast. These two gamma rhythms correspond to different states of the network, but their origin has been not yet clarified. We show that a single inhibitory population can give rise to coexisting slow and fast gamma rhythms corresponding to collective oscillations of a balanced spiking network. The slow and fast gamma rhythms are generated via two different mechanisms: the fast one being driven by the coordinated tonic neural firing and the slow one by endogenous fluctuations due to irregular neural activity. Furthermore, to make a closer contact with the experimental observations, we consider the modulation of the gamma rhythms induced by a slower (theta) rhythm driving the network dynamics. In this context, depending on the strength of the forcing and the noise amplitude, we observe phase-phase coupling with different theta-phases preferences for the two coexisting gamma rhythms.

DY 38.5 Wed 17:00 GÖR 226

Solitary States in Neural Networks — •Leonhard Schülen and Anna Zakharova — Institut für theoretische Physik, Technische Universität Berlin, Deutschland

Understanding mechanisms of desynchronization plays a significant role in the study of neural networks. Dynamical scenario of transition from pathological neural synchrony to a healthy state can involve partial synchronization patterns, such as chimera states or solitary states. The term "solitary" comes from the Latin "solitarius" and can be understood as "alone", "lonely", or "isolated". In the case of chimera states, a network spontaneously splits into coexisting domains of synchronized and desynchronized behavior, which are localized in space. For solitary states, on the contrary, it is typical that individual "solitary" oscillators split off from the synchronized cluster at random positions in space. Here we discuss the formation of solitary states and, in particular, the conditions under which these patterns occur in one-layer and two-layer networks of oscillatory FitzHugh-Nagumo neurons. Furthermore, we present a technique that allows to engineer solitary states. By delaying links of selected nodes we are able to control their position and displacement with respect to the synchronized cluster.

DY 39: Quantum Chaos (joint session DY/TT)

Time: Wednesday 15:00–19:00 Location: HÜL 186

Invited Talk DY 39.1 Wed 15:00 HÜL 186

Supersymmetric Polarization Anomaly in Photonic Discrete-Time Quantum Walks — •Sonja Barkhofen[1], Lennart Lorz[1], Thomas Nitsche[1], Christine Silberhorn[1], and Henning Schomerus[2] — [1]Applied Physics, University of Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom

Quantum anomalies lead to finite expectation values that defy the apparent symmetries of a system. These anomalies are at the heart of topological effects in electronic, photonic, and atomic systems, where they result in a unique response to external fields but generally escape a more direct observation. Here, we implement an optical-network realization of a discrete-time quantum walk, where such an anomaly can be observed directly in the unique circular polarization of a topological midgap state. We base the system on a single-step protocol overcoming the experimental infeasibility of earlier multistep protocols. The evolution combines a chiral symmetry with a previously unexplored unitary version of supersymmetry. Having experimental access to the position and the coin state of the walker, we perform a full polarization tomography and provide evidence for the predicted anomaly of the midgap states. This approach opens the prospect to dynamically distill topological states for quantum information applications.

DY 39.2 Wed 15:30 HÜL 186

Corrected perturbation theory for transverse-electric whispering-gallery modes in deformed microdisks — •Manuel Badel and Jan Wiersig — Postfach 4120, D-39016 Magdeburg, Germany

The perturbation theory by Ge et al. [Phys. Rev. A 87, 023833 (2013)] for transverse-electric polarized modes in weakly deformed microdisks omits terms related to the variation of the normal derivative of the magnetic field along the boundary. We show that these terms are necessary to accurately describe microdisks with a strongly winding boundary. In particular, it is demonstrated that the corrected perturbation theory allows one to describe the counterintuitive phenomenon of Q-factor enhancement due to weak boundary deformation, examplified by the microflower cavity. Good agreement of the corrected perturbation theory with full numerical results is observed.

DY 39.3 Wed 15:45 HÜL 186

Controlling chaos in the quantum regime using adaptive measurements — •Jessica Eastman[1,2,3], Stuart Szigeti[1], Joseph Hope[1], and André Carvalho[3] — [1]Department of Quantum Science, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601, Australia — [2]Centre for Quantum Computation and Communication Technology (Australian Research Council), Griffith University, Brisbane, Queensland 4111, Australia — [3]Centre for Quantum Dynamics, Griffith University, Brisbane, Queensland 4111, Australia

The continuous monitoring of a quantum system strongly influences the emergence of chaotic dynamics near the transition from the quantum regime to the classical regime. Here we present a feedback control scheme that uses adaptive measurement techniques to control the degree of chaos in the driven-damped quantum Duffing oscillator. This control relies purely on the measurement backaction on the system, making it a uniquely quantum control, and is only possible due to the sensitivity of chaos to measurement. We quantify the effectiveness of our control by numerically computing the quantum Lyapunov exponent over a wide range of parameters. We demonstrate that adaptive measurement techniques can control the onset of chaos in the system, pushing the quantum-classical boundary further into the quantum regime.

DY 39.4 Wed 16:00 HÜL 186

Microstar cavities: An alternative concept for the confinement of light — •Julius Kullig[1], Xuefeng Jiang[2], Lan Yang[2], and Jan Wiersig[1] — [1]Institut für Physik, Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany — [2]Department of Electrical and Systems Engineering, Washington University in St. Louis, St. Louis, USA

We report on a novel concept to confine light in a microcavity. In contrast to traditional approaches we exploit neither total internal reflection nor a photonic band gap. Our approach is rather based on the perfect transmission of light at Brewster's angle. Thus, in a properly designed star-shaped cavity light rays can sequentially leave and reenter the cavity along a periodic orbit without loss of intensity. Accordingly, in the wave dynamics long-lived optical modes arise with fascinating and unique properties.

DY 39.5 Wed 16:15 HÜL 186

Investigations on the spectral density of kicked spin chains — •Felix Meier, Daniel Waltner, Petr Braun, and Thomas Guhr — Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Deutschland

We study the semiclassical description of locally interacting spin chains whose individual constituents are identical to the kicked-top model. The magnetic field inducing the periodically applied kicks is chosen so that the model is quantum mechanically non-integrable for all possi-

ble spin representations. The classical analog of the spin chain is a collection of coupled Bloch vectors, whose dynamics is described stroboscopically. The corresponding classical phase space features highly mixed behavior with regular and chaotic motion occuring simultaneously. We investigate the structure of the quantum spectral density for different particle numbers and system parameters, which send the classical analog through a number of bifurcations.

DY 39.6 Wed 16:30 HÜL 186

Many-Body Densities of States on Quantum Graphs — •Adrian Seith[1], Gregor Tanner[2], Stephen Creagh[2], Klaus Richter[1], and Juan-Diego Urbina[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Universitätsstraße 31 D-93053 Regensburg — [2]School of Mathematical Sciences, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

We study the bulk density of states in non-interacting many-body systems on a quantum graph, a one-dimensional network of connected bonds on which the wave function is a solution of the one-dimensional Schrödinger equation.

In [1], Kottos & Smilansky derived a trace formula for the spectrum of a one-particle quantum graph using a secular equation and a transfer operator that describes the dynamics of the system. In [2], Bolte & Kerner show that the DOS of a many-body quantum graph follows an asymptotic Weyl law. We derive an explicit expression of the many-particle DOS on quantum graphs for distinguishable and indistinguishable particles and extend Smilansky's transfer operator approach to many-body systems using Bogomolny's formalism [3] so that we can give a geometric interpretation of many-body quantum graphs and the principle of indistinguishability and pave the way to include interaction effects.

[1] T. Kottos, U. Smilansky. Annals of Physics, Vol. 274 (1999)
[2] J. Bolte, J. Kerner. Journal of Mathematical Physics 55, (2014)
[3] E. B. Bogomolny. Nonlinearity, Vol. 5 (1992)

DY 39.7 Wed 16:45 HÜL 186

New insights on the semiclassical study of many-body interference in Fermionic Fock space: a path integral approach — •Wolfgang Hogger, Juan-Diego Urbina, Falk Bruckmann, and Klaus Richter — Universität Regensburg

A long standing goal of quantum chaos is to establish the classical limit of Fermionic fields and to follow the corresponding semiclassical program. Following Gutzwiller, we propose to apply the stationary phase approximation to the coherent state path integral for bosons on a lattice and transforming a Fermionic system into the latter by subsequent use of Jordan-Wigner transformation and Schwinger-boson mapping. However, it was shown by Wilson and Galitzki in PRL 106, 110401 (2011) how the coherent state path integral breaks down for the Bose-Hubbard model and simple spin systems. Since the issues with the partition function path integral for the aforementioned systems were solved by Bruckmann and Urbina in arXiv:1807.10462v1 through dualization (a known method from lattice quantum field theories), the correct perturbative expansion is now correctly reproduced and one can obtain a path integral for the propagator as well. As a second key ingredient, thanks to a novel transformation in the spirit of Jordan-Wigner providing an exact map from many Fermionic degrees of freedom to a single large spin, we now obtain also a well-defined classical limit. Combining these two insights, a semi-classical theory of generic Fermi-Hubbard models is finally constructed and applied to some simple examples.

15 min. break.

DY 39.8 Wed 17:15 HÜL 186

Geometry of complex instability in four-dimensional symplectic maps — •Jonas Stöber[1,2] and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik — [2]MPI für Physik komplexer Systeme, Dresden

In four-dimensional symplectic maps complex instability of periodic orbits is possible, which cannot occur for the two-dimensional case. We investigate the transition from stable to complex unstable dynamics of a fixed point under parameter variation. The change in the geometry of regular structures is visualized using three-dimensional phase-space slices and in frequency space using the example of two coupled standard maps. The chaotic dynamics is studied using escape time plots and two-dimensional invariant manifolds associated with the complex unstable fixed point. Based on a normal-form description, we investigate the underlying transport mechanism by visualizing the escape paths and the long-time confinement in the surrounding of the complex unstable fixed point. Consequences for the quantum wave-packet dynamics are illustrated.

DY 39.9 Wed 17:30 HÜL 186

Quantum signatures of separatrix crossing: self-trapping in high dimensional Bose-Hubbard systems — •Mathias Steinhuber[1], Steven Tomsovic[2], Remy Dubertrand[1], Klaus Richter[1], and Juan-Diego Urbina[1] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Department of Physics and Astronomy, Washington State University, Pullman, Washington 99164-2814, USA

We generalize the concept and phenomenology of self-trapping in the integrable Bose-Hubbard dimer into systems with non-integrable mean-field dynamics by relating it with crossing of separatrices. To this end, we construct a mapping of site-periodic solutions to find a sub-manifold of integrable dynamics in the non-integrable phase space. This new and powerful concept allows us to analytically explain the numerical observation of a massive transition in the stability properties of mean-field solutions found by Tomsovic in [1]. We also show how this mapping has extensions and generalizations to higher dimensions, opening a door for analytical understanding beyond state of the art numerics, and obtain the Lyapunov spectra of site-periodic fix points, their stabilities and bifurcations. Last we show some quantum signatures of these morphology changes in the classical phases space focusing primarily on the self-trapping transition.

[1] Tomsovic, S. Complex saddle trajectories for multidimensional quantum wave packet and coherent state propagation: application to a many-body system. Phys. Rev. E 98, 023301 (2 Aug. 2018)

DY 39.10 Wed 17:45 HÜL 186

What is the structure of chaotic resonance eigenfunctions? — •Roland Ketzmerick[1,2], Konstantin Clauss[1], Felix Fritzsch[1], and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik — [2]MPI für Physik komplexer Systeme, Dresden

While chaotic eigenfunctions in closed systems are uniformly distributed according to the quantum ergodicity theorem, they show fractal structures in systems with escape. This structure depends crucially on the decay rate of the resonance eigenfunction. It is semiclassically quite well understood for quantum maps with full [1] and partial [2] escape. Here we present the extension to billiard systems, in particular the famous three-disk system (full escape) and the dielectric limaçon billiard relevant for optical microcavities (partial escape).

[1] K. Clauß, M. J. Körber, A. Bäcker, and R. Ketzmerick, Phys. Rev. Lett. **121**, 074101 (2018).
[2] K. Clauß, E. G. Altmann, A. Bäcker, and R. Ketzmerick, Phys. Rev. E **100**, 052205 (2019).

DY 39.11 Wed 18:00 HÜL 186

A PT-symmetric kicked top — Steve Mudute-Ndumbe and •Eva-Maria Graefe — Imperial College London, UK

A PT-symmetric version of the kicked top is introduced to study the interplay of quantum chaos with loss and gain. The classical dynamics arising from the quantum dynamics of the angular momentum expectation values are derived and analysed in some detail. Further, the statistics of the (complex) eigenvalues of the quantum system are investigated.

DY 39.12 Wed 18:15 HÜL 186

Towards universal Hong-Ou-Mandel correlations in topological insulators — •Andreas Bereczuk[1], Juan Diego Urbina[1], Barbara Dietz[2], Jack Kuipers[3], Cosimo Gorini[1], and Klaus Richter[1] — [1]Institut of Theoretical Physics, University Regensburg, Germany — [2]School of Physical Science and Technology, Lanzhou University, China — [3]Department of Biosystems Science and Engineering (BSSE), ETH Zurich, Switzerland

The indistinguishable-distinguishable transition for the transmission probability for two fermions propagating through a quantum point contact is a known manifestation of the celebrated Hong-Ou-Mandel (HOM) effect [1] in electron quantum optics [2]. As shown in [3], universal HOM correlations are expected by substituting the quantum point contact by a chaotic cavity in a mesoscopic regime [3] where universal correlations of the scattering matrix entries at different energies enter. We present here a consistent semiclassical, numerical and

Random Matrix Theory (RMT) analysis of this correlators together we a progress report on its experimental realization in a microwave billard. With this results at hand, we propose a HOM setup with cavities as complex beam splitters and edge states instead of waveguides to observe universal HOM correlations in a topological insulators (TI).

[1] C. K. Hong, Z. Y. Ou and L. Mandel, Phys. Rev. Lett. 59, 2044 (1987)
[2] E. Bocquillon et al., Annalen der Physik 526, 1 (2014)
[3] J. D. Urbina et al., Phys. Rev. Lett. 116, 100401 (2016)

DY 39.13 Wed 18:30 HÜL 186

The Conditioned Real Ginibre Ensemble and PT-Symmetric Quantum Chaos — •Simon Malzard[1], Steve Mudute-Ndumbe[1], Roman Riser[2], Joshua Feinburg[2], and Eva-Maria Graefe[1] — [1]Imperial College London, London, UK — [2]University of Haifa, Haifa, Israel

In Hermitian systems the universality of spectral fluctuations described by the standard Gaussian ensembles is one of the most pronounced fingerprints of chaos in a quantum system. With the recent intense interest in non-Hermitian PT-symmetric systems, it is a natural question whether there are PT-symmetric random matrix ensembles yielding similar universality classes. One candidate for PT-symmetric systems with P^2=1 and T^2=1 which display quantum chaos is the real Ginibre ensemble. Eigenvalues of real Ginibre matrices are real or occur in complex conjugate pairs. The spectral properties of the real Ginibre matrices depend crucially on the number of real eigenvalues. Hence, when studying the eigenvalue distributions and level spacings of PT-symmetric quantum chaotic systems, one should make comparisons to an ensemble of real Ginibre matrices conditioned to have the corresponding number of real eigenvalues. Here we present a numerical method to produce samples of real Ginibre matrices conditioned to have a particular number of real eigenvalues.

DY 39.14 Wed 18:45 HÜL 186

Rate of decoherence and entanglement growth in coupled kicked rotors — •Sanku Paul[1] and Arnd Bäcker[2,1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden 01187, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, Dresden 01069, Germany

The classical-quantum correspondence of a pair of coupled kicked rotors is investigated. In this interacting system, one rotor acts as an environment to the other. This leads to the emergence of decoherence with classical-like behavior at large times. This classical-like behavior is characterized by normal diffusion in energy space and interestingly, it is preceded by an intermediate dynamical localization for weak interactions. It is observed that these different rates of energy diffusion are associated with different regimes of decay of coherence, in particular showing exponential and power-law behavior. We show that the observed decoherence is related to distinct rates of entanglement entropy growth between the rotors which is described by an initial power-law followed by logarithmic growth.

DY 40: Data Analytics, Extreme Events, and Nonlinear Stochastic Systems (joint session DY/SOE)

Time: Wednesday 15:00–17:30 Location: ZEU 118

Invited Talk DY 40.1 Wed 15:00 ZEU 118

I want it all and I want it now! — •Alexander K. Hartmann — University of Oldenburg, Germany

For every random process, all measurable quantities are described comprehensively through their probability distributions. Ideally, they would be obtained analytically, i.e., completely. Since most physical models are not accessible analytically, one has to perform numerical simulations. Usually this means one does many independent runs, allowing one to measure histograms. Since the number of repetitions is limited, maybe 10 million, correspondingly the distributions can be estimated in a range down to probabilities like 10^{-10}. But what if one wants to obtain the full distribution, in the spirit of obtaining all information? Thus, one desires to get the distribution down to the rare events, without waiting for a huge running time.

Here, we study rare events using a very general black-box method [1]. It is based on sampling vectors of random numbers within an artificial finite-temperature (Boltzmann) ensemble to access rare events and large deviations for almost arbitrary equilibrium and non-equilibrium processes. In this way, we obtain probabilities as small as 10^{-500} and smaller, hence (almost) the full distribution can be obtained in a reasonable amount of time. Examples are presented for applications to random graphs [2], traffic flow models, biological sequence alignment, particle diffusion, or calculation of partition functions [3].

[1] A.K. Hartmann, Phys. Rev. E **89**, 052103 (2014)
[2] A.K. Hartmann and M. Mézard, Phys. Rev. E **97**, 032128 (2018)
[3] A.K. Hartmann, Phys. Rev. Lett. **94**, 050601 (2005)

DY 40.2 Wed 15:30 ZEU 118

Constructing accurate and data-efficient molecular force-fields with machine learning — •Igor Poltavskyi, Grégory Fonseca, Valentin Vassilev-Galindo, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg

Employing machine learning (ML) force-fields (FF) is becoming a standard tool in modern computational physics and chemistry. Reproducing potential energy surfaces of any complexity, ML models extend our horizons far beyond the reach of *ab initio* calculations. One can already perform nanosecond-long molecular dynamics simulations for molecules containing up to a few tens of atoms on a coupled-cluster level of accuracy, providing invaluable information about subtle details of intra-molecular interactions [1,2]. Next challenges are constructing ML FFs to molecules with 1000s of atoms and describing far-from-equilibrium geometries without losing accuracy and efficiency. To reach these goals, we developed methods for optimizing reference datasets and partitioning the problem of training global FFs into parts. By minimizing the prediction error for subsets of molecular configurations obtained by clustering, we can build ML FFs equally applicable for the entire range of reference data. Dividing the configuration space into sub-domains by physical and chemical properties, training corresponding ML models, and combining them into one global model enables highly-accurate FFs for molecules containing hundreds of atoms.

[1] Sauceda *et al.*, J. Chem. Phys. **150**, 114102 (2019).
[2] Chmiela *et al.*, Nat. Commun., **9**(1), 3887 (2018).

DY 40.3 Wed 15:45 ZEU 118

Interpretable Embeddings from Molecular Simulations Using Gaussian Mixture Variational Autoencoders — •Yasemin Bozkurt Varolgunes[1,2], Tristan Bereau[1], and Joseph F. Rudzinski[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Koc University, Istanbul, Turkey

Extracting insight from the molecular simulations data requires the identification of a few collective variables (CVs) whose corresponding low-dimensional free-energy landscape (FEL) retains the essential features of the underlying system. Autoencoders are powerful tools for dimensionality reduction, as they naturally force an information bottleneck. While variational autoencoders (VAEs) ensure continuity of the embedding by assuming a Gaussian prior, this is at odds with the multi-basin FELs that typically arise from the identification of meaningful CVs. Here, we incorporate this physical intuition into the prior by employing a Gaussian mixture variational autoencoder (GMVAE), which encourages the separation of metastable states within the embedding. The GMVAE performs dimensionality reduction and clustering within a single unified framework, and is capable of identifying the inherent dimensionality of the input data, in terms of the number of Gaussians required to categorize the data. We illustrate our approach on two toy models and a peptide, demonstrating the anti-clustering effect of the prior relative to standard VAEs. The resulting embeddings stand as appropriate representations for constructing Markov state models, highlighting the transferability of the dimensionality reduction from static equilibrium properties to dynamics.

DY 40.4 Wed 16:00 ZEU 118

The entropy of the longest increasing subsequences: typical and extreme sequences — Phil Krabbe[1], •Hendrik Schawe[1,2], and Alexander K. Hartmann[1] — [1]Carl von Ossietzky Universität

Oldenburg, Germany — [2]Laboratoire de Physique Théorique et Modèlisation, Université de Cergy-Pontoise, France

Consider a game, where you get a sequence of n numbers. Your objective is to circle the maximum amount of numbers such that each circled number is larger than all circled numbers to their left. To circle the maximum amount numbers, one can calculate the *longest increasing subsequence* (LIS). If the sequence of numbers is a random permutation, this problem is remarkably well studied and for the length L, or in our game the number of circles, not only the mean value, but the whole distribution is known [1,2]. In recent time it was shown that this problem is equivalent to certain surface growth and ballistic deposition models, which led to a large interest from physicists.

Note that the LIS is not unique, there are possibly multiple ways to circle L numbers. While this degeneracy M is expected to increase exponentially with the sequence length n [1], we introduce an algorithm to count the number of degenerate LIS and sample uniformly from all LIS of a given sequence. Especially, we obtain the distribution $P(M)$ down into its far tails with probabilities smaller than 10^{-100} using sophisticated Markov chain sampling methods [3].

[1] D. Romik, The Surprising Mathematics of Longest Increasing Subsequences (2015); [2] J. Börjes, H. Schawe, A. K. Hartmann, Phys. Rev. E 99 (4), 042104 (2019); [3] A.K. Hartmann, EPJB 84, 627 (2011)

15 min. break.

DY 40.5 Wed 16:30 ZEU 118

Large-deviation simulation of height distribution for the KPZ equation: dependence on initial conditions and morphologie of extreme configurations — •Alexander K. Hartmann[1], Pierre Le Doussal[2], Alexandre Krajenbrink[2], Baruch Meerson[3], and Pavel Sasorov[4] — [1]University of Oldenburg, Germany — [2]Ecole Normale Supérieure, Paris, France — [3]Hebrew University of Jerusalem, Israel — [4]Keldysh Institute of Applied Mathematics, Moscow, Russia

The distribution of relative free energies H of directed polymers in disordered media is studied, which is in the KPZ universality class. We study the distribution at large temperatures, corresponding to short times in KPZ. Using a statistical mechanics-based *large-deviation approach*, the distribution can be obtained over a large range of the support, down to a probability density as small as 10^{-1000} [1]. We compare with analytical predictions for different types of initial conditions and for full as well as for half space [2]. A very good agreement is found for $H < 0$ and a strong convergence is visible for $H > 0$. Furthermore, we study the morphology of atypical fluctuations [3], compare with analytical results from the *optimal fluctuation method*, and find again a good agreement.

[1] A.K. Hartmann, P. Le Doussal, S.N. Majumdar, A. Rosso and G. Schehr, Europhys. Lett. 121, 67004 (2018).
[2] A.K. Hartmann, A. Krajenbrink, and P. Le Doussal, preprint arXiv:1909.0384.
[2] A.K. Hartmann, B. Meerson, and P. Sasorov, arXiv: 1907.05677.

DY 40.6 Wed 16:45 ZEU 118

Machine Learning on temperature fluctuations in health and disease — •Jens Karschau, Sona Michlíková, Daniel Kotik, Sebastian Starke, Steffen Löck, and Damian McLeod — OncoRay, HZDR, TU Dresden, Dresden, Germany

Rendering disease diagnoses from measurements is a highly complex task. Clinicians train for many years in order to identify pathological events from patient data. Exemplarily, medical expert knowledge recognises subtle differences between normal and tumor-looking features. Today, machine learning (ML) allows us to support not only the clinical decision maker during classification; it also has potential to promptly warn self-monitored individuals. We developed an RNN model that learns on time series temperature data of up to 120 days to detect cancer features in mice. It successfully bins particular days into either tumor vs. no-tumor days. Using out-of-sample data from the same or a different cohort, the model successfully classifies with an accuracy and AUC of up to 0.80. The dynamic time warping dissimilarity measure applied to different days indicates that oscillation patterns contain distinctive features that the RNN model learns. We hypothesise that the model learns features based on oscillatory behaviour at the 150 min time scale: the so-called 'ultradian' rhythm. The double benefit from our method is: (a) it uses non-invasive measurements to classify the disease state and (b) it could be deployed for applications in future on-line monitoring of data from wearable devices. Our next efforts are testing human data to deliver actionable insights in disease control and decision support.

DY 40.7 Wed 17:00 ZEU 118

Using data crawling and flexible semantic data models to enable sustainable research data management — •Alexander Schlemmer[1,2,3], Ulrich Parlitz[1,2,4], and Stefan Luther[1,2,4,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen, Germany — [3]IndiScale GmbH, Göttingen, Germany — [4]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Germany — [5]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Germany

Despite the significant advances in computation power and information technology of the last decades, scientific data management is still lacking widespread adoption in many scientific communities. The absence of standardized workflows and corresponding tools significantly impedes complete transparency and reproducibility of research results.

We discuss key concepts to remove omnipresent barriers in scientific data management. Specifically, data crawling strategies and flexible semantic data models are highlighted. With examples using our open source software CaosDB (https://doi.org/10.3390/data4020083) we show how these concepts can be practically applied in order to achieve sustainable research data management.

DY 40.8 Wed 17:15 ZEU 118

Non-Markovian barrier crossing with two-time-scale memory is dominated by the faster memory component — •Julian Kappler, Victor B. Hinrichsen, and Roland R. Netz — Freie Universität Berlin, Fachbereich Physik, Berlin, Germany

We investigate non-Markovian barrier-crossing kinetics of a massive particle in one dimension in the presence of a memory function that is the sum of two exponentials with different memory times. Our Langevin simulations for the special case where both exponentials contribute equally to the total friction show that the barrier-crossing time becomes independent of the longer memory time if at least one of the two memory times is larger than the intrinsic diffusion time. When we associate memory effects with coupled degrees of freedom that are orthogonal to a one-dimensional reaction coordinate, this counterintuitive result shows that the faster orthogonal degrees of freedom dominate barrier-crossing kinetics in the non-Markovian limit and that the slower orthogonal degrees become negligible, quite contrary to the standard time-scale separation assumption. We construct a crossover formula for the barrier crossing time that is valid for general multi-exponential memory kernels. This formula can be used to estimate barrier-crossing times for general memory functions for high friction, i.e. in the overdamped regime, as well as for low friction, i.e. in the inertial regime.

DY 41: Droplets and Wetting (joint session DY/CPP)

Time: Wednesday 15:00–16:45 Location: ZEU 147

DY 41.1 Wed 15:00 ZEU 147

Coalescence of liquid droplets in a quasi 2D liquid films — •Christoph Klopp, Ralf Stannarius, and Alexey Eremin — Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany

Coalescence of droplets plays a crucial role in nature and modern technology. Various experimental and theoretical studies explored droplet dynamics in 3D and on 2D solid or liquid substrates [1-3]. Here, we demonstrate coalescence of isotropic droplets in thin quasi 2D liquids, an overheated smectic A films. We investigated their dynamics experimentally and measured the shape deformation during the whole merging process using high-speed imaging. This system is a unique example, where the lubrication approximation can be directly applied, and the smectic membrane plays the role of the precursor film. Our

studies reveal the scaling laws of the coalescence time depending on the droplet size and the material parameters. We also compared our results with existing models for liquid lens coalescence on liquid and solid surfaces.

[1] Paulsen et al., Coalescence of bubbles and drops in an outer fluid, Nat. Commun. 5, 3182 (2014)

[2] Aarts et al., Hydrodynamics of Droplet Coalescence, Phys. Rev. Lett. 95, 164503 (2005)

[3] Shuravin et al., Coalescence of viscous two-dimensional smectic islands, Phys. Rev. E 99, 062702 (2019)

DY 41.2 Wed 15:15 ZEU 147

Surface wettability-induced magnitude change and sign inversion of the apparent line tension — •Binyu Zhao[1,4], Shuang Luo[2], Elmar Bonaccurso[3], Günter Auernhammer[4], Zhigang Li[2], and Longquan Chen[1] — [1]University of Electronic Science and Technology of China, Chengdu 610054, China — [2]The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong — [3]Airbus Central R & T, Materials X, Munich 81663, Germany — [4]Leibniz Institute of Polymer Research Dresden, Dresden 01069, Germany

Line tension is defined, thermodynamically, as the excess free energy per unit length of the contact line as postulated by Gibbs in 1878. Despite strenuous research efforts thence, the magnitude and sign of line tension remain in a hot debate. In this study, we determined the apparent line tension from the size-dependent contact angle of sessile nanodroplets on surfaces with different wettabilities via atomic force microscopy measurements. We showed that the apparent line tension changed its magnitude with the surface wettability and its sign changed from positive to negative for droplets on surfaces with an apparent contact angle higher than a critical value. Furthermore, using molecular dynamics simulations, we analysed the potential energy of liquid molecules within the nanodroplet and in the vicinity of the three-phase contact line. This allowed us to explain the surface wettability-induced magnitude change and sign inversion of the apparent line tension form the perspective of surface thermodynamics.

DY 41.3 Wed 15:30 ZEU 147

Characterizing the speed, size and shape of droplets during their flight from an ultrasonic spray coater — •Pieter Verding[1,2], Wim Deferme[1,2], and Werner Steffen[3] — [1]Hasselt University, Institute for Materials Research, Diepenbeek, Belgium — [2]IMEC, Diepenbeek, Belgium — [3]Max-Planck-Institut for Polymer research, Mainz, Germany

Ultrasonic spray coating - USSC is a technology offering numerous possibilities, such as depositing ultrathin homogeneous layers up to 20 nm on large scale. However, its application is limited due to the many process parameters which have a large impact on the quality of the coating. For this reason, measuring the droplet size, speed and concentration during the flight from the ultrasonically generated droplet to the substrate, gives insight in how to tune these parameters. Because thousands of droplets are created at the same time, measuring the properties of the droplets during flight is a complicated task.

Three different measurement techniques have been developed in and around an USSC setup. Dynamic Light Scattering (DLS) shows, after Fourier transformation, shifted peaks, representing the speed of the droplets. By applying Turbidimetry, it is possible to determine the size of the droplets. Droplets size and speed could be measured and gave comparable results as measured with a High Speed Camera (HSC). Furthermore, it was shown that the size and velocity of the droplets depend on the process parameters. It is therefore concluded from this work that a combination of DLS and Turbidimetry is a valuable alternative to measure droplets during their flight from an USSC.

DY 41.4 Wed 15:45 ZEU 147

Simulating the hydrodynamics of droplets on photo-switchable substrates — •Josua Grawitter and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Interfaces between fluids and photo-switchable substrates provide a unique mechanism to precisely manipulate liquid droplets by creating and adapting a heterogeneous wettability landscape. Because droplets respond to changes in wettability, such interfaces provide a means to keep the droplets in non-equilibrium and thereby induce new states of dynamic wetting.

We present a boundary element method to determine the Stokes flow inside a droplet with its curved free surface and its flat interface at the substrate, where we apply the Navier boundary condition to permit motion of the contact line. In our approach we use the Cox-Voinov law [1] and introduce the velocity of the contact-line as a side condition. We also implement an iterative domain-splitting integration scheme capable of treating singular integrands, which are typical for the boundary element method. Using the implemented method, we study how droplets respond to specific spatiotemporal wettability patterns that either move or deform the droplet. Here, we present first studies of the spatio-temporal deformation dynamics induced by oscillating wettability along the contact line and of directed motion initiated by traveling wettability patterns. We specifically investigate how to design the patterns in order to maximize droplet speed.

[1] O. V. Voinov, Fluid Dyn. **11**, 714 (1976).

DY 41.5 Wed 16:00 ZEU 147

A bite of cotton candy physics — •Stephane Dorbolo[3], Floriane Weyer[1], Nicolas Vandewalle[1], and Alexandre Delory[2] — [1]GRASP, UR-CESAM, Departement de Physique, Universite de Liege, Belgium — [2]ESPCI, Paris, France — [3]FNRS, GRASP, UR-CESAM, Departement de Physique, Universite de Liege, Belgium

A cotton candy is made of kilometers of sugar fibers. These thin fibers are easily and quickly soluble into water. The system is generic and found applications in soldering and networks of nano-fibers. First, the wettability of the sugar is measured. The problem is complex since the sessile droplet modifies the substrate made of sugar. Second, the interactions of a sugar fiber with the humidity present in the air and with a single droplet are discussed through experimental investigations. Finally, a model is presented to describe the motion of a droplet along one single fiber.

DY 41.6 Wed 16:15 ZEU 147

Breakup Dynamics of Capillary Bridges on Hydrophobic Stripes — Maximilian Hartmann[1], •Mathis Fricke[2], Lukas Weimar[1], Dirk Gründing[2], Tomislav Maric[2], Dieter Bothe[2], and Steffen Hardt[1] — [1]Nano- and Microfluidics Group, TU Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany — [2]Mathematical Modeling and Analysis Group, TU Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany

The breakup dynamics of a capillary bridge on a hydrophobic stripe between two hydrophilic stripes is studied both experimentally and numerically. The capillary bridge is formed from an evaporating water droplet wetting three neighboring stripes of a chemically patterned surface. The simulations are based on the Volume-of-Fluid (VOF) method implemented in Free Surface 3D (FS3D). By considering the breakup process in phase space, the breakup dynamics can be evaluated without the uncertainty in determining the precise breakup time. It is found that within an intermediate inviscid regime, the breakup dynamics follows a $t^{2/3}$-scaling, indicating that the breakup process is dominated by the balance of inertial and capillary forces. For smaller bridge widths, the breakup velocity reaches a plateau, which is due to viscous forces becoming more important. In the final stage of breakup, the capillary bridge forms a liquid thread that breaks up consistent with the Rayleigh-Plateau instability. The existence of satellite droplets in a regular pattern indicates that the primary breakup process is followed by self-similar secondary breakups.

DY 41.7 Wed 16:30 ZEU 147

Flow structure of marangoni-contracted sessile droplets — O. Ramirez[1], M.A. Hack[2], W. Kwiecinski[3], E.S. Kooij[3], T.J. Seegers[2], J.H. Snoeijer[2], and •S. Karpitschka[1] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Physics of Fluids Group, University of Twente, Enschede, Netherlands — [3]Physics of Interfaces Group, University of Twente, Enschede, Netherlands

A droplet of two miscible liquids should spread over a high-energy surface until complete wetting. However, if one component is more volatile and has a higher surface tension, a quasi-stationary non-vanishing apparent contact angle can be observed. This is caused by the enrichment of the residual component near the contact line and the associated surface tension gradient. A hydrodynamic-evaporative model, using a long-wave approximation for the droplet coupled to diffusion limited evaporation predicts a balance between Marangoni and capillary flows and a power law between the apparent contact angle and the ambient humidity [Karpitschka et al., Langmuir (2017)]. This explanation differs from a recent model, where the low surface tension of a precursor around the droplet is held responsible [Benusiglio et al., Soft Matter (2018)]. A discrimination between possible mechanisms requires experimental resolution of the flow in the drop. We present

uPIV measurements and relate them to the apparent shape of the drop, for aqueous solutions of various short chain carbon diols. Depending on the surface activity of the diol, its concentration, and the ambient humidity, we observe different regimes, indicating that multiple mechanisms lead to the observed angles.

DY 42: Fluid Physics of Life (joint session DY/BP)

Time: Wednesday 15:00–17:45 Location: ZEU 160

Invited Talk DY 42.1 Wed 15:00 ZEU 160

Light-regulated microbial dynamics and self-organization in complex geometries — •Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, D-37077 Göttingen, Germany

Life on Earth has evolved under the periodic exposure to sunlight and many microorganisms are equipped with a photosynthesis machinery enabling them to convert light into chemical energy. Their habitats include liquid-infused soil, porous rocks and microdroplets, featuring complex geometric architectures that induce strong spatial and temporal light fluctuations. Thus, biological functionalities to sense and rapidly respond to light fluctuations are pivotal for microbial life.

In this presentation I will discuss how concepts from non-equilibrium statistical physics, in conjunction with novel experimental approaches from soft matter and biophysics [1], enable us to decipher fundamental physical principles of microbial responses to light cues. We discovered that light regulates the transition of motile microbes from the free-swimming to the surface-adhered state [2]. I will further elaborate on how interfacial interactions govern the motility and navigation of individual cells in complex geometries [3] and demonstrate that the light-regulated motility controls the emergence of self-organization and phase separation of microbial populations in confinement.

[1] M. Backholm & O. Bäumchen, Nature Protocols 14, 594 (2019).
[2] C. Kreis et al., Nature Physics 14, 45 (2018).
[3] T. Ostapenko et al., Phys. Rev. Lett. 120, 068002 (2018).

DY 42.2 Wed 15:30 ZEU 160

Wet-tip versus dry-tip regimes of osmotically driven bile flow in the liver — Oleksandr Ostrenko, Michael Kücken, and •Lutz Brusch — Center for Information Services and High Performance Computing (ZIH), Technische Universität Dresden, Germany

The secretion of osmolites into a lumen and thereby caused osmotic water inflow drive fluid flows like saliva, sweat and bile in organs without a mechanical pump, as opposed to the heart in blood circulation. The effects of elevated fluid pressure and the associated mechanical limitations of organ function remain largely unknown. We consider the pressure profile of the coupled osmolite-flow problem with combined velocity and pressure boundary conditions. Notably, the entire lateral boundary acts as a fluid source, the strength of which is determined by feedback from the emergent pressure solution itself. Hence, the pressure difference between the boundaries is not imposed but self-organises. Our theoretical results reveal fundamental parameter dependencies and a phase boundary separating the commonly considered "wet-tip" regime with steady flow out of the very tip of a channel from a "dry-tip" regime suffering stalled flow and a self-organised block of osmotic water inflow [1]. We validate model predictions against intra-vital video microscopy data from mouse liver [2] and propose a relation between the predicted phase boundary and the onset of zonated cholestasis, a pathological liver condition [3].

[1] Ostrenko et al. (2019) Scientific Reports 9, 4528. [2] Meyer et al. (2017) Cell Systems 4, 277. [3] Segovia-Miranda et al. (2019) Nature Medicine and bioRxiv 572073.

DY 42.3 Wed 15:45 ZEU 160

Memory capacity of a flow network — •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

The slime mould *Physarum polycephalum* is a very simple unicellular but seemingly intelligent organism with a network-like body. Its complex behaviour requires the ability to propagate, store and process information. Recently, it has been shown that *Physarum* propagates information about stimuli with the fluid flows throughout its network. Most inspiringly, *Physarum* was observed to adapt its networks tube radii globally in response to stimuli, reaching a steady-state as a long term response that keeps a memory of the stimuli in its network morphology. Inspired by this observation we here investigate the capacity to store information about previous stimuli in the morphology of an adaptive flow network. We model the organism as a flow network whose radii can change when optimising the network to have the least energy dissipation. We observe how the system reacts to localised changes and the timescale of its responses to applied stimuli by numerical simulation. Through theoretical understanding, we aim to pinpoint the information storing and processing capabilities of adaptive flow networks in general and *Physarum* networks specifically.

DY 42.4 Wed 16:00 ZEU 160

Fluid transport by metachronal waves in cilia chains — •Albert von Kenne, Thomas Niedermayer, and Markus Bär — Physikalisch-Technische Budesanstallt (PTB), Berlin 10587

Motile cilia are hair-like cell extensions that undergo a cyclic motion with the purpose to transport the extracellular fluid at a low Reynolds number, providing crucial functionality of living matter such as cell locomotion or molecular transport in tissue. A striking feature of populations of cilia is a state of collective motion known as metachronal wave. In proximity to a cell surface a symmetry breaking of the flow field is due that affects the properties of metachronal waves and facilitates transport generation. We generalize a simple phase oscillator model for the elastohydrodynamic coupling in ciliated systems [1] to include this asymmetry. We obtain analytical results for the linear stability of metachronal waves in presence of long-range hydrodynamic interactions, illustrate their properties by numerical simulations and relate the change in transport ability to the specific properties of metachronal waves.

[1] Niedermayer et. al., Chaos: 18(3) 2008.

DY 42.5 Wed 16:15 ZEU 160

Boundary conditions for polar active fluids exhibiting mesoscale turbulence — •Sebastian Heidenreich[1], Henning Reinken[2], Daiki Nishiguchi[3], Andrey Sokolov[4], Igor S. Aranson[5], Sabine H. L. Klapp[2], and Markus Bär[1] — [1]Physikalisch Technische Bundesanstalt Braunschweig und Berlin — [2]Technische Universität Berlin — [3]University of Tokyo, Japan — [4]Argonne National Laboratory, USA — [5]Pennsylvania State University, USA

Bacterial suspensions are intriguing examples for active polar fluids which exhibit large-scale collective behaviour from mesoscale turbulence to vortex lattices. The bulk collective motion is well described by a continuum equation with derivatives up to the fourth order [1]. That simple model reproduces experimental findings of mesoscale turbulence and was recently derived from a minimal micro-swimmer model. However, the treatment of boundaries to describe the collective motion in a confinement or near walls remains so far unknown. In the talk, we propose boundary conditions for active polar fluids suitable to describe recent experiments of Bacillus subtilis bacteria moving in an array of lithographic designed pillars [2]. Furthermore, we describe the collective motion of bacteria around single pillars of different sizes in experiments and show that the model with the mentioned boundary conditions reproduces this behavior faithfully.

[1] J. Dunkel, S. Heidenreich, M. Bär and R. E. Goldstein, New. J. Phys. 15, 040516 (2013). [2] D. Nishiguchi, I. S. Aranson, A. Snezhko and A. Sokolov Nat. Comm. 9, 4486 (2018).

15 min. break.

DY 42.6 Wed 16:45 ZEU 160

Artificial topological defects organize bacterial motion — •Henning Reinken[1], Sebastian Heidenreich[2], Daiki Nishiguchi[3], Andrey Sokolov[4], Igor Aranson[5], Markus Bär[2], and Sabine Klapp[1] — [1]Technische Universität Berlin — [2]Physikalisch-Technische Bundesanstalt Berlin — [3]University of Tokyo, Japan — [4]Argonne National Laboratory, USA —

[5]Pennsylvania State University, USA

Active systems spontaneously self-organize into complex spatio-temporal structures such as flocks, bands, vortices, and turbulence. These collective states are susceptible to weak geometrical confinement, as has been demonstrated in experiments on suspensions of *Bacillus subtilis*, where turbulent motion is organized into a highly ordered bacterial vortex lattice by arrays of tiny obstacles [1].
Using a continuum-theoretical approach [2], we show how self-induced topological defects imposed by artificial obstacles guide the flow profile of the active fluid and enable the stabilization of vortex patterns with tunable properties. Beyond the stabilization of square and hexagonal lattices, we also provide a striking example of a chiral, antiferromagnetic lattice induced by arranging the obstacles in a Kagome-like array. In this setup, the interplay of lattice topology, activity and length-scale selection generates a net rotational flow. Further, we investigate how the properties of the stabilized patterns impact the transport of tracer particles in the active fluid.
[1] D. Nishiguchi et al., Nat. Commun. **9**, 4486 (2018).
[2] H. Reinken et al., Phys. Rev. E **97**, 022613 (2018).

DY 42.7 Wed 17:00 ZEU 160

Topological defects in growing bacterial colonies — Anh LP Thai, Arkajyoti Ghoshal, and •Anupam Sengupta — Physics of Living Matter Group, University of Luxembourg, Luxembourg

Bacterial populations are known to mediate vital processes in ecology, medicine and industry. Morphology, a key biophysical trait, has been long studied for its biological relevance in uptake, motility and selection. Yet, only recently we have started to uncover the role of morphology in biophysical interactions between cells or with their micro-environment [1]. Here, I will present recent results that elucidate how non-motile bacteria harness morphology to regulate transport processes over colony scales. We examine the geometric and mechanical properties of growing colonies, with a particular focus on the emergence of topological defects. Our results indicate that the number of topological defects depends on the cell physiology and colony dimensions, which in turn regulate the active dynamics of the colony. We compare our experimental results with MD simulations and continuous modelling [2, 3], and demonstrate that an expanding colony of non-motile cells self-organizes into domains of aligned cells. Topological defects mediate the interactions between domains, ultimately yielding an active nematodynamic system. Topology mediated mechanics can potentially lead to physiological functions due to the active hydrodynamics at scales that are orders of magnitude larger than single cells. [1] A. Sengupta, Microbial Active Matter: A Topological Perspective (under rev.); [2] You, Pearce, Sengupta, Giomi, Phys. Rev. X. 8 (2018); [3] You, Pearce, Sengupta, Giomi, Phys. Rev. Lett. 123 (2019).

DY 42.8 Wed 17:15 ZEU 160

Dynamics of Lithium Chloride Solutions in Nanopores of Various Diameters - a NMR Study — •Christoph Säckel, Sarah Schneider, and Michael Vogel — Institut für Physik kondensierter Materie, TU Darmstadt

We analyse ion transport in aqueous salt solutions confined to nanopores as part of a project that aims to develop a new generation of nanosensors by combining the effectiveness of biological ion channels with the robustness of synthetic silica nanopores. To this end it is necessary to understand the influence of the confinement on the temperature-dependent ion transport. We systematically vary the pore parameters and study effects on the dynamics of aqueous LiCl solutions using ^{2}H and ^{7}Li nuclear magnetic resonance (NMR). We combine homogeneous and gradient field NMR to selectively investigate water and ion dynamics on broad time and length scales from room temperature to the supercooled regime. Both the local and long-range dynamics of ions and water show a slowdown in silica confinement. In addition, our data indicates more heterogeneous dynamics for the liquid in confinement than in bulk. Moreover, NMR studies of solutions in functionalized silica pores reveal a significant influence of the chemical nature of the inner pore surfaces. The observed effects can be explained by a slower layer of solution at the pore walls and bulk-like dynamics in the pore centre. Self-diffusion shows an Arrhenius-like behaviour of the solution in confinements, while bulk samples are best described by a VFT fit.

DY 42.9 Wed 17:30 ZEU 160

Self-organization of active microtubule networks — Smrithika Subramani, •Viswa Maitreyi, and Isabella Guido — Max Planck Institute for Dynamics and Self-Organization, Goettigen, Germany

Transport in nature is a crucial task and simple diffusion is insufficient, especially in the intracellular confinement. Relying on cytoskeletal components and their motor proteins is a strategy that have been evolved to tackle this limitation. It was observed that inside large eukaryotic cells microtubule-motor protein networks display an activity that generates a flow, called cytoplasmic streaming, that contributes to transport and distribution of components. Many efforts have been made to understand the features and function of this intracellular streaming. However, the exact mechanism behind its establishment is still unknown. Here we present a study on a synthetic system made of active microtubule networks. When confined, they self-organize and show an interesting emergent behaviour that presents transitions through different regimes. Such transitions have similarities with the process examined in the intracellular space of Drosophila oocytes during their development. Our results show that the self-assembling of the active network as well as the generated synthetic streaming is dependent on the confinement geometry. This simplified approach allows the characterization of such dependence and can provide a deeper understanding of the natural process.

DY 43: Statistical Physics of Biological Systems II (joint session BP/DY)

Time: Wednesday 15:00–17:30 Location: ZEU 250

Invited Talk DY 43.1 Wed 15:00 ZEU 250

Eavesdropping on fluctuation-driven transport in living matter — •Matthias Weiss — Experimental Physics I, University of Bayreuth, Gemany

The interior of eukaryotic cells is crowded on several length scales by a plethora of macromolecules and membrane-enveloped subcompartments. Self-organization of this complex environment eventually involves fluctuation-driven transport on many scales. Due to a vast number of active processes, living cells are in a genuine non-equilibrium state, endowing fluctuation-driven transport also with a non-thermal noise character.

Using different model systems, from culture cells to developing embryos, we have analyzed fluctuation-driven transport of cell constituents to eavesdrop on the ambient non-equilibrium noise of living matter. In particular, we have used single-particle tracking to quantify the heterogeneous and driven, yet often anomalous diffusion of cellular constituents under varying physiological conditions. Based on a thorough analysis of the experimental data, e.g. in terms of correlation functions and power spectra, and comparison to model simulations, our data provide deep insights into the physics of fundamental steps in cellular self-organization.

DY 43.2 Wed 15:30 ZEU 250

Control of droplet kinetics in active emulsions — •Jacqueline Janssen[1], Marta Tena-Solsona[2,3], Caren Wanzke[2], Fabian Schnitter[2], Hansol Park[4], Benedikt Riess[2], Julianne M. Gibbs[4], Job Boekhoven[2,3], and Christoph A. Weber[1] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Department of Chemistry, Technical University of Munich — [3]Institute for Advanced Study, Technical University of Munich — [4]Department of Chemistry, University of Alberta

Living cells host many membrane-less organelles which originate via liquid-liquid phase separation in both the cytoplasm and the nucleoplasm. Liquid phase separated droplets are crucial in living cells to spatially control chemical reactions. Recent experimental work revealed a new class of active emulsions where the lifetime and the rate of droplet growth can be controlled. This class of active emulsions involves fuel-driven chemical reactions from thermodynamically stable precursor molecules to metastable building blocks. At large enough concentration of building block material, the liquid droplets can form and undergo an anomalously fast ripening towards fewer droplets of larger size. Up to date, there is no theoretical model which would describe such anomalous ripening kinetics of active emulsions. We

have derived a theoretical model which quantitively coincides with the experimental measurements conducted in the Boekhoven Laboratory. Our theory allows to understand how the metastable building blocks determine the lifetime and accelerate the droplet kinetics in this new class of phase separated, active systems.

DY 43.3 Wed 15:45 ZEU 250

Plasticity in vertex model of epithelial tissues — •Marko Popović, Valentin Druelle, and Matthieu Wyart — Institue of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

In order to properly develop and function living organisms are required to change and maintain shape. This can be achieved by reshaping a liquid-like tissue and then changing its material properties to stabilize the final shape. Alternatively, if the tissue is plastic it will respond elastically to stresses below some critical value but higher values of stress will produce a plastic flow leading to a permanent plastic shape change, allowing it to retain the memory of stresses that have acted on it. Plasticity is exhibited by a wide class of amorphous solids such as: colloidal gels, emulsions and foams where it corresponds to a yielding transition. Are there features of yielding transition, such as strong dependence on system preparation and collective particle rearrangements leading to non-linear rheology, that are relevant during biological morphogenesis? Motivated by similarities of disordered tissues and amorphous solids we study plastic properties of vertex model of epithelial tissues, where mechanical properties of individual cells are prescribed and emerging tissue mechanics is obtained from their collective behaviour. We study mechanical properties of elementary plastic event in epithelial tissues, a so called T1 transition, in which two pairs of cells exchange neighborship. We demonstrate that interactions between T1 transitions are analogous to those of particle rearrangements in amorphous solids and that vertex model belongs to the same class of universality.

DY 43.4 Wed 16:00 ZEU 250

Selection via phase separation — •Giacomo Bartolucci[1,2], Yash Rana[1,2], Alexandra Kühnlein[3], Christof Mast[3], Dieter Braun[3], and Christoph A. Weber[1,2] — [1]Max Planck for the Physics of Complex Systems, Dresden — [2]Center for Systems Biology Dresden — [3]Ludwig Maximilian University, München

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

15 min. coffee break

DY 43.5 Wed 16:30 ZEU 250

Sperm chemotaxis in external flows — •Steffen Lange[1,2] and Benjamin Friedrich[1,2,3] — [1]Center for Advancing Electronics Dresden (cfaed) — [2]Cluster of Excellence Physics of Life (PoL) — [3]Institut Theoretische Physik (ITP), TU Dresden, 01062 Dresden, Germany

Chemotaxis - the navigation of biological cells guided by chemical gradients - is crucial for bacterial foraging, immune responses, and guidance of sperm cells to the egg before fertilization.

Previous work on chemotaxis focused predominantly on idealized conditions of perfect chemical gradients. However, natural gradients are subject to distortions, e.g. by turbulent flows in the ocean.

Recent experiments with bacteria [1] and sperm cells from marine invertebrates [2] have surprisingly revealed the existence of an optimal turbulence strength at which the chemotaxis is more effective than for still water conditions with perfect gradients.

Using sperm chemotaxis in shear flow as a prototypical example, we reproduce an optimal turbulence strength in numerical simulations. We can understand the origin of this optimum and quantify it:

For this we apply a theory of sperm chemotaxis to the concentration filaments, which are typical for scalar turbulence. We explain how external flows distort sperm swimming paths and concentration gradients, but at the same time extend the spatial range of these gradients. Together, these two competing effects set the optimal turbulence strength. We compare our theoretical results to previous experiments and find good agreement.

[1] Taylor, Stocker; Science 2012 [2] Zimmer, Riffell; PNAS 2011

DY 43.6 Wed 16:45 ZEU 250

Extracting the degree of order in the bacterial chromosome using statistical physics — •Joris Messelink[1], Jacqueline Janssen[2], Muriel van Teeseling[3], Martin Thanbichler[3], and Chase Broedersz[1] — [1]Arnold Sommerfeld Center for Theoretical Physics, LMU München — [2]Max Planck Institute for the Physics of Complex Systems, Dresden — [3]Faculty of Biology, Philipps University Marburg

Elucidating the three-dimensional spatial organization of the bacterial chromosome is essential to understand how genomic processes are spatially regulated inside the cell. Recent Hi-C chromosome conformation capture experiments provide contact frequency maps of the chromosome. These experiments reveal structural organization beyond that of an amorphous polymer. However, despite such experimental advances, the degree of spatial organization of the bacterial chromosome remains unclear. To investigate this, we develop a maximum entropy approach to extract the three-dimensional structure of the bacterial chromosome from such data. Using this approach, we obtain a coarse-grained model for the full distribution of chromosome configurations for the bacterium C. crescentus. We validate the predictive power of our model by experiments on the localization of chromosomal loci in the cell. Our model reveals novel features of spatial chromosome organization on various length scales. Our approach is not organism-specific, and opens up a new way of analyzing spatial chromosome organization.

DY 43.7 Wed 17:00 ZEU 250

Rewarding cargo-carrier interactions: cell-mediated particle transport — •Valentino Lepro[1,2], Robert Grossmann[1], Oliver Nagel[1], and Carsten Beta[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

As society paves its way towards devices miniaturization and precision medicine, micro-scale actuation and guided transport become increasingly prominent research fields, with high potential impact in both technological and clinical contexts. To accomplish directed motion of micron-sized cargos towards specific target sites, a promising strategy is the usage of living cells as smart biochemically-powered carriers, developing so-called *bio-hybrid systems*. In this talk, we discuss eukaryotic active particle transport, using *Dictyostelium discoideum* as a model organism. We shed light on the underlying mechanics and the emerging dynamics governing such cell-mediated transport. A simple yet powerful model is proposed which reproduces the observed phenomenology and, moreover, elucidates the role of cell-cargo interactions for the long-time mass transport efficiency.

DY 43.8 Wed 17:15 ZEU 250

Effective spin glass theories for gene regulatory networks — •Fabrizio Olmeda[1] and Steffen Rulands[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany

The development and maintenance of complex organs relies on precisely regulated cell fate decisions. Understanding the molecular mechanisms underlying these decisions is one of the central questions in stem cell biology.

The primary layer of regulation is the expression of genes and their interaction in gene regulatory networks. Here, by rigorously mapping the stochastic dynamics of gene regulatory networks to bipartite spin glasses, we develop an effective theory for describing fluctuations in gene regulatory networks during cellular decision making.

Performing a replica calculation, we describe the phase diagram that emerges in terms of the parameters of the gene network and demonstrate the existence of a spin glass phase.

In addition to the highly efficient simulation of gene networks our work, for the first time, allows using single-cell sequencing experiments to link fluctuations in gene expression to mechanisms of cellular decision making.

DY 44: Modelling and Simulation of Soft Matter II (joint session CPP/DY)

Time: Wednesday 15:00–16:45 Location: ZEU 255

DY 44.1 Wed 15:00 ZEU 255

Machine Learning Inter-Atomic Potentials Generation Driven by Active Learning: A Case Study for Amorphous and Liquid Hafnium dioxide — •Anand Narayanan Krishnamoorthy[1,2], Ganesh Sivaraman[3], Matthias Baur[1], Christian Holm[1], Chris Benmore[6], Marius Stan[4], Gabor Csanyi[5], and Álvaro Vázquez–Mayagoitia[7] — [1]Institute for Computational Physics, University of Stuttgart — [2]Helmholtz Institute Muenster — [3]Leadership Computing Facility, Argonne National Laboratory - USA — [4]Applied Materials Division, Argonne National Laboratory, USA — [5]Department of Engineering, University of Cambridge, UK — [6]X-ray Science Division, Argonne National Laboratory, USA — [7]Computational Science Division, Argonne National Laboratory, USA

We propose a novel active learning scheme for automatically sampling a minimum number of uncorrelated configurations for fitting the Gaussian Approximation Potential (GAP). We apply this scheme to a Hafnium dioxide (HfO2) dataset generated from a melt-quench ab initio molecular dynamics (AIMD) protocol. Our results show that the active learning scheme, with no prior knowledge of the dataset is able to extract a configuration that reaches the required energy fit tolerance. Further, molecular dynamics (MD) simulations performed using this active learned GAP model on 6144-atom systems of amorphous and liquid state elucidate the structural properties of HfO2 with near ab initio precision and quench rates (ie 1.0 K/ps) not accessible via AIMD.

DY 44.2 Wed 15:15 ZEU 255

BoltzmaNN: Heuristic inverse design of pair potentials using neural networks — •Fabian Berressem, Mihir Khadilkar, and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University Mainz, Germany

In this work, we investigate the use of neural networks (NNs) to devise effective equations of state from a given isotropic pair potential using the virial expansion of the pressure. We train the NNs with data from molecular dynamics simulations, sampled in the NVT ensemble at densities covering both the gas- and liquid-like regime. We find that the NNs provide much more accurate results compared to the analytic estimate of the second virial coefficient derived in the low density limit. Further, we design and train NNs for computing the potential of mean force from the radial pair distribution function, g(r), a procedure which is often performed for coarse-graining applications. Here, we find that a good choice for the loss function is crucial for an accurate prediction of the pair potentials. In both use cases, we study in detail how providing additional information about forces and the density impacts the performance of the NNs. We find that including this additional information greatly increases the quality of the predictions, since more correlations are taken into account. Further, the predicted potentials become smoother and are in general much closer to the target potential.

DY 44.3 Wed 15:30 ZEU 255

Prediction of iSCFT chemical potentials via machine learning — •Lucia Milena Wesenberg, Ludwig Schneider, and Marcus Müller — Institute for Theoretical Physics, Georg-August University Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

We explore the use of machine learning to enhance the simulation of polymeric nanostructures. Self-assembly of symmetric diblock copolymers is the chosen testing system for this purpose. Such polymers consist of two equally long blocks of different monomer types. As the two monomer types are incompatible but linked in the center of each polymer, microphase separation occurs.

Simulations of such systems often pose a challenge for particle-based models as large systems and concomitantly long time scales need to be simulated. Thus, continuum models are employed, where the dynamics can be conceived as the relaxation towards the local minimum of a free-energy basin and jumps between such basins. These models reduce the degrees of freedom by integrating out the molecular degrees of freedom. The most detailed continuum model investigated here is the Self-Consistent Field Theory (SCFT). Unfortunately, dynamic SCFT requires the chemical potential of a non-equilibrium morphology that is computationally expensive to obtain. The SCFT potential calculation is an iterative process, and the stability of the algorithm depends heavily on the starting conditions. Our machine learning approach provides suitable initial conditions for the algorithm. The predicted starting conditions reduce the computational effort considerably.

DY 44.4 Wed 15:45 ZEU 255

PolyEC - an event-chain framework — •Tobias A. Kampmann, David Müller, and Jan Kierfeld — TU Dortmund University, Germany

PolyEC is a MC event chain framework suitable for simulation of various colloidal systems. We focus on modularity and extensibility to simulate heterogenous systems. In event-chain simulations only one particle is active and interactions can be treated independently by factorization, which allows for a highly modular approach for particle-based simulations. Albeit ECMC is a monte-carlo method, a single event-chain is deterministic (although there are modifications where this is not true). One crucial feature of this method is that each state a piece-wise deterministic event-chain visits between events are properly (Boltzmann-) weighted. This opens the possibility to measure observables like pressure or the distribution of energy *on the fly*. As examples we show needle-colloid mixtures and an active particle system.

DY 44.5 Wed 16:00 ZEU 255

Analytical and computational study of advection-diffusion-reaction processes in catalytic fibrous membranes — •Gabriel Sitaru and Stephan Gekle — Biofluid Simulation and Modeling, Theoretische Physik VI, Universität Bayreuth

We investigate the efficiency of multi-step catalytic systems where a reactant species is flown through a set of fibrous catalytic membranes. The complexity of such systems arises from the interplay of three different time scales: advection, diffusion and reaction. A theory based on infinitely long cylindrical catalytic sites is developed for the steady-state of an advection-diffusion limited reaction. Additionally, the time-dependent concentration profiles are computed using a Lattice-Boltzmann based solver for both the advection-diffusion-reaction and the Navier-Stokes equations. The comparison shows a good agreement between the theory and the numerical results, our model breaking down only in the very low-Péclet regime (i.e. diffusive flow). Both methods can be easily used to predict the efficiency of a multi-step catalysis in fibrous membranes with various geometries.

DY 44.6 Wed 16:15 ZEU 255

The stability field of the chiral CO2 water hydrate from molecular dynamics simulations — •Marcello Sega[1], Jakob Michl[2], and Christoph Dellago[2] — [1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Germany — [2]Faculty of Physics, University of Vienna, Austria

Recent experimental evidence[1] shows that the water network characterizing the high-pressure CO2 hydrate[2] is, in fact, ice XVII, which possesses open helicoidal channels giving the structure a chiral nature. The question of the stability field boundaries of this hydrate is still open, and we report on recent molecular dynamics simulations[3] in which we found that the CO2-filled ice XVII is more stable than the sI clathrate and than the mixture of ice VI and dry ice at pressure values ranging from 6 to 18 kbar and in a wide temperature range. We propose a phenomenological correction to take into account the limitation of the model potentials, suggesting that the stability should more realistically range from 6.5 to 13.5 kbar. Our simulation results support the current hypothesis that the chiral CO2 hydrate is stable at temperatures above the melting curve of ice VI.

[1]L. Del Rosso, M. Celli, and L. Ulivi, Nat. Comm. 7, 13394 (2016)

[2]H. Hirai, K. Komatsu, M. Honda, T. Kawamura, Y. Yamamoto, and T. Yagi, The J. Chem. Phys. 133, 124511 (2010)

[3]J. Michl, M. Sega, and C. Dellago, J. Chem. Phys. 151, 104502 (2019)

DY 44.7 Wed 16:30 ZEU 255

Mechanics of shape-shifting droplets — •Ireth Garcia-Aguilar[1], Piermarco Fonda[1], Eli Sloutskin[2], and Luca Giomi[1] — [1]Instituut-Lorentz, Universiteit Leiden, The Netherlands — [2]Department of Physics and Institute of Nanotechnology & Advanced Materials, Bar-Ilan University, Ramat-Gan, Israel

It has been long understood that dispersed liquid droplets are spherical in order to minimize the tension at their interface. Surprisingly, oil emulsion droplets in water have been observed to spontaneously deform into polyhedral shapes when cooling down the system. The equilibrium shape of a droplet at some temperature depends on its initial volume but all deformations take place below the freezing point of the surfactant monolayer, while the bulk oil and water remain liquid. The frozen interface forms an hexagonal lattice which is topologically constrained to accommodate defects. These produce large stresses that induce in and out-of-plane deformations in the crystal which in turn are opposed by the interfacial tension between oil and water. Initially, it was thought that this competition determines the droplet shape; however, this alone can not explain the size dependence of the deformations. By modeling the interface as a 2D elastic surface and studying its equilibrium geometry, we found a mechanism that explains the size-scaling behaviour. Interestingly, crystalline defects are not the only peculiarity playing a role in shaping the droplets.

DY 45: Microfluidics (joint session DY/CPP)

Time: Wednesday 17:00–18:30 Location: ZEU 147

DY 45.1 Wed 17:00 ZEU 147

Near-field acoustic manipulation in a confined evanescent Bessel beam — •Pierre-Yves Gires[1,2] and Cédric Poulain[1,3] — [1]University Grenoble Alpes, CEA LETI — [2]University of Bayreuth, Experimental Physics I — [3]University Grenoble Alpes, CNRS, Grenoble INP, Institut Néel

Microparticles such as cells can be manipulated in a suspension by the application of an ultrasonic acoustic field. Following the path taken in the development of optical tweezers, we demonstrate the potential of working in the evanescent regime, with both sub-wavelength confinements and resonators [1]. We generate an evanescent acoustic Bessel beam in liquid above a thin, circular, axisymmetrically excited plate. In the sub-MHz domain, the resulting radiation force causes the particles to assemble at the pressure antinodes along concentric circles corresponding to the Bessel profile. By imposing an axial confinement in the evanescent region, the sub-wavelength two-plate sandwich system becomes resonant, increasing the radiation force magnitude. Resonances occur for some well-defined gaps for which whole numbers of antinodal circles are observed. Through fine tuning, particles as small as bacteria can be patterned. Further amplification can be obtained by trapping a microbubble in the Bessel beam axis.

[1] Pierre-Yves Gires and Cédric Poulain. Near-field acoustic manipulation in a confined evanescent bessel beam. Communications Physics, 2(1):1-8, 2019.

DY 45.2 Wed 17:15 ZEU 147

Theoretical and numerical investigation of an EWOD-driven micro pump — •Sebastian Bohm and Erich Runge — Technische Universität Ilmenau, Theoretische Physik 1, Weimarer Straße 25, 98693 Ilmenau

We show how the EWOD (electrowetting-on-dielectric) effect can be used to realize a micro pump that uses no moveable components at all, see patent [1]. The flow is generated due to the periodic movement of liquid-vapor interfaces in a large number ($\approx 10^6$) of microcavities ($\Delta V \approx 1$ pl per cavity). The total flow resulting from all microcavities adds up to a few hundred nanolitres per cycle. Tesla-Diodes are used as valves to completely forgo on moving parts. They must be optimized to generate a reasonable valve action even at the small Reynolds numbers that are typical for micro pumps.
The theoretical description of the pumping mechanism is a challenge due to the coupling of the fluid- and electrodynamics and the intrinsic multi-scale character of the system. In each microcavity, the flow can be modelled as multiphase flow with time-dependent wetting properties as boundary conditions. It is implemented via a boundary element method. Additionally, an approximation is presented that allows the fast calculation of the stationary shape of liquid/vapor interfaces in electrical fields. Topological optimization methods for the optimization of the Tesla-Diodes are presented, in which the complete micro pump system is considered as well.
[1] Hoffmann, M., Dittrich, L., Bertko, M.; German patent DE11 2011 104 467 (2012)

DY 45.3 Wed 17:30 ZEU 147

Digital magnetofluidics with planar Hall effect sensors — •Julian Schütt[1], Rico Illing[1], Oleksii Volkov[1], Tobias Kosub[1], Pablo Granell[1,2], Hariharan Nhalil[3], Jürgen Fassbender[1], Lior Klein[3], Asaf Grosz[4], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany — [2]Escuela de Ciencia y Tecnología, UNSAM, Buenos Aires, Argentina — [3]Department of Physics & Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel — [4]Department of Electrical and Computer Engineering, Ben-Gurion University of the Negev, Israel

The detection of magnetic nanoparticles is of major importance in biomedical and biological applications. Here, the trend goes towards improvements of state-of-the-art methods in the spirit of high-throughput analysis at ultra-low volumes. Microfluidics addresses these requirements as it deals with the control and manipulation of liquids in confined microchannels. Sensor elements utilizing the planar Hall Effect (PHE) are exceptionally suited for this conjunction and were already applied in continuous flow microfluidics. We present a sensing strategy relying on PHE sensors in digital microfluidics for the detection of a multiphase liquid flow. We show the detection of nanoliter-sized superparamagnetic droplets with a concentration of 0.58mg/cm3, biased in a geomagnetic field, down to 0.04mg/cm3 in a magnetic field of 5mT. We are convinced that the tracking of microfluidic droplets can greatly contribute to state-of-the-art magnetoresistive sensing with dramatic downscaling of the analyzed volume.

DY 45.4 Wed 17:45 ZEU 147

Positioning of Gold Nanoparticles by Thermo-Osmotic Flows in Electrolytes — •Martin Fränzl and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

The application of gold nanoparticles as plasmonic sensors in fluidic applications requires exact positioning which is often only achieved by rigid templating using physical or chemical lithography. Here we investigate the control of single and multiple gold nanoparticles with the help of optically induced thermo-osmotic flows in electrolyte solution. Our control is using a thin gold film on substrates to allow for a local heating of an electrolyte solution in a liquid film. The local temperature rise at the gold induces thermo-osmotic flows at the gold electrolyte solution. By tuning the electrolyte concentration, we to confine the mobility of the gold-nanoparticles to a two-dimensional layer at a distance of a few 10 nanometers from the gold film in which a positioning with the help of thermo-osmotic flows is easily possible. The experimental results of the gold nanoparticle dynamics are compared the theoretical predictions.

DY 45.5 Wed 18:00 ZEU 147

Flow in Responsive Porous Media — •Thomas Darwent[1], Enrico Segre[2], Ran Holtzman[3], and Lucas Goehring[1] — [1]Nottingham Trent University — [2]Weizmann Institute of Science — [3]Coventry University

Fluid flows in porous media, such as sand, rocks and biological tissues, are controlled by the geometry of that media and the properties of the fluids. Here, we explore the situation where the properties of the fluid and solid are coupled, such that an invading fluid modifies the structure of a porous medium around it. Specifically, we look at the case where the porous matrix is deformable, and we show that a new invasion pattern is seen: capillary fracturing. This results from the fluid pushing and pulling on individual grains making up the solid body, which changes the pressures required to flow past, or invade, those grains. This effect occurs in hydrocarbon recovery and CO2 sequestration where fluids are injected underground and deform the local structure. To study this problem, we use soft lithography and microfluidic techniques to produce PDMS micromodels, allowing us to tune the elasticity and disorder of a model porous medium. Along with numerical simulations, we show that deformation caused by the fluid leads to localised fingering patterns in more compliant materials, and that this effect is restricted by increasing the disorder in the system.

DY 45.6 Wed 18:15 ZEU 147

Actuation of soft particles in oscillating Poiseuille flow — •Winfried Schmidt[1], Sebastian W. Krauss[2], Andre Förtsch[1], Matthias Laumann[1], and Walter Zimmermann[1] — [1]Theoretische Physik 1, Universität Bayreuth, 95447 Bayreuth, Germany — [2]Experimentalphysik 1, Universität Bayreuth, 95447 Bayreuth, Germany

What is the dynamical behavior of soft particles in oscillatory (pulsating) Poiseuille flow at low Reynolds number? By investigating the overdamped motion of 2D bead-spring models, as well as 3D capsules and red blood cells, we predict particle actuation in the case of vanishing mean flow. This effect is generic as it does not depend on the model. We show that symmetric particles propagate for asymmetric flow oscillations with non-equal flow sections. The mean actuation (swim) velocity of a particle is caused by its varying shape in both parts of the flow period. Since the actuation steps depend also on the size and the rigidity of soft particles, this novel actuation (passive swimming) mechanism is also appropriate for particle sorting.

DY 46: Many-body Quantum Dynamics I

Time: Thursday 9:30–12:30 Location: HÜL 186

Invited Talk DY 46.1 Thu 9:30 HÜL 186

Nanofriction in Ion Coulomb Systems — •Tanja Mehlstäubler — QUEST-Institut an der PTB, Bundesallee 100, 38116 Braunschweig

Single trapped and laser-cooled ions in Paul traps allow for a high degree of control of atomic quantum systems. They are the basis for modern atomic clocks, quantum computers and quantum simulators. Our research aims to use ion Coulomb crystals, i.e. many-body systems with complex dynamics, for precision spectroscopy. This paves the way to novel optical frequency standards for applications such as relativistic geodesy and quantum simulators in which complex dynamics becomes accessible with atomic resolution.

The high-level of control of self-organized Coulomb crystals open up a fascinating insight into the non-equilibrium dynamics of coupled many-body systems, displaying atomic friction and symmetry-breaking phase transitions. We discuss the creation of topological defects and Kibble-Zurek tests in 2D crystals and present recent results on the study of tribology and transport mediated by the topological defect.

DY 46.2 Thu 10:00 HÜL 186

Charge-density-wave melting in the one-dimensional Holstein model — •Jan Stolpp[1], Jacek Herbrych[2], Florian Dorfner[3], Elbio Dagotto[4], and Fabian Heidrich-Meisner[1] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Wroclaw University of Science and Technology — [3]Arnold Sommerfeld Center for Theoretical Physics, Universität München — [4]Department of Physics and Astronomy, University of Tennessee and ORNL

In a recent preprint [1] we study the real-time dynamics in the half-filled Holstein model starting from different initial states that are charge-density-wave (CDW) ordered. The regime where the relaxation dynamics is dominated by electron-phonon coupling is considered (complementary to the case studied in [2] where strong electron interactions were present) and we focus on the far-from-equilibrium regime. Here, a clear separation of time scales between electron relaxation and phonon equilibration is identified. In the transient dynamics we observe effects like a temporal self trapping of the electrons. The study of such regimes is enabled by extending the time-evolving block decimation algorithm with local basis optimization, previously applied to single-polaron dynamics [3], to a half-filled system.

[1] Stolpp et al., arXiv:1911.01718 (2019)
[2] Hashimoto and Ishihara, PRB 96, 035154 (2017)
[3] Brockt et al., PRB 92, 241106(R) (2015)

DY 46.3 Thu 10:15 HÜL 186

Confinement Quench Dynamics on a Quantum Computer — •Joseph Vovrosh[1] and Johannes Knolle[1,2,3] — [1]Blackett Laboratory, Imperial College London, London, SW7 2AZ, United Kingdom — [2]Department of Physics, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Confinement is a phenomenon that occurs when the attraction between two particles grows with their distance, most prominently found in quantum chromodynamics (QCD) between quarks. In condensed matter physics, similar phenomena occur in quantum spin chains, for example, in the one dimensional transverse field Ising model with an additional longitudinal field or as measured in scattering experiments on cobalt niobate. It turns out that confinement effects also lead to clear signatures in the non-equilibrium dynamics after a quantum quench. This makes confinement an ideal quantum effect to test the capabilities of quantum computers. Here, the underlying physics of confinement is explored in relation to quantum simulation on state of the art quantum computers. Quantum confinement is a non-perturbative interaction effect and its quantum simulation opens the possibilities to explore new quantum phenomena beyond the capabilities of classical computers.

DY 46.4 Thu 10:30 HÜL 186

Preparing Atomic Topological Quantum Matter by Adiabatic Non-Unitary Dynamics — Simone Barbarino[1], Jinlong Yu[2,3], Peter Zoller[2,3], and •Jan Carl Budich[1] — [1]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Center for Quantum Physics, Faculty of Mathematics, Computer Science and Physics, University of Innsbruck, Innsbruck A-6020, Austria — [3]Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, Innsbruck A-6020, Austria

Motivated by the outstanding challenge of realizing low-temperature states of quantum matter in synthetic materials, we propose and study an experimentally feasible protocol for preparing topological states such as Chern insulators. By definition, such (non-symmetry protected) topological phases cannot be attained without going through a phase transition in a closed system, largely preventing their preparation in coherent dynamics. To overcome this fundamental caveat, we propose to couple the target system to a conjugate system, so as to prepare a symmetry protected topological phase in an extended system by intermittently breaking the protecting symmetry. Finally, the decoupled conjugate system is discarded, thus projecting onto the desired topological state in the target system. By construction, this protocol may be immediately generalized to the class of invertible topological phases, characterized by the existence of an inverse topological order. We illustrate our findings with microscopic simulations on an experimentally realistic Chern insulator model of ultracold fermionic atoms in a driven spin-dependent hexagonal optical lattice.

DY 46.5 Thu 10:45 HÜL 186

Hierarchy of double-time correlations for quenches in the Bose-Hubbard model — •Friedemann Queisser[1,2,3] and Ralf Schützhold[1,2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

The hierarchy of correlations is an analytical approximation method which allows us to study non-equilibrium phenomena in strongly interacting quantum many-body systems on lattices in higher dimensions (with the underlying idea being somewhat similar to dynamical mean-field theory). So far, this method was restricted to equal-time correlators such as $\langle \hat{A}_\mu(t)\hat{B}_\nu(t)\rangle$. Using the method of complete induction, we generalize this method to double-time correlators such as $\langle \hat{A}_\mu(t)\hat{B}_\nu(t')\rangle$, which allows us to study effective light cones and Green functions and to incorporate finite initial temperatures. As an application, we study the non-equilibrium dynamics after quantum quenches of the Bose-Hubbard model in the Mott insulator phase.

Reference: arXiv:1909.10938

15 min. break.

DY 46.6 Thu 11:15 HÜL 186

Boltzmann relaxation dynamics in the strongly interacting Fermi-Hubbard model — •Friedemann Queisser[1,2,3] and Ralf Schützhold[1,2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany — [2]Helmholtz-

Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

Via the hierarchy of correlations, we study the Mott insulator phase of the Fermi-Hubbard model in the limit of strong interactions and derive a quantum Boltzmann equation describing its relaxation dynamics. In stark contrast to the weakly interacting case, we find that the scattering cross sections strongly depend on the momenta of the colliding quasi-particles and holes. Therefore, the relaxation towards equilibrium crucially depends on the spectrum of excitations. For example, for particle-hole excitations directly at the minimum of the (direct) Mott gap, the scattering cross sections vanish such that these excitations can have a very long life-time.

Reference:

F. Queisser and R. Schützhold, Phys. Rev. A **100**, 053617 (2019)

DY 46.7 Thu 11:30 HÜL 186

Boltzmann relaxation dynamics of strongly interacting spinless fermions on a lattice — •Friedemann Queisser[1,2,3], Sebastian Schreiber[1], Peter Kratzer[1], and Ralf Schützhold[1,2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

Motivated by the recent interest in nonequilibrium phenomena in quantum many-body systems, we study strongly interacting fermions on a lattice by deriving and numerically solving quantum Boltzmann equations that describe their relaxation to thermodynamic equilibrium. The derivation is carried out by inspecting the hierarchy of correlations within the framework of the 1/Z expansion. Applying the Markov approximation, we obtain the dynamic equations for the distribution functions. Interestingly, we find that in the strong-coupling limit, collisions between particles and holes dominate over particle-particle and hole-hole collisions – in stark contrast to weakly interacting systems. As a consequence, our numerical simulations show that the relaxation timescales strongly depend on the type of excitations (particles or holes or both) that are initially present.

Reference: arXiv:1909.12802

DY 46.8 Thu 11:45 HÜL 186

Enhancement of local pairing correlations in periodically driven Mott insulators — •Francesco Peronaci[1,2,3], Olivier Parcollet[1,4], and Marco Schiró[1] — [1]Institut de Physique Théorique (IPhT), CEA, CNRS, UMR 3681, 91191 Gif-sur-Yvette, France — [2]CPHT, Ecole Polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France — [3]Max Planck Institute for the Physics of Complex Systems, Dresden 01187, Germany — [4]Center for Computational Quantum Physics, Flatiron Institute, 162 Fifth Avenue, New York, NY 10010, USA

We investigate a model for a Mott insulator in presence of a time-periodic modulated interaction and a coupling to a thermal reservoir. The combination of drive and dissipation leads to non-equilibrium steady states with a large number of doublon excitations, well above the maximum thermal-equilibrium value. We interpret this effect as an enhancement of local pairing correlations, providing analytical arguments based on a Floquet Hamiltonian. Remarkably, this Hamiltonian shows a tendency to develop long-range staggered superconducting correlations. This suggests the possibility of realizing the elusive eta-pairing phase in driven-dissipative Mott Insulators.

DY 46.9 Thu 12:00 HÜL 186

Hilbert space average of transition probabilities — •Nico Hahn and Daniel Waltner — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

The typicality approach and the Hilbert space averaging method as its technical manifestation are important concepts of quantum statistical mechanics. Extensivley used for expectation values we will extend them to transition probabilities. We find that the transition probability of two random uniformly distributed states is connected to the spectral statistics of the considered operator. We will demonstrate our quite general result for a kicked spin chain.

DY 46.10 Thu 12:15 HÜL 186

Quenched Fermi systems mediating time delayed interactions — •Conor Jackson and Bernd Braunecker — University of St Andrews, St Andrews, UK

Impurity quenches in Fermi systems are known to substantially reorganise the Fermi sea, most dramatically illustrated by Anderson's orthogonality catastrophe. We investigate how the influence of the catastrophe is transmitted through the system, finding singular behaviour at the boundary of the light cone emanating from the quench. We examine how states localised some distance away from the impurity display the influence of the spreading shake up of the Fermi sea and explore using the long range effect of the quench to induce a time delayed interaction between such states. Such a coherent coupling via a largely incoherent medium may have uses in quantum information processing.

DY 47: Focus Session: Nonlinear Dynamics of the Heart I (joint session DY/BP)

Time: Thursday 9:30–12:45 Location: ZEU 118

Invited Talk DY 47.1 Thu 9:30 ZEU 118

Nonlinear dynamics of cardiac arrhythmias in the long QT syndrome — •Alain Karma — Northeastern University, Boston, USA

Long QT syndrome is associated with fatal ventricular arrhythmias promoted by triggered activity in the form of early afterdepolarizations (EADs). This talk will review recent progress to understand the genesis of EADs and associated life-threatening arrhythmias at cellular and tissue scales using a combination of computational and experimental studies. Computational studies make use of a physiologically detailed computational model of calcium (Ca2+) cycling and membrane voltage dynamics that bridges the submicron scale of individual couplons of plasmalemmal L-type Ca2+ channels clusters and sarcoplasmic reticulum (SR) Ca2+ release units (CRUs) and the whole cell. Experimental studies make use of large animal transgenic rabbit models that mimic human mutations associated with most common forms of the long QT syndrome types 1 and 2. The results, obtained by iterations between modeling and experiments spanning ion channels, cellular, and organ scales, highlight the important roles of the coupling between intracellular Ca2+ cycling and voltage dynamics in the genesis of cellular EADs and tissue-scale spatial heterogeneities in the initiation of arrhythmogenic premature ventricular contractions.

DY 47.2 Thu 10:00 ZEU 118

Understanding the origin of line defects in heart tissue. — •Marcel Hörning[1], Alessio Gizzi[2], and Alessandro Loppini[2] — [1]University of Stuttgart, Stuttgat, Germany — [2]University Campus Bio-Medico of Rome, Rome, Italy

Spatiotemporal patterns are observed in a wide range of excitable systems. They have important and diverse regulatory functions, such as regulation of cell migration of Dictyostelium cells, synchronization of electrophysiological dynamics in the cerebral neocortex, and maintenance of the contractility and cardiovascular blood circulation in mammalian hearts. In the heart, excitable waves can form complex oscillatory and chaotic patterns even at an abnormally higher frequency than normal heart beats, which increase the risk of fatal heart conditions by inhibiting normal blood circulation. Previous studies suggested that the occurrence of line defects in alternans play a critical role in the stabilizion of those undesirable patterns. However, this nonlinear phenomenon is still poorly understood. It remains to be elucidated, how nodal lines form, what their origin is, and how they stabilises. Here we show new insights in the stability of those by observing and analysing nodal line dynamics in spiral waves that exhibit stable alternans, and giving first clues on the origin of those.

DY 47.3 Thu 10:15 ZEU 118

Optogenetic Control Spiral Wave Dynamics in Cardiac Tissue — •Sayedeh Hussaini[1,2,4], Rupamanjari Majumder[1,4], Valentin Krinski[1,4], Ulrich Parlitz[1,4], Stefan Luther[1,2,3,4], and Claudia Richter[1,4] — [1]Max Planck Institute for Dynamics and Self-

Organization, Goettingen, Germany — [2]Institute for the Dynamics of Complex Systems, Goettingen, Germany — [3]Institute of Pharmacology and Toxicology, Goettingen, Germany — [4]German Center for Cardiovascular Research, Goettingen, Germany

Cardiac optogenetics may be used as a tool to elucidate the mechanisms underlying the dynamics and control of the spiral waves in the heart. Here we present a simulation study based on the ionically realistic Bondarenko model of mouse ventricular cardiomyocytes, coupled to a model for the light-activated protein Channelrhodopsin-2. We show that constant global sub-threshold illumination increases the resting membrane voltage, decreases the amplitude and the conduction velocity of the excitation wave. Periodic global illumination of the two-dimensional domain results in the transition of the spiral wave core of the trajectory from circular to epicycloidal and hypocycloidal. Using structured sub-threshold illumination, we induced spiral drift towards the boundary and subsequent termination. In the presence of an intensity gradient, the spiral wave drifts towards higher intensities.

DY 47.4 Thu 10:30 ZEU 118

Dynamics of scroll waves in a cylinder jacket geometry — Christian Bruns[1] and •Marcus Hauser[2] — [1]Institut für Biometrie und Medizinische Bioinformatik, Universität Magdeburg, Magdeburg, Germany — [2]Insitut für Biologie, Universität Magdeburg, Magdeburg, Germany

The dynamics of scroll waves in a narrow cylinder jacket-shaped reactor is investigated experimentally by optical tomography using a chemical model system. The fate of the scroll waves of excitation in the Belousov-Zhabotinsky reaction depend on the thickness of the cylinder jacket. While at sufficiently wide cylinder jackets vertically oriented scroll waves remain stable, the probability that the filaments of the scrolls hit a lateral wall increase with the shrinking width of the cylinder jacket. This may lead to the rupture of the initial filament and pinning of the filament ends at the lateral walls. Filaments that pin to opposite lateral walls shrink and reorient to a horizontal orientation; such a reorientation corresponds to a transition from an intramural to a transmural scroll wave. The kinetics of the reorientation and shrinkage of the scrolls were studied. Furthermore, we find that no new filaments were generated upon collision of excitation waves at the side of the cylinder jacket opposite to the scroll wave. Thus, under the studied conditions, we do not observe any new generation of filaments due to a phenomenon like reentry.

DY 47.5 Thu 10:45 ZEU 118

Synchronization of viscoelastically coupled cardiomyocytes — •Florian Spreckelsen[1,2,3], Stefan Luther[1,2,3], and Ulrich Parlitz[1,2,3,4] — [1]Max Planck Institute for Dynamics and Self-organization, Göttingen, Germany — [2]University of Göttingen, Institute for the Dynamics of Complex Systems, Göttingen, Germany — [3]DZHK (German Center for Cardiovascular Research), Partner Site Göttingen, Germany — [4]University Medical Center Göttingen (UMG), Institute of Pharmacology and Toxicology, Göttingen, Germany

Periodically beating cardiomyocytes coupled mechanically by a viscoelastic extracellular matrix are modelled as viscoelastically coupled excitable oscillators. Their synchronization dynamics depends on the stiffness of the coupling matrix [1].

Systems of two coupled cells and linear chains are investigated numerically. At high stiffness of the viscoelastic coupling, full in-phase synchronization is found. Partial n:n synchronization is observed in case of intermediate stiffness. In the special case of purely elastic coupling, two cells show antiphase synchronization while antiphase chimera states are found in linear chains.

The conditions necessary for the synchronization of viscoelastically coupled cardiomyocytes may give a mechanistic explanation for the importance of fibroblasts to the engineering of cardiac tissue [2,3].

[1] Spreckelsen, Luther, Parlitz, Phys. Rev. E 100, 2019
[2] Tiburcy et al., Circulation 135, 2017
[3] Schlick et al., Prog Bio Mol Bio 144, 2019

15 min. break.

Invited Talk DY 47.6 Thu 11:15 ZEU 118

Wave-particle duality of dissipative vortices and implications for cardiology — •Irina V. Biktasheva — University of Liverpool, Liverpool, UK

Recent theoretical and experimental advancements in study of dynamics of dissipative vortices (aka spiral waves) brought these studies closer to practical impact and applications than ever before.

A dissipative vortex divides homogeneous system into the core, defined by it's rotation centre, or organising filament, and the periphery synchronised by signals from the core. Perturbed vortex slowly changes frequency and location of the core. Regime synchronises all available space, though it behaves as localised object sensitive only to perturbations affecting the core. The wave-particle duality is due to localisation of vortex's Response Functions (RFs) in immediate vicinity of the core. RFs allow quantitative prediction of drift caused by small perturbations of any nature, which makes RFs as fundamental characteristics for spiral waves as mass is for the matter.

We use cardiac re-entry's RFs to predict iscaemic border zone dynamics, and define basal tissue conditions for re-entry's escape into recovered tissue to either collapse or develop fibrillation. In human atrium, we demonstrate functional effects of anatomical structures on re-entry's spontaneous drift along pectinate muscles (PM) and crista terminalis, anchor to PM-atrial wall junctions or to some locations with no obvious anatomical features. The insights might improve patient specific ablation and low-voltage defibrillation protocols.

DY 47.7 Thu 11:45 ZEU 118

Control and self-termination of spiral wave chaos — •Thomas Lilienkamp[1,2] and Ulrich Parlitz[1,2,3] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]German Center for Cardiovascular Research (DZHK), Göttingen, Germany — [3]Institut für Dynamik Komplexer Systeme, Georg-August Universität, Göttingen, Germany

During life threatening cardiac arrhythmias like ventricular fibrillation the electrical excitation dynamics inside the heart is governed by chaotic spiral/scroll wave propagation. In experiments, it is frequently observed that the chaotic dynamics can also terminate by itself. This phenomenon can also be reproduced in numerical simulations. We demonstrate in simulations, how a system of chaotic spiral wave dynamics can be controlled using small but finite perturbations which are locallized in space and time, by exploiting the state space structure. With this, we show that a control of such systems can be achieved in principle by a minimal interaction with the system.

DY 47.8 Thu 12:00 ZEU 118

Constitutive modeling for failing heart regeneration — Moritz Kalhöfer-Köchling[1,3], Wolfram Zimmermann[2,3], Eberhard Bodenschatz[1,3], and •Yong Wang[1,3] — [1]MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]University Medical Center Göttingen, 37075 Göttingen, Germany — [3]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen, Göttingen, Germany

Heart failure is a common, costly, and potentially fatal condition in which the heart cannot pump enough blood to meet the body's needs. It is mainly caused by myocardial infarction, and associated with changes both in structure and function of the heart. Employing nonlinear solid mechanics, constitutive modeling is adopted to study cardiac mechanics and guide new therapy such as tissue engineered heart repair. To simulate the infarcted tissue as well as implanted engineered heart muscle, a novel class of constitutive models is proposed by considering fiber dispersion. Compared with their predecessors, those models improve the numerical stability, compute faster and are easier to implement. We also investigate the mechanical properties of heart muscle experimentally. This work was supported by the Max Planck Society and the German Center for Cardiovascular Research.

DY 47.9 Thu 12:15 ZEU 118

Synchronization-based reconstruction of the electrical dynamics of the heart — •Baltasar Rüchardt[1,3], Jochen Bröcker[4], Stefan Luther[1,2,3], and Ulrich Parlitz[1,2,3] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August-Universität Göttingen, Institute for Nonlinear Dynamics, Göttingen, Germany — [3]German Center for Cardiovascular Research (partnersite Göttingen), Göttingen, Germany — [4]University of Reading, Reading, UK

For more than a century, the electrocardiogram (ECG) is the standard diagnostic tool to assess cardiac electrophysiological function. The relation between the electrical excitation of the heart and the electrical potential on the surface of the body is well understood. The reconstruction of the source distribution on the heart from given ECG measurements is challenging, because information is lost when the electrical signal travels through the body in a diffusion-like process. This problem is called inverse problem of electrocardiography.

The standard methods to handle this loss are regularization methods which impose pre-defined assumptions on the problem until a solution can be found. This can exclude the true solution and, in general, does not rely on information of the underlying dynamical processes. In contrast, we show the reconstruction of the electrical state of the heart from sensor signals with reduced spatial information by means of synchronization, based on a model of the spatial-temporal electrical dynamics. We show this for a 2D excitable media heart tissue model and discuss the application to three dimensions.

DY 47.10 Thu 12:30 ZEU 118

Real-time Processing of Optical Fluorescence Videos showing Contracting Hearts using Neural Networks — •Jan Lebert[1,2,3] and Jan Christoph[1,2,3] — [1]University Medical Center Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]German Center for Cardiovascular Research, Partnersite Göttingen, Germany

Optical mapping is an established fluorescence imaging technique for studying electrophysiological wave phenomena in isolated, intact hearts and cardiac cell cultures. Mechanical contraction of the cardiac tissue, however, can lead to severe motion artifacts in the recorded optical signals. Pharmacological electromechanical uncoupling agents have been used to compensate for these artifacts. However, recently numerical motion tracking and post-processing algorithms were developed to suppress motion artifacts and separate the recorded electrical waves from mechanical contraction.

Here, we present a deep convolutional neural network (CNN) approach for the real-time tracking of contracting and fluorescing hearts in optical mapping videos. Our approach provides a dramatic speed-up in the processing of optical mapping data and superior performance over conventional optical flow estimation algorithms, which are sensitive to noise and can be irritated by fluorescence-encoded wave patterns, as they assume brightness consistency. After training the network on various experimental and synthetically generated optical mapping data, we evaluated the network's performance and found it to perform robustly under various conditions.

DY 48: Statistical Physics far from Thermal Equilibrium

Time: Thursday 9:30–12:15 Location: ZEU 147

DY 48.1 Thu 9:30 ZEU 147

Entropy Production in Open Systems: The Predominant Role of Intraenvironment Correlations — •Krzysztof Ptaszyński[1] and Massimiliano Esposito[2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań, Poland — [2]Complex Systems and Statistical Mechanics, Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We show [1] that the entropy production in small open systems coupled to environments made of extended baths is predominantly caused by the displacement of the environment from equilibrium rather than, as often assumed, the mutual information between the system and the environment. The latter contribution is strongly bounded from above by the Araki-Lieb inequality, and therefore is not time-extensive, in contrast to the entropy production itself. Furthermore, we show that in the thermodynamic limit the entropy production is associated mainly with generation of the mutual information between initially uncorrelated environmental degrees of freedom. We confirm our results with exact numerical calculations of the system-environment dynamics.

[1] K. Ptaszyński, M. Esposito, Phys. Rev. Lett. 123, 200603 (2019)

DY 48.2 Thu 9:45 ZEU 147

Tuning Interaction in Long-Range Models Changes Dynamical Scaling During Aging — •Henrik Christiansen[1], Suman Majumder[1], Malte Henkel[2,3], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [2]Laboratoire de Physique et Chimie Théoriques (CNRS UMR 7019),Université de Lorraine Nancy, 54506 Vandaeuvre-lès-Nancy Cedex, France — [3]Centro de Física Teórica e Computacional, Universidade de Lisboa, 1749-016 Lisboa, Portugal

Aging in phase-ordering kinetics of the long-ranged $d = 2$ Ising model is studied via Monte Carlo simulations. The dynamical scaling and aging behavior is analyzed. The dynamical scaling of the spin-spin two-time autocorrelation function is best described by sub-aging in the regime of long-range interactions and by simple aging for effective short-range interactions. The sub-aging exponent μ and the nonequilibrium autocorrelation exponent λ depend explicitly on the range parameter σ. Our data support the relation $\lambda = \sigma$ for $\sigma \leq 1$ and $\lambda = 1.25$ for $\sigma > 1$.

DY 48.3 Thu 10:00 ZEU 147

Thermodynamic Uncertainty Relation for the Kardar-Parisi-Zhang Equation — •Oliver Niggemann and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

Recently, we have proposed a field-theoretic thermodynamic uncertainty relation for a generic field theory [arXiv: 1908.05560]. In this talk, we first formulate a framework which describes quantities like current, entropy production and diffusivity in the case of a generic field theory. We will then apply this general setting to the one-dimensional Kardar-Parisi-Zhang equation, a paradigmatic example of a non-linear field-theoretic Langevin equation. In particular, we will treat the dimensionless Kardar-Parisi-Zhang equation with an effective coupling parameter measuring the strength of the non-linearity. It will be shown that a field-theoretic thermodynamic uncertainty relation holds up to second order in a perturbation expansion with respect to a small effective coupling constant. The calculations show that the field-theoretic variant of the thermodynamic uncertainty relation is not saturated for the case of the Kardar-Parisi-Zhang equation due to an excess term stemming from its non-linearity.

DY 48.4 Thu 10:15 ZEU 147

Domain wall fluctuations between extremal current phases of driven lattice gases — •Marco Bosi, David Locher, and Philipp Maass — Fachbereich Physik, Osnabrück Universität, Germany

Driven lattice gases are systems where fundamental aspects of non-equilibrium physics can be conveniently studied. In addition they have many applications in biology and other fields. In bulk-driven open system coupled to particle reservoir, phase transitions occur, where, the bulk density in stationary states exhibits a singular behaviour upon varying the parameters of the system-reservoir couplings (analogous to first and second transitions known in equilibrium).Self-organized phases can appear with bulk densities equal to values where the bulk current is minimal or maximal[1][2].

In the presence of repulsive nearest-neighbour interactions degenerate maxima in the bulk current-density relation emerge[3], which allow for coexisting maximal current phases[4]. We report on the behaviour of the fluctuations of the domain walls separating those coexisting phases.

[1]J. Krug, *Phys. Rev. Lett.* 67, 1882 (1991).
[2]G. M. Schütz, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz (Academic Press, London, 2001), Vol. 19, pp. 1-251.
[3]M. Dierl, M. Einax, and P. Maass, *Phys. Rev.* E 87, 062126 (2013).
[4]P. Maass, M. Dierl, and M. Wolff, in *On Phase Transitions in Biased Diffusion of Interacting Particles* (Springer International, Cham, 2018), Chap. 9, pp. 147-168.

DY 48.5 Thu 10:30 ZEU 147

Diffusion System with Lorentz Force — •Iman Abdoli[1], Hidde Derk Vuijk[1], Holger Merlitz[1], Jens-Uwe Sommer[1,2], Joseph Michael Brader[3], and Abhinav Sharma[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, 01069 Dresden, Deutschland — [2]Technische Universität Dresden, Institut für Theoretische Physik, 01069 Dresden, Deutschland — [3]Department de Physique, Université de Fribourg, CH-1700 Fribourg, Suisse

In the presence of Lorentz force arising from an external magnetic field the Fokker-Planck equation picks up a tensorial coefficient, which reflects the anisotropy of the particle's motion. Lorentz force gives rise to diffusive or irrotational fluxes and Brownian vortexes or solenoidal fluxes along and perpendicular to the density gradients, respectively. We first study the systems in which these Brownian vortexes can be ignored in the time evolution of the density. We then investigate how these vortexes influence the probability density function (or PDF) of the particle's positions in the nonequilibrium stationary state of a diffusion system under stochastic resetting with Lorentz force. Next,

we show, analytically and computationally, that the solenoidal fluxes persist in the stationary state of a diffusive system with two different temperatures.

15 min. break.

DY 48.6 Thu 11:00 ZEU 147

Acceleration of non-equilibrium relaxations from long-range initial conditions — •Malte Henkel — MPIPKS, Noethnitzer Strasse 38, D - 01187 Dresden, Germany

Physical ageing is a widespread phenomenon which arises typically after a complex many-body system is quenched from some initial state to a more ordered state, where characteristically several equivalent equilibrium states compete in the control of the long-time evolution. Here we study those ageing processes which may arise in systems which undergo *biased* transport, in a preferred direction. Specific examples, notably the exact solution of the one-dimensional biased Glauber-Ising chain, show that the dynamical exponent z, defined through the relevant cluster size $L(t) \sim t^{1/z}$ at large times t, can depend on the chosen initial conditions. In particular, we shall show that sufficiently long-range initial correlations can lead to a cross-over from effectively diffusive transport, where $z = 2$, to ballistic transport with $z = 1$. This leads to a considerable acceleration of the dynamics, whose possible applications will be explored.

M. Henkel, S. Stoimenov, J. Stat. Mech. 084009 (2019) [arxiv:1810.09855].

DY 48.7 Thu 11:15 ZEU 147

Ageing and non-markovian effects in the exactly solved quantum $O(n)$-model — •Sascha Wald[1], Alessio Chiocchetta[2], Malte Henkel[3], and Andrea Gambassi[4] — [1]Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, 01187, Dresden, Germany — [2]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [3]Laboratoire de Physique et Chimie Théoriques (CNRS UMR 7019), Université de Lorraine Nancy, B.P. 70239, 54506 Vandoeuvre lès Nancy, France — [4]SISSA - International School for Advanced Studies and INFN, via Bonomea 265, I-34136 Trieste, Italy

The effects of quantum noise on the non-equilibrium dynamics of many-body quantum systems, after a quantum quench, are analysed. Quantum noise, as opposed to the classical white noise, is inherently non-Markovian and the resulting dynamics is affected by memory effects, which lead to changes compared to Markovian white noises. In order to systematically analyse these effects, we study the quantum $O(n)$-model at large n, in contact with a bath at zero temperature. Starting from the quantum Langevin equation, the dynamical equations are explicitly solved. The universal properties of the dynamics, as given by the quantum noise and after a quantum quench, are analysed by studying the two-time correlation and response functions. Quantum coarsening and quantum ageing in these observables are highlighted and compared with their classical counterparts. In particular, the validity of the fluctuation-dissipation theorem after a quantum quench is studied in detail.

DY 48.8 Thu 11:30 ZEU 147

A quantum heat engine based on dynamical material design — •Gerhard Tulzer[1], Levan Chotorlishvili[2], Martin Hoffmann[1], Robert Zillich[1], Jamal Berakdar[2], and Arthur Ernst[1] — [1]Institute for Theoretical Physics, Johannes Kepler University, Linz, Austria — [2]Institute of Physics, Marthin Luther University Halle-Wittenberg, Halle (Saale), Germany

We investigate the practical usability of a magneto-electric working substance (Cr_2O_3) for a quantum Otto cycle. The new approach here is the exploitation of a new type of driving during the adiabatic work strokes, where non-linear phonon processes controlled by high-intensity terahertz optical pulses are employed to induce structural changes in the magnetic ordering of the system, being described as a spin chain with spin-3/2. The isochoric heating and cooling strokes are based on the coupling to a phonon thermostat. This type of system appears to be very promising due to its swiftness, but still needs a thorough investigation due to the nonlinearity in its dynamics and the much richer energy spectrum compared to toy models.

After confirming that we actually obtain a thermodynamic cycle we investigate the practical feasibility using the Lindblad master equation. Two quantities of interest in this regard are the efficiency as well as the output power and their relation to the experimental control parameters. We then consider the effects of different thermostat settings, and also investigate relaxation times and work stroke duration in order to find the optimal timing for high efficiency and output power.

DY 48.9 Thu 11:45 ZEU 147

Analytical solutions for non-Markovian Brownian systems far from thermal equilibrium — •Timo Dörries, Sarah A.M. Loos, and Sabine H.L. Klapp — Institut für Theoretische Physik, Hardenbergstr. 36, TU Berlin, 10623 Berlin, Germany

Markovian Langevin equations are an established tool to describe stochastic motion. However, in many real-world systems, memory effects play a crucial role and e.g. complex environments can yield to stochastic motion characterized by different timescales. Analytical solutions are in general difficult to obtain here. We propose (linear) toy models where we non-reciprocally couple auxiliary variables to a Brownian particle, each auxiliary variable corresponding to one characteristic timescale. Projecting out the auxiliary variables, we obtain a non-Markovian Langevin equation with memory and colored noise.

By deriving closed expressions for up to three auxiliary variables, we can systematically study the connection between the coupling topology and the resulting autocorrelation functions. Further, by studying the connection between topology and thermodynamical properties, we demonstrate that models with non-reciprocal coupling automatically have a net heat production, i.e. describe nonequilibrium systems [1,2].

Finally, we show that a minimal model with two auxiliary variables yields correlation functions similar to those describing hydrodynamic backflow in an optical trap [3].

[1] S.A.M. Loos et al., arXiv:1910.08372 (submitted)
[2] S.A.M. Loos and H.L. Klapp, Scientific Reports 9, 2491 (2019)
[3] Franosch et al., Nature **478**, 85-88 (2011)

DY 48.10 Thu 12:00 ZEU 147

Dynamics of active hard cross-shaped particles in two-dimensional lattice system — •Rakesh Chatterjee[1], Nimrod Segall[1], Carl Merrigan[1], Kabir Ramola[2], Bulbul Chakraborty[3], and Yair Shokef[1] — [1]Tel Aviv University, Israel — [2]Tata Institute of Fundamental Research Hyderabad, India — [3]Brandeis University, Waltham, USA

We analyse the dynamics of an active tracer particle embedded in a thermal lattice gas. All particles are subject to exclusion up to third nearest neighbours on a square lattice, which leads to slow dynamics at high densities. With no rotational diffusion of the tracer, we derive an analytical expression for the resulting drift velocity of the tracer in terms of non-equilibrium density correlations involving the tracer particle and its neighbours. For the case where the tracer undergoes rotational diffusion, we relate its diffusion coefficient to the thermal diffusion coefficient and drift velocity. We also study dynamics where the rotation of the tracer is limited by the presence of neighbouring particles.

Next we explore phase separation and kinetic arrest when all particles are active and have infinite persistence time of their active orientation. The passive limit of the model quenches into the two-phase coexistence region represent an ageing passive glass. Adding small persistent active bias to the particle dynamics creates states that resemble the passive glass at lower densities. For large active bias, the dense, immobile clusters proliferate until a spanning network bridges the system leading to percolation of an arrested phase.

DY 49: Wetting and Liquids at Interfaces and Surfaces I (joint session CPP/O/DY)

Time: Thursday 9:30–13:00 Location: ZEU 255

DY 49.1 Thu 9:30 ZEU 255

Designing Pickering Emulsions for Catalysis: Influence of Nanoscale Particle Properties on Microscale Droplets — •Sebastian Stock[1], Annika Schlander[1], Kai Spanheimer[1], Maresa Kempin[2], Dmitrij Stehl[1], Anja Drews[2], Markus Gallei[3], and Regine von Klitzing[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]HTW Berlin, Berlin, Germany — [3]Universität des Saarlandes, Saarbrücken, Germany

Pickering Emulsions (PEs) describe emulsions stabilized by surface-active particles. The aim of the present work is to design PEs as a reaction environment for catalytic reactions. As a model reaction the hydroformylation of 1-dodecene is investigated. Due to the PEs high stability separation methods with outstanding energy efficiency are applicable e. g. the separation of the oil phase by nanofiltration. Many microscopic and macroscopic PE properties are dominated by the nanoscale properties of the particles. In order to distinguish the impact of particle surface charge both positively and negatively charged silica spheres were prepared. This was achieved by adequate surface modification. The resulting nanoscale particle properties concerning size, shape, charge, and hydrophobicity were investigated via Transmission Electron Microscopy (TEM), ζ-potential and sessile drop measurements, the effect on the microscopic emulsion properties were studied with microscopy and the PEs reaction behavior including yield and stability was evaluated.

DY 49.2 Thu 9:45 ZEU 255

A Thermodynamic Consistent, Instantaneous Dividing Surface to Study Wetting Phenomena — •Amal Kanta Giri and Marcello Sega — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Fürther Straße 248, 90429 Nürnberg, Germany

A detailed knowledge of the microscopic structure and dynamics in the interfacial region of soft materials is a necessary step on the way to develop novel materials and is also key to a deeper understanding of the statistical mechanics of fluid interfaces out of equilibrium. The presence of thermal capillary waves, however, hinders efforts to investigate the local structure of interfaces by smearing out observable quantities computed in the global reference frame. To recover a detailed picture of the interface neighborhood, one needs to compute observables in the local, instantaneous reference frame located at the interface, although the determination of this frame is, in general, not unique.

Here, we report on the possibility of using computational geometry approaches to determine the set of instantaneous surface atoms in a way which is thermodynamically consistent with the Gibbs (equimolar) dividing surface. We apply these methods to the determination of the instantaneous, fluctuating contact line of droplets on solid substrates, with an outlook on the problem of dynamic wetting of soft, deformable substrates.

DY 49.3 Thu 10:00 ZEU 255

Concentration measurements in binary liquids via Raman spectroscopy — •Alena K. Bell and Robert W. Stark — Physics of Surfaces, Materialwissenschaften, TU Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt, Deutschland

The optical measurement of concentration gradients in liquid mixtures plays a crucial role in understanding transport processes in various technical applications such as printing or medical technology. In particular Raman spectroscopy offers a direct approach to identify the substances and to quantify the concentration of the components in a binary liquid. In order to quantify concentration gradients confocal Raman spectroscopy can provide the necessary spatial and temporal resolution that is needed to monitor transport processes as they occur during the evaporation of binary droplets or during mixing processes in microchannels. To this end, chemically similar substances such as alcohols of different molecular weight need to be differentiated either through the analysis of the fingerprint region or through chemical labelling. However, using the weak Raman signals in fingerprint region reduces the temporal resolution drastically which makes chemical labelling much more convenient. We discuss the advantages and disadvantages of chemical labelling in order to discriminate spectroscopically between the components of a binary liquid. By using this approach concentration gradients can be calculated by comparing relative peak intensities and correlating these results with calibration curves. Thus, the temporal and spatial evolution of concentration gradients in binary mixtures of chemically similar fluids can be analysed.

DY 49.4 Thu 10:15 ZEU 255

Hard sphere electrolyte solutions at heterogeneously charged substrates — •Maximilian Mussotter[1], Markus Bier[2], and S. Dietrich[1] — [1]Max-Planck Institut für Intelligente Systeme und Universität Stuttgart, 70569 Stuttgart, Germany — [2]University of Applied Sciences Würzburg-Schweinfurt, 97421 Schweinfurt, Germany

The structure of a dilute electrolyte solution close to a surface carrying a non-homogeneous surface charge distribution is investigated by means of classical density functional theory (DFT) within the approach of fundamental measure theory (FMT). In the case of electrolyte solutions, the effects of these inhomogeneities are particularly severe due to the corresponding length scale being the Debye length, which is large compared to molecular sizes. A fully three-dimensional investigation is performed, which accounts explicitly for the sol- vent particles, and thus provides insight in effects of ion-solvent coupling. The present work introduces a powerful framework to study a broad range of possible surface charge heterogeneities even beyond the linear response regime, showing a sensitive dependence of the density profiles of the fluid components and of the electrostatic potential on the magnitude of the charge as well as on the short ranged details of the surface charge pattern.

DY 49.5 Thu 10:30 ZEU 255

Core-shell latex colloids as interfaces for tailoring wetting properties — Calvin J. Brett[1,2,3], Joakim Engström[3,4], Volker Körstgens[5], Peter Müller-Buschbaum[5,6], Eva Malmström[4], and •Stephan V. Roth[1,4] — [1]DESY, 22603 Hamburg, Germany — [2]KTH, Dept. Mechanics, SE-10044 Stockholm, Sweden — [3]WWSC, SE-10044 Stockholm, Sweden — [4]KTH, Dept. Fibre and Polymer Technology, SE-10044 Stockholm, Sweden — [5]TUM, Physik Department, 85748 Garching, Germany — [6]MLZ, TUM, 85748 Garching, Germany

Facile surface functionalisation of latex colloids makes them most promising materials for broad thin film applications. However, the effect of these colloids on chemical film and wetting properties is not easily evaluated. Core-shell particles can deform and coalesce on the nanoscale during thermal annealing yielding tailored physical properties. We investigated two different core-shell systems (soft and rigid) with identical shell but with chemically different core polymer and core size. These core-shell colloids are probed during thermal annealing on surfaces in order to investigate their behavior as a function of nanostructure size and rigidity. X-ray scattering allows us to follow the re-arrangement of the colloids and the structural evolution in situ during annealing. Evaluation by real-space imaging techniques reveals a disappearance of the structural integrity and a loss of colloids' boundaries. We present the possibility to tailor and fine-tune the wettability by tuning the core-shell colloid morphology in thin films, thus providing a facile template methodology for repellent surfaces.

DY 49.6 Thu 10:45 ZEU 255

Depleting Hydrogels with Oil Flows — •Philipp Baumli[1], Emanuela Lorusso[2], Lukas Hauer[1], Azadeh Sharifi-Aghili[1], Katharina Hegner[1], Maria D'Acunzi[1], Burkhard Duenweg[1], Jochen Gutmann[2], Hans-Jürgen Butt[1], and Doris Vollmer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Deutsches Textilforschungszentrum Nord-West ÖP GmbH, Adlerstraße 1, 47798 Krefeld, Germany.

Hydrogels are ubiquitous in our daily lives. Applications range from jelly pudding and diapers to scaffolds in tissue engineering. A hydrogel-coating is covalently attached to a micropillar array. Swelling the hydrogel-coating with water establishes a liquid-infused surface (LIS). On LIS, liquid-depletion is synonymous with loss of functionality.

We demonstrate that the hydrogel-based LIS can be kept lubricated upon a shear-flow of oil for a wide variety of flow conditions independent of the exact nature of the hydrogel-coating. Dehydration of the hydrogel-coating is followed by confocal laser scanning microscopy and progresses linearly independent of flow conditions and hydrogel. The mechanism is explained with the help of an extended diffusion model.

DY 49.7 Thu 11:00 ZEU 255

Tracking nematic flows at microscales using small angle X-ray scattering — •Paul Steffen[1], Eric Stellamanns[2], Michael Sprung[2], Fabian Westermeier[2], and Anupam Sengupta[3] — [1]Göttingen — [2]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [3]Physics of Living Matter, Dept. of Physics and Materials Science, University of Luxembourg, Luxembourg

Liquid crystal microflows play a fundamental role in materials, modern display technologies, and biological systems. However, a quantitative, dynamic and spatially resolved measurement of the director field and surface anchoring remain a significant challenge. Here we present small angle X-ray measurements on stationary flows of 4-Cyano-4-pentylbiphenyl (5CB) in circular Kapton capillaries (under homeotropic and random planar anchoring) at temperatures between 280 and 310 K, and Ericksen numbers ranging from 0 to 200, with a spatial resolution of 1/1000 of the capillary dimension. The angular dependence of the scattering peaks from both periodic length scales was approximated by a double Gaussian fit with four parameters: amplitude, angle, width and background amplitude. The peak angles were found to be in good agreement with the director fields calculated using the Leslie-Ericksen theory. The width and the amplitude of the scattering patterns obtained from the larger length scale are less affected by the temperature than those from the smaller length scale.

15 min. break

DY 49.8 Thu 11:30 ZEU 255

Macroscopic Capillary Number for Characterization of Two-phase Flow in Porous Media — •Hu Guo and Rudolf Hilfer — Institute for Computational Physics, Universität Stuttgart, Stuttgart, Germany

The Capillary number (Ca) defined as the ratio of viscous force to capillary force is widely used to qualitatively characterize multiphase flow in porous media as in carbon dioxide geologic sequestration and chemical enhanced oil recovery (EOR). The main difficulty is to characterize forces porperly. There exists 22 definitions for Ca (Guo et al, IOR 2020). The most concise definition is $Ca = \frac{v\mu}{\sigma}$ with velocity v, viscosity μ and interfacial tension σ (Saffman and Taylor, 1958). It is supported by core flooding tests and most widely used. However, this definition is less sound than the one that involves the wettability parameter (Moore and Slobod, 1955). Meanwhile, the values of these Ca are regarded as too small to reflect the actual force balance (Dullien, 1979). It was shown theoretically, that this Ca is microscopic in nature and incorrectly used (Hilfer and Øren, 1996, Trans. Porous Media).

We study the new macroscopic capillary number $Ca = \frac{\mu\phi vL}{KP_b}$ with viscosity μ, porosity ϕ, velocity v, permeability K, length L and capillary breakthrough pressure P_b (Hilfer et al, 2015, Physical Review E). The new Ca explains some of the latest observations (Doorwar and Mohanty, 2017, SPE J; Qi et al, 2017, SPE J; Rabbani et al, 2018, PNAS; Zhao et al, 2019, PNAS) that contradict predictions obtained from the microscopic Ca. EOR field practice also verified that the macroscopic Ca is more profound.

DY 49.9 Thu 11:45 ZEU 255

Drop Impact on Hot Plates: Contact, Lift-Off and the Formation of Holes — •Kirsten Harth[1,2], Sang.Hyeon Lee[3], Maaike Rump[2], Minwoo Kim[3], Detlef Lohse[2], Kamel Fezzaa[4], and Jung Ho Je[3] — [1]Institute of Physics, Otto von Guericke University Magdeburg — [2]Physics of Fluid and Max Planck Center, University of Twente, The Netherlands — [3]X-Ray Imaging Center, Pohang University of Science and Technology, Korea — [4]X-Ray Science Division, Argonne Ntnl. Laboratory, USA

Everyone who poured water into a hot pan has experienced the manifold boiling behaviours of drops impacting on a hot plate, a problem which is of high relevance in many technical applications. When the drop is gently deposited, and the surface temperature is sufficiently high, it hovers on a vapour layer (Leidenfrost effect). For impacting drops, this critical temperature for a contact-less rebound is substantially increased, and much harder to determine. In fact, determining contact times between drops and smooth substrates from side view imaging is impossible for most temperatures above the boiling point.

We combine High-Speed Total Internal Reflection and synchrotron X-Ray measurements to reliably determine contact times and the Leidenfrost temperature for drops impacting on smooth hot surfaces. Furthermore, we study the lift-off characteristics. A local minimum in lift-off times correlates with spontaneous lamella rupture and the morphology of the contact.

DY 49.10 Thu 12:00 ZEU 255

Lucas-Washburn equation applies for four phase contact point — •Peyman Rostami[1,2] and Günter Auernhammer[1,2] — [1]Max Planck Institute for Polymer Research, 55128, Mainz, Germany — [2]Leibniz Institute of Polymer Research, 01069, Dresden, Germany

A four-phase contact point, e.g., in merging of immiscible drops, is the point where the liquid-liquid interface advances along the contact line of one drop. The dynamics of drop merging involve various driving and dissipating forces in the dynamics of the four-phase contact point. The viscous friction, i.e. the flow field, within liquids is influenced by the different boundary conditions on the different interfaces (liquid-gas, liquid-liquid, liquid-solid). Additionally, Marangoni stresses between the two liquids and the spreading coefficients along the contact lines play a role. Effectively, these effects lead to a capillary force acting on the four-phase contact point. In total, the situation resembles the capillary flow in open V-shaped groove. The important difference is that, in the classical problem, the grooves are made out of two solid walls, but in the present case one of the *walls* is liquid, i.e., flowable and deformable. We investigate a range of liquids with different combination of physical properties (viscosity ratio, surface and interfacial tensions). The results show a good qualitative agreement for different liquids of the experimental results with the classical Washburn equation (h~square root of time), where h is the filled length of the *groove*.

DY 49.11 Thu 12:15 ZEU 255

Simulations of Thermal Fluctuations with a Thin Film Lattice Boltzmann Model — •Stefan Zitz[1], Jens Harting[1,2], and Andrea Scagliarini[3] — [1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Nuremberg, Germany — [2]Eindhoven University of Technology, Eindhoven, The Netherlands — [3]Consiglio Nazionale delle Ricerche, Rome, Italy

The effect of thermal fluctuations on thin film flows is an interesting yet challenging phenomenon. Although in experiments their presence is undeniable thermal fluctuations are often neglected in the analysis of the results. Also in simulations their inclusion is far from being trivial due to the stochastic nature of the fluctuations.

Here we present a numerical approach to include the influence of thermal fluctuations. Based on our newly developed lattice Boltzmann method we show how to effectively match the thin film regime and further how to include thermal fluctuations in a self consistent matter [1].

One problem of deterministic thin film simulations is the discrepancy between experimental and simulated rupture times in dewetting experiments. It has been shown that the experimental rupture times are shorter than the ones predicted by deterministic simulations. We will show that adding fluctuations does reduce the rupture time to better match the experimental results. To this end we will also address the importance of the fluid substrate interaction, e.g. the equilibrium contact angle θ_{eq}.

S. Zitz, J. Harting et al., Phys. Rev. E 100:3, 033313, 2019

DY 49.12 Thu 12:30 ZEU 255

Impact of submillimetre-sized droplets on freely suspended liquid membranes — •Florian von Rüling, Alexey Eremin, and Ralf Stannarius — Otto von Guericke University Magdeburg, Germany

Droplet impact and splashing phenomena at solid and fluid interfaces remain an exciting research topic with vast application possibilities [1]. Impact scenarios are primarily governed by capillary forces, inertia, oscillation dynamics of the droplets, and the dynamics of the thin air cushion entrapped between droplet and surface during impact [2,3]. We experimentally investigated the impact of large submillimetre- to millimetre-sized droplets on freely suspended smectic films. We were able to vary the droplet diameter from several hundred microns to one millimetre. Droplets can either be trapped or reflected by the film or tunnel through it, depending on geometrical and dynamical parameters. The film remains intact in all these scenarios. In addition to the drop size and impact velocity, material properties and the film thickness can affect the behaviour of both droplet and film.

[1] A. M. Worthington, The Splash of a Drop; Romance of Science. Society for the Promotion of Christian Knowledge, London, 1895.

[2] C. Antonini, A. Amirfazli, M. Marengo, Drop impact and wettability: From hydrophilic to superhydrophobic surfaces, Phys. Fluids

24 102104 (2012).

[3] S. Dölle, R. Stannarius, Microdroplets impinging on freely suspended smectic films: three impact regimes, Langmuir 31 6479 (2015).

DY 49.13 Thu 12:45 ZEU 255

Imbibition-Induced Deformation Dynamics in Nanoporous Media — •Juan Sanchz[1], Zhuoqing Li[2], Michael Froeba[3], and Patrick Huber[4] — [1]Institute of Materials Physics, Hamburg University of Technology — [2]Institute of Materials Physics, Hamburg University of Technology — [3]Institute of Anorganic and Applied Chemistry, Hamburg University — [4]Institute of Materials Physics, Hamburg University of Technology

We present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths (carbon and silica) upon spontaneous, capillarity-driven invasion of water. We find two distinct dynamical regimes. One of them can be quantitatively traced to deformations originating in changes in the surface stress at the inner pore walls (dynamic Bangham's regime) upon water invasion, whereas the second one results from Laplace pressure effects. Our study demonstrates that it is possible to dynamically monitor imbibition dynamics by simple dilatometry measurements.

DY 50: Granular Matter and Granular Dynamics II

Time: Thursday 10:00–11:45 Location: ZEU 160

DY 50.1 Thu 10:00 ZEU 160

Granular Rheology from First Principles — •Till Kranz[1], Olfa Lopez[2], Olivier Coquand[2], and Matthias Sperl[2,1] — [1]Institut für Theoretische Physik, Uni Köln — [2]Institut für Materialphysik im Weltraum, DLR Köln

We have recently demonstrated that the *Granular Integration Through Transients* (GITT) formalism allows to derive a constitutive equation for the shear stress σ as a function of the shear rate $\dot{\gamma}$ for arbitrary shear rates and high densities [1] of a granular fluid. Here we extend the formalism to derive a constitutive equation for the pressure $p(\dot{\gamma})$. This allows us to discuss flow curves at constant pressure and the *effective friction* $\mu = \sigma/p$. The phenomenological $\mu(I)$ rheology [2] relates the friction μ to the dimensionless inertial number I. We will discuss the relation between the GITT expressions and $\mu(I)$ rheology. In addition, we will present experimental stress measurements on fluidised glass beads covering several orders of magnitude in shear rate and displaying all the rheologigcal regimes predicted by GITT, namely, Newtonian rheology, as well as shear thinning and shear thickening behaviour.

[1] W. T. Kranz, F. Frahsa, A. Zippelius, M. Fuchs and M. Sperl, PRL **121**, 148002 (2018); arXiv:1710.04475
[2] GDR Midi, EPJ E **14**, 341 (2004)

DY 50.2 Thu 10:15 ZEU 160

Is Janssen's effect still valid when simply filling a silo with non-moving bottom? — •Diego Sancho Martinez[1], Ralf Stannarius[1], Robin Shädel[1], and Tamas Börzsönyi[2] — [1]Otto von Guericke Universität, Magdeburg, Germany — [2]Wigner Institute for Solid State Physics, Budapest, Hungary

Grain storage has been a matter of special interest during the past centuries. In former times storage containers were small compared to current silos. The biggest problem that occurs in large silos is that the walls bear much of the weight contained in it. The saturation of the pressure at the base of the silo with height in a granular system was described in detail by Janssen and supported by posterior studies. Several recent studies show, that with mobilized contact forces (realized e.g. by slowly moving the silo wall upwards) the pressure saturates at small filling heights (comparable to the silo diameter D). Without mobilization the pressure depends on the history of the system. Here, we investigate the case of simple filling (without moving walls) for different materials: soft and nearly frictionless hydrogels, soft and highly friction round-shaped sponges as well as hard particles such as glass beads and airsoft beads. We find that the pressure at the bottom of the silo as a function of filling height does not saturate up to filling heights of 20D, but keeps increasing. The rate of increase appears to be constant above filling heights of about 3D.

DY 50.3 Thu 10:30 ZEU 160

Applyig Edwards' theory for a 2+ϵ dimensional frustrated granular system — •Sára Lévay[1], David Fischer[2], Ralf Stannarius[2], Tamás Börzsönyi[3], Ellák Somfai[3], and János Török[1,4] — [1]Budapest University of Technology and Economics, Budapest, H. — [2]Otto-von-Guericke-University, Magdeburg, G. — [3]Wigner Research Centre for Physics, Budapest, H. — [4]MTA-BME Morphodynamics Research Group, Budapest, H.

Despite the inherent athermal features of granular materials, treating jammed granular systems in analogy to thermal equilibrium statistical mechanics was proposed by Edwards by using a volume ensemble of equiprobable jammed states, and introducing a configurational temperature named compactivity. Since then this concept was successfully used to derive the volume fraction of random loose and random close packing. We use Edwards' theory to describe a 2+ϵ dimensional frustrated system of monodisperse spherical particles. This is a flat cuboid cell at the transition between two and three dimensions: slightly thicker than the diameter of a particle. If the container is only slightly larger than the particle diameter, the optimal packing is a triangular lattice in two dimensions and particles are building alternating stripes in the third direction. It was observed that the system does not reach its ground state using mechanical agitation by shaking. In order to understand this puzzle we performed analytic calculations of the volume and the expected number of specific local configurations of particles in our system according to Edwards' theory, and successfully matched them with numerical simulations and experiments.

DY 50.4 Thu 10:45 ZEU 160

Configuration statistics of sphere packings in geometrical confinement — •David Fischer[1], Jonas Schulze[1], Ralf Stannarius[1], Sára Lévay[2], Tamás Börzsönyi[3], and János Török[2] — [1]Otto von Guericke University Magdeburg, Germany — [2]Budapest University of Technology and Economics, Hungary — [3]Wigner Research Centre for Physics, Budapest, Hungary

While regular packings of spheres in 2 and 3 dimensions are satisfactorily understood today, random packings still bear unsolved mysteries. Granular materials are athermal, thus temperature and free energies are not appropriate parameters to describe the statistics of local configurations. Edwards introduced a different concept with local volumes of configurations replacing energies and compactivity replacing temperature. We apply this concept to a 2+epsilon dimensional spatially restricted system, a cuboid cell filled with monodisperse spheres slightly smaller than the cell thickness. Experiments and numerical simulations are compared.

DY 50.5 Thu 11:00 ZEU 160

Flow study for transparent model system of concrete and cement paste — •Himanshu P Patel[1] and Günter K Auernhammer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Straße 6, D-01069 Dresden, Germany — [2]Max Planck Institute for Polymer Research, Ackermannweg 10 - D-55128 Mainz, Germany

The study of internal dynamics and particle migration in a complex granular suspension, such as flowing concrete, poses couple of scientific challenges. Concrete due to opacity restricts the possibility of optical observations of the flow induced particle migration (FIPM). Non-optical techniques such as ultrasonic velocity profiler and sliper test provides limited understanding.

We here demonstrate the development of highly transparent model system for concrete. The system is an optically transparent dense granular suspension (42% to 48% by volume) that mimics rheology behavior of concrete on the parameters of yield stress and plastic viscosity. Further, we analyze the flow in continuous phase using specific experimental setup. The setup allows flow analysis, to understand shear and plug flow in addition to insight about segregation of particles. The study is part of understating FIPM for dense granular suspensions.

The flow profile and FIPM of model concrete is observed using high-speed camera and Laser sheet Microscopy.

DY 50.6 Thu 11:15 ZEU 160

Is the hourglass always flowing with a constant speed? — •Tamás Börzsönyi[1], Tivadar Pongó[1,2,3], Viktória Stiga[1], János Török[3], Sára Lévay[3], Balázs Szabó[1], and Ralf Stannarius[4] — [1]Wigner Research Centre for Physics, H-1525 Budapest, Hungary — [2]Universidad de Navarra, Pamplona, Spain — [3]Institute of Physics BME, Budapest, Hungary — [4]Otto-von-Guericke-University, D-39106 Magdeburg, Germany

For usual granular materials the discharge rate from a bin is known to be time independent (constant flow rate). This is opposed to the case of a liquid for which the decreasing height leads to decreasing pressure, resulting in gradually decreasing flow rate during a discharge process. We performed laboratory experiments and numerical simulations with traditional (frictional hard) granular materials, grains with reduced surface friction and hardness, as well as non-spherical particles which develop orientational ordering during flow. We show, that grains with a small (<0.1) surface friction coefficient discharge with decreasing flow rate, while for frictional elongated grains the development of orientational ordering leads to increasing flow rate.

DY 50.7 Thu 11:30 ZEU 160

Dunes of frozen methane sand on Pluto — •Eric Josef Ribeiro Parteli — Department of Geosciences, University of Cologne

Sand dunes, which require a supply of granular particles at the surface and a boundary layer of sufficient efficacy to enable transport of these particles by fluid forces, have been detected in surprising locations of our solar system, including Mars, Venus and Saturn's moon Titan. Continuum simulations of wind-blown sand transport have been pushing forward our understanding of dune physics on Earth and these extra-terrestrial environments. In this talk I will report the discovery of dunes on Pluto, where the atmosphere is 100,000 times less dense than the Earth's. While terrestrial dunes consist of quartz grains, Pluto dunes are made of methane ice grains. I will present insights about the formative wind regime, particle size of Pluto dunes and the characteristics of sediment transport on Pluto from numerical simulations, which I developed in the framework of a collaboration with the New Horizons Science Team. Moreover, I will present challenging open questions about dune physics, and discuss how dune modeling will help us to improve climate simulations and our understanding of sediment landscape dynamics on Earth and extra-terrestrial environments.

DY 51: Focus Session: Nonlinear Dynamics of the Heart II (joint session DY/BP)

Time: Thursday 14:00–15:45 Location: ZEU 118

Invited Talk DY 51.1 Thu 14:00 ZEU 118

Dyadic structure-function relationships in ventricular cardiac myocytes: from sparks to action potentials — •Martin Falcke[1,2], Filippo G. Cosi[3], Wolfgang Giese[1], Wilhelm Neubert[1], Stefan Luther[3], and Ulrich Parlitz[3] — [1]Max Delbrück Center, Berlin — [2]Dept. of Physics, Humboldt University Berlin — [3]MPI for Dynamics and Self-Organization, Göttingen

Cardiovascular disease is often related to defects in molecular and subcellular components in cardiac myocytes, specifically in the dyadic cleft, which include changes in cleft geometry and channel placement. Modelling of these pathological changes requires both spatially resolved cleft as well as the whole cell level descriptions. We use a multiscale model to create dyadic structure-function relationships in order to explore the impact of molecular changes on whole cell electrophysiology and calcium cycling. This multiscale model incorporates stochastic simulation of individual L-type calcium channels (LCC) and ryanodine receptor channels (RyRs), spatially detailed concentration dynamics in dyadic clefts, rabbit membrane potential dynamics, and a system of partial differential equations for myoplasmic and lumenal free Ca^{2+} and Ca^{2+}-binding molecules in the bulk of the cell.

We create models with varying dyadic cleft properties including RyR and LCC clustering, stochastic opening and closing rates as well as changes in LCC and RyR calcium currents. We investigate biomarkers describing action potential, Ca^{2+} transient and Ca^{2+} spark dynamics. We quantify sensitivity and parameter uncertainty and derive cellular functional implications from molecular level properties.

DY 51.2 Thu 14:30 ZEU 118

Multiscale modeling of dyadic structure-function relation in ventricular cardiac myocytes — •Filippo Cosi[1,4,5], Wolfgang Giese[2], Wilhelm Neubert[2], Stefan Luther[1,4,5], Nagaiah Chamakuri[3], Ulrich Parlitz[1,4,5], and Martin Falcke[2,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Max Delbrück Center for Molecular Medicine in the Helmholtz association, Berlin, Germany — [3]Institute of Applied Mathematics, University of Hohenheim, Stuttgart, Germany — [4]Georg-August-Universität Göttingen, Institute for the Dynamics of Complex Systems, Göttingen, Germany — [5]DZHK (German Center for Cardiovascular Research), Partnersites Göttingen and Berlin, Germany

Understanding how defects in the subcellular components of single cardiomyocytes affect the calcium cycling in single cells can help to pin down the origin of cardiovascular disease. A multiscale model is used, which combines the stochastic nature of subcellular components (as Ryanodine Receptors, RyR or L-type Calcium Channels, LCC), their spatial arrangement as well as spatio-temporal calcium and buffer gradients at the whole-cell level. Recent findings regarding the geometrical clustering of RyRs and LCCs inspired us to include the physiological description of it into our mathematical model. The included structure modifications showed a dramatic effect on the model's outputs; in detail the arrangement of RyRs has a strong impact on cell functions. Our study aims to lay a quantitative fundament for the analysis of defect cardiomyocytes under physiologically conditions to deepen the understanding of how diseased heart tissue might be treated.

DY 51.3 Thu 14:45 ZEU 118

Simple mechanism for low-energy antifibrillation pacing — Pavel Buran, Thomas Niedermayer und •Markus Bär — Physikalisch-Technische Bundesanstalt (PTB), Berlin

Rotating excitation waves and electrical turbulence in cardiac tissue are associated with arrhythmias such as life-threatening ventricular fibrillation. Experimental studies have shown that a sequence of low-energy electrical far-field pulses is able to terminate fibrillation with less energy than a single large energy shock [1]. Previous theoretical approaches to understand this low-energy antifibrillation pacing (LEAP) have often focused on unpinning and removal of a small number of rotating spirals in quasi-two-dimensional situations. These theories, however, cannot explain the defibrillation of spatiotemporal chaos. Based on a systematic simulation study, we present an alternative mechanism for the success of LEAP in two dimensions, which explains both, the termination of stable spirals as well as spatiotemporal chaos. It turns out that actually each pulse during LEAP annihilates all excitation fronts, however, that new fronts could arise at the borders between refractory and excitable parts of the tissue. The success probability of each individual pulse can thus be simply interpreted as the probability that no new front arises. Furthermore, we will show that the success probability depends exponentially on the total length of these refractory boundaries and that successful LEAP is characterized by pulses causing a gradual decrease of this length simultaneously increasing the success probability of subsequent pulses until complete defibrillation.
[1] Luther et al., Nature **475**, 235-239 (2011)

DY 51.4 Thu 15:00 ZEU 118

Feedback-based protocol for low-energy defibrillation — •Pavel Buran, Thomas Niedermayer und Markus Bär — Physikalisch-Technische Bundesanstalt (PTB), Berlin

Low-energy antifibrillation pacing (LEAP) is a method where electrical turbulence characteristic for atrial or ventricular fibrillation is suppressed by a series of low energy pulses [1]. Systematic simulation studies show that the choice of the right pacing period is crucial for successful LEAP [2]. However, the range of those successful pacing periods is a priori not known for a given tissue. Methods that efficiently determine the range of successful pacing periods are therefore of high interest. We have found, that termination probability of each individual pulse during LEAP depends exponentially on the total length of the interfaces between refractory and excitable parts of the tissue. Based on this finding, we present a feedback controlled protocol that ensures that pulses are applied in such a way to minimize the mentioned interface length in line with our earlier findings about the mechanism of LEAP. This protocol does not need any a priori information about the system

and can thus also be used as an efficient method to determine the optimal pacing period.
[1] Luther et al., Nature **475**, 235-239 (2011)
[2] Buran et al., Chaos **27**, 113110 (2017)

DY 51.5 Thu 15:15 ZEU 118

General equilibrium approach to resolve ventricular calcium homeostais — •Enrique Alvarez-Lacalle[1], Blas Echebarria[1], Angelina Peñaranda[1], Inmaculada R. Cantalapiedra[1], Yohannes Shiferaw[2], and David Conesa[1] — [1]Departament de Física. Universitat Politècnica de Catalunya (UPC-BarcelonaTech), Barcelona, Spain. — [2]Department of Physics. California State University Nortridge, Los Angeles, USA.

The ventricular contraction in the heart is roughly proportional to the amount of calcium released from the Sarcoplasmic Reticulum during systole. The change in the membrane potential triggers the opening of thousands of Ryanodine Receptor clusters in the SR membrane, being the release larger when pre-systolic calcium levels are larger. While it is rather straightforward to measure calcium levels and contractibility under different physiological conditions, the complexity of calcium handling during systole and diastole has made the prediction of its release at steady-state from measurements away from steady-state impossible. In this contribution, we present a general equilibrium framework to understand how homeostasis can be understood and analyzed to make predictions about its level when key properties of ionic channels or buffers (due to phosphorylation, genetic mutation,etc..) involved in calcium handling are changed. This framework should be useful to describe why different animals have such different homeostatic behavior upon changes in the pacing rate and provide a physiological mechanism for SERCA gene therapy failure.

DY 51.6 Thu 15:30 ZEU 118

Synchronization-based reconstruction of electromechanical wave dynamics in elastic excitable media — Jan Lebert[1,2,3] and •Jan Christoph[1,2,3] — [1]University Medical Center Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]German Center for Cardiovascular Research, Partnersite Göttingen, Germany

Reconstructing electrical excitation wave dynamics within the heart muscle remains a major scientific challenge. Recently, it was shown using high-resolution 4D ultrasound that it is possible to identify mechanical filament-like phase singularities within the contracting, fibrillating heart wall, suggesting that the tissue mechanics reflect three-dimensional electrical scroll wave dynamics.

Here, we present a mechano-electrical data assimilation approach with which it is possible to reconstruct electrical excitation wave dynamics, including electrical vortex filaments, within the volume of deformable excitable media. By observing the spatio-temporal deformation patterns, which occur in response to the electrical excitation, the mechanical data is assimilated in a numerical replication of the observed elastic excitable system, and within this replication the data drives the intrinsic excitable dynamics, which then co-evolve and correspond to a reconstruction of the original dynamics. We provide a numerical proof-of-principle and demonstrate the performance of the approach by recovering even complicated three-dimensional scroll wave patterns.

DY 52: Quantum Dynamics, Decoherence and Quantum Information

Time: Thursday 15:00–18:15 Location: HÜL 186

DY 52.1 Thu 15:00 HÜL 186

Distributed Multipartite Entanglement Generation in Coupled Cavities — •Marc Bostelmann, Frederik Lohof, and Christopher Gies — Institute for Theoretical Physics, University of Bremen, Germany

Generation of spatially distributed entanglement is important for the realization of quantum information protocols and quantum computing. Coupled cavities offer a platform to create this kind of entanglement between spatially separated qubits [1]. By carefully tailoring excitations with external light pulses we theoretically examine the generation of entangled states, such as GHZ or Dicke states. Starting with a system of two qubits for generating bipartite entanglement, we extend the discussion to the multipartite case, exploiting symmetries of the system. Bridging the gap to experimental realizations, we study robustness of the generated entangled states to dissipation and asymmetry in the system. [1] Aron et al., PRA, 90, 062305 (2014).

DY 52.2 Thu 15:15 HÜL 186

Gaussian Approximation of the Wigner Function for the Stochastic Schrödinger Equation — •Robson Christie, Jessica Eastman, and Eva-Maria Graefe — Imperial College London, UK

Stochastic Schrödinger equations arise in many contexts in quantum mechanics, for example as an unravelling of the Lindblad equation. Here the time evolution of the Wigner function of a Gaussian state evolving along a trajectory of the stochastic Schrödinger equation for arbitrary Lindbladians is investigated in the semiclassical limit. The resulting coupled stochastic differential equations are compared to the full quantum dynamics for example systems.

DY 52.3 Thu 15:30 HÜL 186

Improving non-perturbative approximations of open-system dynamics using fermionic duality — •Valentin Bruch[1], Konstantin Nestmann[1], Maarten Wegewijs[1,2,3], Jens Schulenborg[4], and Janine Splettstoesser[5] — [1]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany — [2]JARA-FIT, 52056 Aachen, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [4]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen — [5]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, SE-41298 Göteborg

The evolution of a large class of fermionic open quantum systems with strong memory effects obeys an exact relation known as "fermionic duality". Given any description of the evolution of states (Schrödinger picture), it explicitly provides the corresponding description of the evolution of observables (Heisenberg picture) by a parameter substitution and some simple operations. We apply this to a non-perturbative semigroup approximation that is both completely positive and trace-preserving, as well as to its correction by a so-called "initial slip", and present a detailed comparison of these two approximations. We show that, surprisingly, the initial slip correction can be constructed for a large part using only the duality relation, circumventing further model-specific calculations. The main features of both approximations can already be seen in the exactly solvable resonant level model with strong coupling to a fermionic reservoir at finite temperature.

DY 52.4 Thu 15:45 HÜL 186

Relaxing (Quantum-) Master Equations — •Bernd Fernengel and Barbara Drossel — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulst. 6, 64289 Darmstadt, Germany

Quantum Master Equations are special kinds of transport equations. The Gorini*Kossakowski*Sudarshan*Lindblad Equation in particular describes the time evolution of both the probabilities of, and the coherences between the quantum mechanical states.

We give several necessary and sufficient criteria for (Quantum-) Master Equations being asymptotically stable (also called *relaxing*). Instead of looking at the Lindblad Equation directly, we study a stochastic differential equation of of the ket-state vector (a so called *unravelling*) that is consistent with the Lindblad Equation. The condition for the Lindblad Equation being relaxing can then be mapped to the classical case.

DY 52.5 Thu 16:00 HÜL 186

Bose condensation of squeezed light — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics-UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

Light with an effective chemical potential and no mass is shown to possess a general phase-transition curve to Bose-Einstein condensation. This limiting density and temperature range is found by the diverging in-medium potential range of effective interaction. While usually the absorption and emission with Dye molecules is considered, here it is proposed that squeezing can create also such an effective

chemical potential. The equivalence of squeezed light with a complex Bogoliubov transformation of interacting Bose system with finite lifetime is established with the help of which an effective gap is deduced. This gap phase creates a finite condensate in agreement with the general limiting density and temperature range. The phase diagram for condensation is presented due to squeezing and the appearance of two gaps is discussed. Phys. Rev. B 99 (2019) 205124

DY 52.6 Thu 16:15 HÜL 186

Coherent States for a Bosonic Atom-Molecule Conversion Systems — •Wasim Rehman[1] and Eva-Maria Graefe[2] — [1]Imperial College, London, UK — [2]Imperial College, London, UK

Coherent states are of great importance in quantum mechanics, in particular for the investigation of quantum-classical correspondence. Here I will consider a simple two-state quantum model of atom-molecule conversion in cold atom systems, where bosonic atoms can combine into diatomic molecules and vice versa. The many-particle system can be expressed in terms of the generators of a deformed SU(2) algebra. In this context the question of what the relevant coherent states are had so far not been fully addressed. Here I will present candidates for the coherent states for this system and analyse their properties and resulting phase-space structures.

15 min. break.

DY 52.7 Thu 16:45 HÜL 186

Dynamics of disordered dissipative spin-boson systems at strong coupling — Eliana Fiorelli[1,2], Pietro Rotondo[1,2], Federico Carollo[1,2], •Matteo Marcuzzi[1,2], and Igor Lesanovsky[1,2,3] — [1]School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK — [2]Centre for the Mathematics and Theoretical Physics of Quantum Non-equilibrium Systems, University of Nottingham, Nottingham NG7 2RD, UK — [3]Institut fur Theoretische Physik, University of Tuebingen, Auf der Morgenstelle 14, 72076 Tuebingen, Germany

Spin-boson Hamiltonians are an effective description for numerous quantum many-body systems such as atoms coupled to cavity modes, quantum electrodynamics in circuits and trapped ion systems. While reaching strong light-matter couplings has become practicable, the understanding of the physics in this parameter regime remains a challenge. We investigate a particular example where sufficient amounts of dissipation and disorder over the local couplings make it possible to map the spin dynamics onto an effective classical master equation; the latter is, in turn, approximately governed by a fully-connected energy function, the Hopfield model, studied in the past as a simple model for an associative memory. We highlight similarities and differences in the stationary and dynamical properties of the two systems.

DY 52.8 Thu 17:00 HÜL 186

Statistics of the bifurcation in quantum measurement — Karl-Erik Eriksson and •Kristian Lindgren — Department of Space, Earth and Environment, Chalmers University of Technology, Gothenburg, Sweden

Quantum mechanics is at the basis of all modern physics and fundamental for the understanding of the world that we live in. As a general theory, quantum mechanics should apply also to the measurement process. From the general experience of non-destructive measurements, we draw conclusions about the interaction between the observed system and the measurement apparatus and how this can be described within quantum mechanics [1].

We model quantum measurement of a two-level system μ. Previous obstacles for understanding the measurement process are removed by basing the analysis of the interaction between μ and the measurement device on quantum field theory. This formulation shows how inverse processes take part in the interaction and introduce a non-linearity, necessary for the bifurcation of quantum measurement. A statistical analysis of the ensemble of initial states of the measurement device shows how microscopic details can influence the transition to a final state. We find that initial states that are efficient in leading to a transition to a final state result in either of the expected eigenstates for μ, with ensemble averages that are identical to the probabilities of the Born rule. Thus, the proposed scheme serves as a candidate mechanism for the quantum measurement process.

[1] Eriksson & Lindgren, Entropy (2019): doi.org/10.3390/e21090834

DY 52.9 Thu 17:15 HÜL 186

The Periodical Driven, Anharmonic Oscillator — Mattes Heerwagen and •Andreas Engel — Carl von Ossietzky Universität, Oldenburg, Germany

In the thermodynamics of nanoscopic systems the correspondence between classical and quantum mechanical description is of particular importance. To scrutinize this relationship we study an anharmonic oscillator driven by a periodic external force with slowly varying amplitude both classically and within the framework of quantum mechanics. More precisely, we are interested in the energy change of the oscillator induced by the external drive. It is closely related to the distribution of work in the system. Since the amplitude $\lambda(t)$ of the external drive increase from zero to a maximum λ_{max} and than decrease back to zero initial and final Hamiltonian coincide. Our main quantity of interest is the probability density $P(E_f|E_i)$ for transitions from initial energy E_i to final energy E_f.
In the classical case non-diagonal transitions with $E_f \neq E_i$ mainly arise due to the mechanism of separatrix crossing. It is most efficiently analyzed using action-angle variables. Within the pendulum approximation analytical results for the transition probability can then be compared with numerical simulations. In the quantum case numerically exact results are complemented with analytical arguments employing Floquet techniques. The latter highlight in particular the mechanism behind the periodical variation of $P(E_f|E_i)$ with the maximal amplitude λ_{max} of the drive.

DY 52.10 Thu 17:30 HÜL 186

Extended coherently delocalized states in a frozen gas — Ghassan Abumwis, Matthew T. Eiles, and •Alexander Eisfeld — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany

The long-range dipole-dipole interaction between excited states of atoms can create highly delocalized states due to the exchange of excitation between the atoms. We show that even in a random gas many of the single-exciton eigenstates are surprisingly delocalized, composed of roughly one quarter of the participating atoms. We identify two different types of eigenstates: one which stems from strongly-interacting clusters, resulting in localized states, and one which extends over large delocalized networks of atoms. These two types of states can be excited and distinguished by appropriately tuned electromagnetic pulses.

DY 52.11 Thu 17:45 HÜL 186

Relaxation dynamics in a Hubbard dimer coupled to fermionic baths — Eric Kleinherbers[1], •Nikodem Szpak[1], Jürgen König[1], and Ralf Schützhold[1,2,3] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47048 Duisburg — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden

We study relaxation dynamics in a strongly-interacting two-site Fermi-Hubbard system coupled to fermionic baths. Starting with an ab initio approach, we apply several approximations leading through the real-time diagrammatics to obtain a Lindblad master equation for the dimer system itself. The latter offers a direct phenomenogical interpretation of the particle flows between the dimer and the baths. However, the approximations must be chosen and performed carefully, as for instance the local-bath approximation seems to be in contradiction with the Gibbbs final equilibrium state. In particular, at temperature zero, conserved quantities apear which lead to deceherence-free sectors. We demonstrate that the relaxation takes place in several steps on different time-scales and discuss problems related to intruduction of different approximations [1].

[1] E. Kleinherbers, N. Szpak, J. König, and R. Schützhold, arXiv: 1910:04130 (2019)

DY 52.12 Thu 18:00 HÜL 186

Spin-mapping approach for nonadiabatic molecular dynamics — •Johan E. Runeson and Jeremy O. Richardson — Laboratory of Physical Chemistry, ETH Zurich, 8093 Zurich, Switzerland

An open problem in computational physics and chemistry is to rigorously combine the quantum description of nonadiabatic processes with the simple classical trajectories of molecular dynamics (MD) simulations. Nonadiabatic processes are relevant for many modern applications, for example light harvesting in chromophores, and are characterized by the breakdown of the Born-Oppenheimer approximation.

In my talk I will show a simple way to achieve this for a general N-level quantum system in a classical environment, without invoking the

surface-hopping ansatz. The key idea is to assign additional variables to each trajectory to describe the electronic states, in addition to the nuclear coordinates and momenta. These variables originate from a Wigner-like representation of the Bloch vector, that can be viewed as a classical spin. We have showed[1] how to derive a mixed quantum-classical method in this way, which shares the same equations of motion as in Ehrenfest dynamics, but differs in an important way in how initial distributions and observables are defined. This vastly improves results in benchmark systems of population dynamics compared to the conventional Ehrenfest method, without adding computational cost.

[1] J. E. Runeson and J. O. Richardson, *J. Chem. Phys.* **151**, 044119 (2019)

DY 53: Poster: Quantum Dynamics, Chaos and Information; Many Body Systems

Time: Thursday 15:00–18:00 Location: P1A

DY 53.1 Thu 15:00 P1A

Thermalization properties of a system with topological flat bands and impurities — •Stefan kleine Brüning and Thomas Dahm — Universität Bielefeld

Topological insulators posses edge states, which are gapless in contrast to the bulk states. Bi_2Se_3 is of particular interest, because of its relatively simple Hamiltonian and, most importantly, under the influence of a Zeeman field flat bands appear in thin stripes of this material[1].

Due to the zero group velocity of electrons in flat bands there is no thermalization for a localized initial state. The question arises how this non-thermalization behaviour and the localization changes in the presence of impurities. In this work we focus on disorder, which modifies the on-site energy of the material. The influence of this disorder is investigated numerically using time evolution. The observable of interest is a quantity which is related to the localization of the wavepacket. The behaviour of this observable under change of strength and number of impurities is compared to a situation without a flat band. To investigate the question of thermalization it is probed whether the eigenstate thermalization hypothesis holds. To do this we employ a method suggested by Steinigeweg et al.[2]. This method uses random state vectors and scaling behaviour to decide this matter.

[1] Paananen, T., & Dahm, T. Physical Review B, 87, 195447(2013).
[2] Steinigeweg, R., et al. Physical Review Letters, 112, 130403 (2014).

DY 53.2 Thu 15:00 P1A

Wave Functions in White Noise Potential: Spreading or Localization? — •Marco Hofmann and Barbara Drossel — Institute of Condensed Matter Physics, Technische Universität Darmstadt, Hochschulstr. 6, 64289 Darmstadt, Germany

We study the dynamics of a quantum wave function on a 1D lattice subject to a fluctuating potential that is described as uncorrelated Gaussian white noise. Starting from a stochastic Schrödinger equation, we derive the corresponding Lindblad equation. This Lindblad equation, in turn, can be unravelled in terms of stochastic wave function dynamics in several different ways, all of which are empirically equivalent, as the density matrix alone determines the outcome of measurements. Two of these unravellings are widely used in the theory of Open Quantum Systems, namely the Quantum State Diffusion Model and the Quantum Jump Method. We show that the degree of localization or spreading of the wave function depends on the type of unravelling used, and in particular on the way the trace-conserving term of the Lindblad equation is implemented in the wave function dynamics. Part of the implementations lead to the localization of the wave function on a limited number of lattice sites. Our results raise interesting questions related to the interpretation of the wave function.

DY 53.3 Thu 15:00 P1A

Sources and coupling in billiards for light — •Marika Federer, Rebecca Cizek, Michel Hendriks, Jule Katharina Schnepfer, Martí Bosch, Jakob Kreismann, Jaewon Kim, and Martina Hentschel — Institute of Physics, Technical University Ilmenau, Germany

Optical microresonators, or billiards for light, have proven to be a rich model system for nonlinear dynamics, quantum chaos, and optics. Here, we study how the presence of sources affects the intracavity dynamics and the far-field emission of these open systems. To this end, we use ray modelling as well as wave simulations and compare their results in the spirit of ray-wave correspondence in real and phase space. Furthermore, we relate the presence of sources to coupling phenomena and study coupled microcavities in arrays and how coupling affects the emission properties of the complex optical system.

DY 53.4 Thu 15:00 P1A

A PT-Symmetric Kicked Rotor — •Joseph Hall and Eva-Maria Graefe — Imperial College, London, UK

PT-symmetric quantum mechanics has attracted a large amount of research interest over the last decade. Thus far most theoretical investigations have focused on simple model systems, which are open counterparts of integrable and often even analytically solvable systems. However little investigation has been undertaken into the properties of PT-symmetric chaotic systems. Here we investigate this phenomenon for the example of a PT-symmetric generalisation of the kicked rotor. We present signatures of chaos arising in both the classical and quantum descriptions of the system.

DY 53.5 Thu 15:00 P1A

Structure of resonance eigenfunctions for chaotic systems with partial escape — •Konstantin Clauss[1], Eduardo Altmann[2], Arnd Bäcker[1,3], and Roland Ketzmerick[1,3] — [1]TU Dresden, Institut für Theoretische Physik — [2]School of Mathematics and Statistics, University of Sydney — [3]MPI für Physik komplexer Systeme, Dresden

Physical systems are often neither completely closed nor completely open, but instead they are best described by dynamical systems with partial escape or absorption. We introduce classical measures that explain the main properties of resonance eigenfunctions of chaotic quantum systems with partial escape [1]. We construct a family of conditionally-invariant measures with varying decay rates by interpolating between the natural measures of the forward and backward dynamics. We show numerically, that these classical measures describe the main features of quantum resonance eigenfunctions: their multifractal phase space distribution, their product structure along stable and unstable directions, and their dependence on the decay rate. The (Jensen-Shannon) distance between classical and quantum measures goes to zero in the semiclassical limit for long- and short-lived eigenfunctions, while it remains finite for intermediate cases.

[1] K. Clauß, E. G. Altmann, A. Bäcker, and R. Ketzmerick, Phys. Rev. E **100** (2019), 052205.

DY 53.6 Thu 15:00 P1A

Real-time dynamics and thermalization of quantum-classical hybrid systems — •Nicolas Lenzing and Michael Potthoff — I. Institute of Theoretical Physics, Department of Physics, Universität Hamburg

The real-time dynamics of a noninteracting system of fermions is strongly constrained due to a macroscopically large number of conserved quantities such that thermalization of the system in the long-time limit is generally not expected.

We test this expectation for a slightly different setup, namely by coupling a classical degree of freedom to the Fermi-gas system, i.e., we consider fermions confined by an infinite potential well and treat one of the "walls" as a classical dynamical variable.

The time-dependent wall position is governed by a Newtonian equation of motion, including the Fermi-gas pressure, which must be solved simultaneously with the von-Neumann-type equation of motion for the one-particle reduced density matrix of the Fermi subsystem.

In a first step, we discuss fundamental aspects of the dynamics of quantum-classical hybrid systems for the case of a single quantum particle in contact with the classical wall.

In a second step, we study the time evolution towards a thermal state for the case of a Fermi gas in contact with a classical wall which is additionally subjected to an external force and compare with the predictions of thermodynamics.

DY 53.7 Thu 15:00 P1A

Violation of eigenstate thermalization in an interacting flat-band system — •Mirko Daumann and Thomas Dahm — Univer-

sität Bielefeld, Germany

Flat-band systems are characterized by the presence of completely dispersionless bands. They have interesting properties, because they possess a macroscopic degeneracy, zero group velocity and infinite effective mass. Recently, flat bands have been realized experimentally in various different physical systems.

Here we investigate the role of a particle-particle interaction on the thermalization in a quasi one-dimensional flat band system. By time evolution, we show that thermalization is not reached both in terms of the inverse participation ratio (IPR) and local operator expectation values. We further validate our results by showing that our system violates the eigenstate thermalization hypothesis (ETH) even in the presence of a particle-particle interaction.

DY 53.8 Thu 15:00 P1A

Fermionic duality beyond weak coupling: General simplifications of open-system dynamics — •Valentin Bruch[1], Konstantin Nestmann[1], Maarten Wegewijs[1,2,3], Jens Schulenborg[4], and Janine Splettstoesser[5] — [1]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany — [2]JARA-FIT, 52056 Aachen, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [4]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen — [5]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, SE-41298 Göteborg

The dynamics of a large class of open fermionic quantum systems with strong memory effects obeys an exact relation known as "fermionic duality". These are essentially impurity-type quantum transport models with arbitrarily complex and strong local interactions exhibiting various low-temperature many-body effects. Here we present a new, more elementary derivation of this and extend it to all prominent approaches to open system dynamics, including the time-nonlocal (Nakajima-Zwanzig) and the time-local (TCL) quantum master equation with its generalized Lindblad form, and the Kraus operator decomposition. Whereas in some of these formulations this yields a strong restriction on eigenvalues and eigenvectors, in others it can be exploited to completely by-pass nontrivial time-evolution calculations. This establishes that for fermionic open systems there exists a powerful analogue of the symmetry of hermitian conjugation in closed systems.

DY 53.9 Thu 15:00 P1A

Many-Body Localization in the Hartree-Fock Approximation — •Paul Pöpperl[1], Elmer Doggen[2], Konstantin Tikhonov[2], Igor Gornyi[1,2], and Alexander Mirlin[1,2] — [1]Institut für Theorie der kondensierten Materie, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

We investigate the quench dynamics of a spinless disordered Fermi-Hubbard model in the Hartree-Fock (HF) approximation. The one-dimensional model is expected to show a transition to a many-body localized (MBL) phase with increasing disorder at a fixed interaction strength. Surprisingly, the simple HF approximation qualitatively captures the MBL phenomenology [1]. We compare results from the HF approach to exact calculations and results obtained by the time-dependent variational principle (TDVP) [2] in order to illuminate the benefits and limitations of the HF approach.

[1] Weidinger, Simon et al (2018).
Self-consistent Hartree-Fock approach to many-body localization.
Physical Review B. 98. 10.1103/PhysRevB.98.224205.
[2] Doggen, Elmer V. H. et al (2018).
Many-body localization and delocalization in large quantum chains.
Physical Review B. 98. 10.1103/PhysRevB.98.174202.

DY 53.10 Thu 15:00 P1A

Prediction of Floquet oscillations and Zitterbewegung in driven Dirac systems — •Vanessa Junk, Phillipp Reck, Cosimo Gorini, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

The modification of solid state systems by time periodic driving has been a very vivid research topic in the last years. A special proof of Floquet engineering's power was the discovery of Floquet topological insulators [1]. However, the search for similarities between Bloch and Floquet systems is still ongoing.

Here, we predict an analogue of Bloch oscillations [2] occuring in Floquet systems. We numerically demonstrate these Floquet oscillations in a spatially continuous but time-periodically driven Dirac system [3]. A particle is driven through the resulting Floquet band structure by a static electric field and performs a motion similar to Bloch oscillations. Since the features of the Floquet bands are mimicked by these oscillations, the latter could provide a way to directly measure the Floquet bands. Due to the Dirac character of our model system, we can also observe Zitterbewegung with frequency equal to the energy difference of the Floquet bands.

[1] N. H. Lindner, G. Refael, and V. Galitski, Nature Physics **7**, 13368 (2016)
[2] K. Leo, P. Haring Bolivar, F. Brüggemann, R. Schwedler, and K. Köhler, Solid State Comm. **84**, 943 (1992)
[3] V. Junk, P. Reck, C. Gorini, and K. Richter, arXiv:1906.04446v1

DY 53.11 Thu 15:00 P1A

Dynamics of visons in weakly perturbed Kitaev models — •Aprem Joy and Achim Rosch — Institute of Theoretical Physics, University of Cologne, Germany

The Kitaev honeycomb model is a paradigmatic model which realizes a spin liquid phase and is exactly solvable. Candidate materials for Kitaev spin liquids are best described by Kitaev interactions perturbed by other spin exchange couplings which breaks the exact solvability of the model.

We study the dynamics of topological vison excitations coupled to the Majorana fermions in the Kitaev honeycomb model under weak perturbations, e.g., Heisenberg coupling, magnetic field and symmetric-anisotropic (Γ) interactions. The pure Kitaev model can be exactly solved thanks to the underlying static nature of the visons which effectively separates the model into free majoranas hopping in the background of a static Z_2 gauge field. But in the presence of perturbations, these visons are no more static but acquire dynamics also modifying the Majorana sector.

DY 53.12 Thu 15:00 P1A

Interplay of quantization and chaotic behaviour in ring-coupled condensates — •Damian Wozniak[1,2], Johann Kroha[3], and Anna Posazhennikova[1,2] — [1]Institut für Physik, Universität Greifswald, 17487 Greifswald, Germany — [2]Department of Physics, Royal Holloway, University of London, Egham, Surrey TW20 0EX, United Kingdom — [3]Fachbereich Physik, Universität Bonn, D-53115 Bonn, Germany

We study large rings of weakly-coupled Bose-Einstein condensates and analyse in detail their dynamics and its dependence on the system size. Since we are interested in circulating currents and their quantisation, we consider initial conditions which result in potential maximisation of such current: equal site occupation and equal phase differences between neighbouring sites. Within the Gross-Pitaevskii approximation we show that the current is quantised (exhibits sharp delta peaks) if the phase difference takes certain discrete values in the interval (Pi/2; 3Pi/2). The peaks, however, gradually average out to zero with increasing interaction due to chaos inherent to the system of many condensates. This kind of behaviour does not happen for smaller phase differences because of energetic reasons. Eventually, the quantisation ceases to occur for a macroscopic number of sites and the circular current manifests sinusoidal behaviour readily derived from the noninteracting limit. This marks the transition to the continuous limit.

DY 53.13 Thu 15:00 P1A

Partial transport barriers in 4D symplectic maps — •Markus Firmbach[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik — [2]MPI für Physik komplexer Systeme, Dresden

The transport across partial barriers in systems with a higher-dimensional phase space is of great interest for physical applications as well as from a conceptual point of view. We consider the 4D standard map and construct partial transport barriers of co-dimension one which are based on invariant objects in phase space, namely families of periodic one-tori. We compute the 4D flux across these partial barriers by volume- and transport measurements. This agrees with a flux formula using just the invariant objects.

DY 53.14 Thu 15:00 P1A

Entanglement in integrable-chaotic bipartite systems — •Maximilian Kieler[1] and Arnd Bäcker[1,2] — [1]TU Dresden, Insti-

tut für Theoretische Physik — [2]MPI für Physik komplexer Systeme, Dresden

We investigate entanglement of eigenstates and time-evolved states for the four-dimensional coupled quantum standard map where one subsystem is integrable and the other is chaotic. An analytic description of the eigenstate transition from unentangled to entangled is governed by a single transition parameter. The time evolution is investigated with respect to the initial state ensembles of unperturbed eigenstates, random states, and coherent states. Each ensemble exhibits different initial time behaviour and asymptotic values of the entropy.

DY 53.15 Thu 15:00 P1A

Entanglement in coupled kicked tops with chaotic dynamics — •Tabea Herrmann[1], Maximilian Kieler[1], Felix Fritzsch[1], and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik — [2]MPI für Physik komplexer Systeme, Dresden

The entanglement of eigenstates in two coupled, classically chaotic kicked tops is studied in dependence of their interaction strength. Governed by a universal scaling parameter, the statistics of level spacings, entanglement entropies, and the Schmidt eigenvalues undergo a transition from the non-interacting system towards full random matrix behavior [1]. Universality is found not only for equally sized large subsystems but also when one subsystem is small. Introducing a suitable random matrix transition ensemble allows for deriving the transition parameter. Combining the random matrix approach with perturbation theory leads to an accurate description of the initial phase of the transition. In the case of the entanglement entropies this can be extended to the whole transition.

[1] arXiv:1910.13447 [quant-ph] (2019)

DY 53.16 Thu 15:00 P1A

Resonance–Assisted Tunneling in Deformed Optical Microdisks with a Mixed Phase Space — •Felix Fritzsch[1], Roland Ketzmerick[1,2], and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik — [2]MPI für Physik komplexer Systeme, Dresden

In optical microcavities dynamical tunneling allows for finite lifetimes of whispering gallery modes, which are classically confined by total internal reflection. The lifetimes of such modes may drastically decrease by resonance–assisted tunneling due to the presence of classical nonlinear resonances in the ray dynamics. We present an intuitive semiclassical description which is based on classical properties and gives good agreement with numerically obtained lifetimes [1]. Moreover, we employ a perturbative description of resonance–assisted tunneling in order to predict complex wave numbers and to reconstruct both the intensity distribution of the nearfield as well as the phase-space distribution of whispering gallery modes.

[1] Fritzsch, Ketzmerick, Bäcker, Phys. Rev. E **100**, 042219 (2019)

DY 53.17 Thu 15:00 P1A

Relaxation dynamics in a Hubbard dimer coupled to fermionic baths: phenomenological vs. microscopic description — •Eric Kleinherbers[1], Nikodem Szpak[1], Jürgen König[1], and Ralf Schützhold[2,3] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47048 Duisburg — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden

We study relaxation dynamics in a strongly-interacting two-site Fermi-Hubbard model that is induced by fermionic baths. On the one hand, we model the dynamics with a Lindblad equation where the jump operators are chosen on pure phenomenogical grounds in the spirit of a local-bath approximation. On the other hand, we employ the real-time diagrammtic technique and derive the generalized master equation microscopically. Analyzing the characteristic time scales of relaxation processes, we find and discuss qualitative differences between the phenomenological and the microscopic approach. [1]

[1] E. Kleinherbers, N. Szpak, J. König, and R. Schützhold, arXiv: 1910:04130 (2019)

DY 53.18 Thu 15:00 P1A

Towards a numerical implementation of the Quench Action Approach — •Philipp Jaeger[1,2], Andreas Klümper[2], and Jesko Sirker[1] — [1]University of Manitoba, Department of Physics and Astronomy, Winnipeg, MB, Canada — [2]Bergische Universität Wuppertal, Fachbereich C - Fachgruppe Physik, Wuppertal, Germany

In the framework of integrable models the Quench Action approach was developed in recent years. This formalism in principle allows to calculate intermediate-time dynamics exactly by considering certain infinitesimal excitations around the GGE, all belonging to the same macro-state. However it is notoriously difficult to determine the relevant states and to evaluate the integrals. So far, this method has proven very useful to calculate GGE states and their convergence behaviour to the sub-leading order.

The two main ingredients are a spectrum and a measure of entropy, which can in principle be obtained using exact diagonalization (ED). To determine the relevant excitations, the n-String states from Bethe Ansatz must be identified in the numerics. To that end, we must consider sufficiently large systems which makes the ED algorithm quite complicated.

DY 53.19 Thu 15:00 P1A

Disentanglement Approach to Many-Body Quantum Spin Systems — •Stefano De Nicola — IST Austria

The disentanglement approach provides an exact description of many-body quantum spin systems in terms of classical variables. The resulting formulation can be equally seen as a field theory, amenable to analytical treatments, and a numerical method, whereby quantum dynamics is exactly mapped to an average over an ensemble of classical stochastic trajectories. The disentanglement method is applicable to integrable and non-integrable systems, including those in higher dimensions, within a unified framework, and can be applied both in and out of equilibrium. After discussing the general features of the disentanglement formalism, I illustrate the method by considering in particular its application to quantum quenches in paradigmatic many-body quantum spin systems. In this context, I show that the method can be used to obtain a wide range of observables, computed by numerically evaluating a set of formulae of broad applicability. Further insights on the quantum dynamics can be obtained by investigating the underlying quantum-to-classical correspondence, as recently shown in the case of dynamical quantum phase transitions. Finally, I discuss the strengths and limitations of the current implementation of the method, outlining directions for further developments.

DY 53.20 Thu 15:00 P1A

Performance of locally purified TN states as Ansatz-class for physical systems — •Lennart Bittel[1], Albert H. Werner[2], and Martin Kliesch[1] — [1]Heinrich Heine Universität, Düsseldorf, Germany — [2]University of Copenhagen, Copenhagen, Denmark

Tensor network models have proven to be a useful tool for the simulation of interacting quantum many-body systems and have also been extended from closed to open quantum systems. Matrix product density operators (MPDO) provide a common ansatz class to simulate quantum states under nearest neighbour Lindblad dynamics. Alternatively, locally purified tensor networks can be used to avoid positivity issues and to to obtain trace norm control for the simulation errors. However, It is known that some states can be approximated less efficiently compared to MPDO. Moreover, purifications of quantum states have a unitary gauge freedom, which can lead to significant errors in simulation if not appropriately fixed. In this work, we investigate use cases and develop algorithms for open tensor networks like state approximation, Lindblad dynamics and finding the respective equilibrium state and show that purified networks can outperform MPDO for relevant physical systems.

DY 53.21 Thu 15:00 P1A

Rydberg Composites — •Matthew Eiles, Andrew Hunter, Alexander Eisfeld, and Jan-Michael Rost — Max Planck Institute for the Physics of Complex Systems, 38 Noethnitzer Str. Dresden 01187

Rydberg states of atoms can be large enough that, in a dense cloud of ground state atoms, the electron can scatter off of many hundreds of impurities. Such a system, combining a Rydberg atom with a dense environment of localized scatterers, is called a Rydberg Composite. In conjunction with the high degeneracy of electronic states, the scattering from the localized impurities leads to a variety of heavily perturbed electronic states which, since the impurity atoms can be arranged in either crystalline or amorphous structures, shares many similarities with phenomena in solid-state materials. We will discuss some of these properties in this poster, for example the appearance of a band-like structure in the electronic density of states in a two-dimensional Composite and the existence of Anderson localization in a circular Composite.

DY 54: Poster: Active Matter and Microswimmers (joint session DY/TT)

Time: Thursday 15:00–18:00 Location: P1A

DY 54.1 Thu 15:00 P1A

Colloidal rods with visual perception: a simple cone of sight model. — •Anton Lüders, Philipp Stengele, and Peter Nielaba — Universität Konstanz, Konstanz, Deutschland

We introduce a simple model system of two-dimensional colloidal spherocylinders which become self-propelled under visual stimuli triggered by their neighboring particles. Via conventional Brownian dynamics simulations, the clustering phenomena and the collective motion in systems of multiple colloidal rods with visual perception are analyzed. In our model system, every particle is linked to a predefined cone of sight. A specific particle moves according to active Brownian motion if there is another particle's center inside the corresponding cone of sight but fluctuates according to normal passive Brownian motion otherwise. By analyzing the clustering phenomena of large systems we find a regime dominated by a clustering mechanism characteristic for the rods with visual perception in the range of small number densities. This regime leads to an unusual enhancement of the mean cluster size by reducing the number density of the system. Furthermore, it is studied how a small number of grouped spherocylinders with visual perception spread inside an infinite system. We find that the dynamics of rods inside this system is based on metastable states of passive Brownian motion and small flocks of activated particles. The dynamics of the particles inside the infinite system is further compared to more complex model systems of colloidal spherocylinders with visual perception.

DY 54.2 Thu 15:00 P1A

Inertial effects in collective microswimmer hydrodynamics — •Jan Cammann and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen

Microswimmers, such as bacteria, sperm cells, and motile algae, are typically found in regimes where the relevant length and velocity scales allow their hydrodynamic interactions to be studied in the limit of low Reynolds numbers. This simplifies the Navier-Stokes to the Stokes equations. In this approximation, inertial effects are completely neglected. For individual swimmers, this approximation is known to work well, whereas for the collective motion of a large number of swimmers the situation is less clear. For dense suspensions, the hydrodynamic flows produced by the individuals may interfere constructively, making inertial effects relevant. To elucidate this, we perform direct numerical simulations of swimmers immersed in a fluid described by either the Navier-Stokes or the Stokes equations. By directly comparing the dynamical properties, we probe the limits of this approximation for the collective hydrodynamics.

DY 54.3 Thu 15:00 P1A

Target search of active agents in complex environments. — •Luigi Zanovello[1,2], Michele Caraglio[1], Pietro Faccioli[2], and Thomas Franosch[1] — [1]Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria — [2]Statistical and Biological Physics Group, Dipartimento di Fisica, Università degli studi di Trento, Via Sommarive 14, 38123 Trento, Italy

Often living microorganisms, i.e. bacteria, move in complex landscapes in search of some target, i.e. nutrients, and use self propulsion to optimize their search.

Transport properties of single active Brownian particles in disordered environments are here investigated by computer simulations. Typically, in such random environments many paths exist connecting a starting region to the target. Furthermore, reaching the target likely involves the overcome of many barriers, which introduces a separation of time scales and makes the target search a rare event. Thus, with naive brute force molecular dynamics, characterizing the transition paths ensemble can be very demanding, if not unfeasible.

To cope with these issues, we design enhanced sampling techniques for active Brownian particles, which are inspired from methods used for the determination of rate constants in chemical reactions and protein folding. In particular, we design an active particle's version of transition path sampling and self-consistent path sampling. As a case study, the transition paths properties of active particles are compared with those of passive ones in simple potential landscapes with few local minima.

DY 54.4 Thu 15:00 P1A

Shearing an Active Glass — •Rituparno Mandal[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, Göttingen, Germany — [2]King's College London, London, United Kingdom

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 54.5 Thu 15:00 P1A

Collective behaviour of self-propelled elliptical particles — •Ashreya Jayaram, Andreas Fischer, and Thomas Speck — Institute of Physics, Johannes Gutenberg-University Mainz, Germany

Ensembles of anisotropic self-propelled particles exhibit a rich variety of emergent phases. A combination of short-ranged excluded volume interactions, which induce inter-particle forces and torques, and self-propulsion determines the resulting macroscopic structure. Starting from a point in parameter-space which displays motility-induced phase separation (MIPS) for isotropic particles, we systematically increase the aspect ratio of the constituent ellipses. On doing so, first, MIPS breaks down paving way to a spatially homogeneous state comprising polar domains. Secondly, at sufficiently large aspect ratios, particles aggregate into polar bands. We rationalize these observations from simulations by extracting two effective parameters, *viz.*, the force imbalance coefficient and the coupling to the local polarization, that enter the mean-field description of the system.

DY 54.6 Thu 15:00 P1A

Chimera states and waves in cilia arrays — •Albert von Kenne, Markus Bär, and Thomas Niedermayer — Physikalisch-Technische Budesanstallt (PTB), Berlin 10587

The study of coupled oscillators revealed a multitude of collective dynamics including synchronous motion, asynchronous motion, wave-like motion and a peculiar synchronization pattern known as chimera state. Here, a population of identical oscillators branches into coexisting subpopulations that are synchronized and desynchronized, respectively. Particularly, the constituents of living matter often exhibit cyclic processes with a tendency to synchronize. For example motile cilia and flagella – hair-like projections of eukaryotic cells that push fluid in motion to cause transport phenomena. We study numerically a generalized version of a simple phase oscillator model for the coupling of cilia. The model is linked to wave formation [1] and encompasses the features relevant for the emergence of chimera states [2]. We investigate chimera states and waves in cilia arrays and discuss its properties with respect to transport generation and switching of motility states.

[1] Niedermayer et. al., Chaos: 18(3) 2008; [2] Niedermayer et. al., DPG Spring Meeting 2017: Contributed talk DY 52.1

DY 54.7 Thu 15:00 P1A

Nanoscale Temperature Imaging using Liquid Crystal Phase Transitions — •Martin Fränzl and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

With the growing number of applications of thermoplasmonics in a variety of different fields there is a need to for a simple and reliable temperature measurement of optically heated metal nanostructure. We present a method to study such temperature distributions at the nanoscale utilizing the 5CB liquid crystal nematic-isotropic phase transition. The technique is based on a conventional optical microscopy and capable of imaging isothermal contours around heated nanostructures as well as to retrieve the absolute temperature increment. The setup is easy to implement with any conventional optical microscope requiring no external modifications of additional components. We demonstrate our technique for various plasmonic nanostructures such as gold nanoparticles, Janus particles and continuous gold films. The

spatial resolution of this technique is diffraction limited and temperature variations smaller than 0.1 K can be detected.

DY 54.8 Thu 15:00 P1A

Random Caustics in active random walks in random environments — •King Hang Mok[1,2] and Ragnar Fleischmann[1] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany — [2]Institut für Dynamik komplexer Systeme, Georg-August-Universität Göttingen

The trail patterns of Argentine ants can show striking resemblance to the branched flow patterns of waves in correlated random environments. Branched flow is a general phenomenon that is widely observable in nature, such as in the electron flow in semiconductors, tsunami waves in the ocean or the propagation of light and sound through turbulent media. An important mechanism in branched flows is the formation of random caustics, singularities in the ray density corresponding to the wave flow.

We study the density fluctuations of active random walks biased by correlated random environments, resembling the motion of Argentine ants in Gaussian random fields of pheromones. We analyse in which parameter regimes reminiscences of the caustics of the deterministic dynamics in quenched disorder can be observed in the random walk.

DY 54.9 Thu 15:00 P1A

Can a passive colloid in an active bath be modeled as an active Brownian particle? — •Jeanine Shea[1], Friederike Schmid[1], and Gerhard Jung[2] — [1]Johannes Gutenberg University — [2]University of Innsbruck

Passive colloids in baths of active particles exhibit vastly different behavior than passive colloids in thermal baths. In particular, Wu and Libchaber [1] found experimentally that a passive colloid immersed in an active bath exhibits superdiffusive behavior on short time scales and normal diffusive behavior in the long-time limit. This behavior is analogous to that of an active particle, which is characterized by this transition between superdiffusive and diffusive behavior. Although Wu and Libchaber were able to relate this crossover time to experimental observables such as the length scale of collective motion, they did not explicitly relate the parameters of the system of active particles, such as the density, the rotational diffusion coefficient, or the force of active particles, to this characteristic crossover time. We investigate the detailed mechanisms that lead to the "activity" of the passive colloid and aim to explicitly map the dynamics of a passive colloid in an active bath to the model of an Active Brownian Particle.

[1] Wu, X.-L., and A. Libchaber, 2000, "Particle diffusion in a quasi-two-dimensional bacterial bath," Phys. Rev. Lett. 84, 3017-3020.

DY 55: Poster: Turbulence; Complex Fluids; Microfluidics; Droplets and Wetting

Time: Thursday 15:00–18:00 Location: P1A

DY 55.1 Thu 15:00 P1A

High Performance Free Surface LBM on GPUs — •Moritz Lehmann, Fabian Häusl, and Stephan Gekle — Biofluid Simulation and Modeling, Theoretische Physik VI, Universität Bayreuth

By combining the lattice Boltzmann method (LBM) with the Volume-of-Fluid (VoF) model, free surfaces can be simulated. Besides the challenge of running VoF alongside LBM with massive parallelism on the GPU, the core difficulty of VoF is surface tension calculation using piecewise linear interface construction (PLIC), which until now had no complete analytic solution and so far was solved iteratively - thereby severely slowing down the simulation. We present the full analytic solution for PLIC and apply it to a GPU implementation of VoF-LBM. This excellent performance enables close to real-time simulations of complex free surface phenomena such as drop impacts with all the variety of emerging effects such as crown- and jet-formation or the Plateau-Rayleigh instability. The model is validated by comparison to analytic solutions and experimental data.

DY 55.2 Thu 15:00 P1A

Dynamics of gel networks on different time and length scales — •Matthias Gimperlein and Michael Schmiedeberg — Institut für Theoretische Physik 1, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany

Gelation is connected to a slow-down in dynamics, the onset of percolation and an increasing number of neighboring particles. The slow-down occurs on different time scales depending on the studied length scales.

Using Brownian Dynamics simulation for a system of colloidal particles interacting due to a modified square well potential we investigate the properties of gel networks on different time and length scales.

The square well potential is modified by introducing an additional interaction range α to flatten the walls of the square well such that Brownian dynamics simulations are possible. The phase diagram was determined by fitting the gas-liquid coexistence binodal. In the square well limit ($\alpha \to 0$) the result shown in [1] is recovered.

Further research includes distinguishing dynamic regimes or structures on different length and time scales, investigating the history/protocol dependency of the development (*i. e.* starting from different initial configuration by varying particle density or system structure) and finding stable or metastable structures to describe the evolution of gel networks not on the particle level anymore, but on a coarse grained level.

[1] Speck *et al.*, J. Chem. Phys. **148**, 241101 (2018)

DY 55.3 Thu 15:00 P1A

Defects and phasonic flips during the growth of soft quasicrystals — •Stefan Wolf[1,2], Michael Engel[1], and Michael Schmiedeberg[2] — [1]Institute for Multiscale Simulation, Friedrich-Alexander-University Erlangen-Nuremberg, Erlangen, Germany — [2]Institut für Theoretische Physik I, Friedrich-Alexander-University Erlangen-Nuremberg, Erlangen, Germany

An important but not yet well-understood mechanism during the growth of defect-free quasicrystals is the repair of defects or excitations via phasonic flips. We simulate a one-component quasicrystals in order to study the growth and the influence of phasonic flips. We developed a Monte Carlo method to fathom the growth of quasicrystals without and with phasonic flips. To speed up the simulations, the possible directions of the growth are limited to positions given by fixed vectors. For the calculation of the energy, and therefore for the probability of occupation of a position, an oscillating pair potential is used. First results show the formation of structures with 10-fold rotational symmetry for low temperatures without phasonic flips. In the next step, phasonic flips are taken into account in order to reveal how they influence the growth of quasicrystals.

DY 55.4 Thu 15:00 P1A

The parameter space of thermohaline stairs — •Axel Rosenthal and Andreas Tilgner — Institute of Geophysics, Göttingen, Germany

Convection and diffusion in water can be observed when a gradient in temperature or in salinity takes effect on density in presence of gravity. Both gradients can force or stabilize the process. We conducted experiments where the salt gradient is the driving force and simultaneously the temperature gradient is stabilizing in opposite direction, observed by particle image velocimetry. The question is at which gradients, expressed by Rayleigh numbers, does the transport occure in stable so called "thermohaline stairs"? Thermohaline stairs are a sequence of two flow systems, a finger regime and a large scale circulation.

DY 55.5 Thu 15:00 P1A

Droplet evaporation/condensation in the lattice gas — •Manuel Maeritz — Universität Tübingen, Institut für Angewandte Physik

We investigate the droplet evaporation/condensation of the lattice gas in two and three dimensions within the framework of density functional theory. First, we construct improved free energy functionals by mapping the lattice gas to the Asakura-Oosawa model and formulate a functional using a suggestion by Cuesta et al. (Highlander functional) [1]. Comparison to standard mean-field results shows a clear improvement of the phase diagram. Second, we apply the functional to droplets in finite boxes and extract droplet surface tensions. A comparison to recent simulation results by Tröster et al. is given [2].

[1] J. Cuesta, L. Lafuente and M. Schmidt, Phys. Rev. E 72, 031405 (2005).

[2] A. Tröster, F. Schmitz, P. Virnau, K. Binder, J. Phys. Chem. B

122, 3407-3417 (2018).

DY 55.6 Thu 15:00 P1A

Characterizational Measurements of a Model Wind Turbine in a Variable Density Wind Tunnel — •Birte Thiede[1], Christian Küchler[1], Julian Jüchter[2], Michael Hölling[2], Eberhard Bodenschatz[1], Joachim Peinke[2], and Michael Wilczek[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]ForWind, Institute of Physics, University of Oldenburg, Oldenburg

Wind tunnel experiments with small-scale models are an essential part of wind turbine research as they offer a highly controllable environment for the investigation of various research questions. Due to the limited size of wind tunnels, the Reynolds numbers that can typically be achieved in such experiments are significantly smaller than those in actual wind turbine systems.
The Variable Density Turbulence Tunnel at the Max Planck Institute for Dynamics and Self-Organization can be filled with the dense gas SF6 and pressurized up to 15 bar, which leads to sufficiently high Reynolds numbers $\left(\text{up to } 2 \cdot 10^7\right)$ to perform wind turbine experiments at dynamic similarity.
In this tunnel, we study the power generation as well as the wake characteristics for different turbulent inflow conditions (generated by an active grid) and a range of Reynolds numbers of the MoWiTO 0.6, a model wind turbine built at the ForWind Center for Wind Energy Research Oldenburg, which is equipped with a pitch- and a load control.

DY 55.7 Thu 15:00 P1A

Upscaling of dielectrophoretic continuous-flow separation in a microfluidic system — •Jakob Derksen, Dario Anselmetti, and Martina Viefhues — Experimental Biophysics and Applied Nanoscience, Bielefeld University, Germany

High throughput analysis and separation of biomolecules or nanoparticles is an important task for many biological and medical applications such as separating DNA fragments and purification of gene vaccines. Thus, new separation techniques are requested. In this work, we present a sufficient microfluidic concept for upscaling of continuous-flow separation by means of dielectrophoresis (DEP).

DEP describes the movement of an electrically polarizable object in a non-uniform electric field. The advantages are that it is non-invasive, label-free and it provides selective manipulation of samples. A current disadvantage of this method is the limitation to small sample volumes and associated with that, the enormous purification time for reasonably sample volumes in the range of millilitre.

Here, we demonstrate the upscaling of a dielectrophoretic continuous-flow separation method in a microfluidic system. For that purpose, we created a system with two parallel separation channels in one device. We successfully demonstrated the separation of 100 nm and 40 nm beads and 10 kbp and 5 kbp DNA and harvesting in separate reservoirs. With these experiments, we firstly demonstrated an upscaling of separation throughput in a microfluidic device, paving the way to high-throughput applications.

DY 55.8 Thu 15:00 P1A

Two-point velocity statistics from ocean surface drifter observations in the Benguela upwelling system: In search of the inverse energy cascade — •Julia Draeger-Dietel[1], Alexa Griesel[1], and Dhruv Balwada[2] — [1]Institut für Meereskunde, Universität Hamburg, Hamburg, Germany — [2]Courant Institute of Mathematical Sciences, New York University, New York, NY, USA

Lagrangian trajectories from surface drifters in the ocean constitute a time evolving, highly non-uniform spatial grid. The corresponding drifter velocity observations can be treated as scattered point Eulerian measurements, which can help in deducing the turbulent properties of the flow. Here we examine the probability distribution $P(\Delta u_\ell|s)$ of relative longitudinal velocity Δu_ℓ, as a function of spatial separation s, from surface drifters deployed in the upwelling region off Namibia. We find the $P(\Delta u_\ell|s)$ to be positively skewed for relative separations s of 10 km - 80 km. The rescaled 3rd order structure function, $\left\langle \Delta u_\ell^3 \right\rangle / s$, reveals a (positive) plateau, supporting an inverse energy cascade with energy transfer rate $\epsilon \simeq 2.4 \cdot 10^{-8} m^3/s^2$. The combination with former findings of Richardson scaling of pair separations, $\left\langle s^2(t) \right\rangle = g\epsilon t^3$, yield a reduced Obhukov constant g close to the finding in laboratory experiments. The reduced Obhukov constant can be traced back to an algebraic decay $s^{-\alpha}$ with $\alpha \simeq -5/3$ in the central regime of the corresponding probability distribution $P(s|t)$ of relative separations s for fixed time t. An algebraic decay with $1 < \alpha < 2$ points to the relevance of Levy walk models in the stochastic description of the turbulent transport process in the ocean.

DY 55.9 Thu 15:00 P1A

Charged Liquid Bridges — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

A new solution of a charged catenary is presented which allows to determine the static and dynamical stability conditions where charged liquid bridges are possible. The creeping height, the bridge radius and length as well as the shape of the bridge is calculated showing an asymmetric profile in agreement with observations. The flow profile is calculated from the Navier Stokes equation leading to a mean velocity which combines charge transport with neutral mass flow and which describes recent experiments on water bridges. The velocity profile in a water bridge is reanalyzed. Assuming hypothetically that the bulk charge has a radial distribution, a surface potential is formed that is analogous to the Zeta potential. The Navier*Stokes equation is solved, neglecting the convective term; then, analytically and for special field and potential ranges, a sign change of the total mass flow is reported caused by the radial charge distribution. [Water 9 (2017) 353, Phys. Rev. E 86 (2012) 026302, errata Phys. Rev. 86 (2013) 069904]

DY 55.10 Thu 15:00 P1A

Small-scale simulations of high Reynolds number turbulence — •Niklas Schnierstein[1,2] and Michael Wilczek[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August University, Göttingen, Germany

Three-dimensional turbulence is a multi-scale problem, in which energy is transferred from the largest, energy-containing scales to the smallest, dissipative scales. The separation of these scales increases with the Reynolds number. Thus, resolving all scales of a turbulent flow in direct numerical simulations (DNS) is for many realistic problems computationally prohibitive. However, in some problems, one is only interested in certain scales of the flow. One example is the formation of microdroplets in clouds, for which small-scale turbulence is of crucial importance. For this reason, we explore the possibility of generating a realistic small-scale turbulent flow while adequately modeling the larger scales using stochastic processes. By controlling the parameters of these processes, we can precisely impose key statistical quantities on the flow, such as the energy spectrum and the correlation time. We investigate different methods of coupling the modeled and the resolved scales, characterize the generated flow field, and compare it to fully resolved DNS to analyze the advantages and limitations of this approach.

DY 55.11 Thu 15:00 P1A

Effect of disorder on dispersive transport in porous media — •Felix Jonathan Meigel[1,4], Thomas Darwent[3], Lucas Goehring[3], and Karen Alim[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — [2]Physics Department, Technical University Munich, Germany — [3]School of Science and Technology, Nottingham Trent University, Nottingham, United Kingdom — [4]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Transport by the means of fluid flow through porous media is central for many processes in our daily life. Porous media show a large variety of morphologies that may change over time. How does the morphology interplay with the transport of solute particles through the medium? Here, we show how changing the disorder in a medium affects transport through the porous medium. We connect the dynamics on the level of single pores with the macroscopic transport through the whole medium. Using a first passage time formalism, we describe how macroscopic transport statistics emerge from the interplay of individual pores. We find dynamics that deviate from Fickian descriptions and cannot be explained using an effective advection diffusion equation. Using a two-dimensional model porous medium in which we can control the disorder, we focus on the variance of the dispersive front of a medium being filled up to saturation with solute particles. We find that the variance changes non-monotonically as either the disorder or the Peclet number is altered. We find these results both in simulation and experiments and give a theoretical explanation of our findings.

DY 55.12 Thu 15:00 P1A

Rheology and self-assembly of mixtures of magnetic and non-magnetic liquid crystals under shear and external field —

•Ferdinand Schönerstedt, Nima H. Siboni, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

Doping liquid crystals (LC) with magnetic nanoparticles (MNP) has proven a successful strategy to obtain magnetic field responsive materials. In this work, motivated by recent advances in MNP manufacturing technology [1], we investigate the effect of the external field on rheology and self-assembly of LC-MNP mixtures where the MNPs have the same shape and the same size of the LC particles.

It is noteworthy that even in the absence of the magnetic dipole-dipole interactions, such mixtures show an interesting demixing at strong fields, and as a consequence, an intriguing non-monotonic field dependence of the shear stress emerges [2]. By considering a finite dipole-dipole interaction in a non-equilibrium molecular dynamics simulation setup, we explore the interplay between the self-assembly of MNPs (under the influence of the external field [3]), and the shear- and magnetic field-induced orderings.

[1] A. Mertelj, D. Lisjak, M. Drofenik, and M. Čopič, Nature **504**, 237 (2013).

[2] N. H. Siboni, G. P. Shrivastav, and S. H. L. Klapp, arXiv:1908.10815 (2019).

[3] C. E. Alvarez, and S. H. L. Klapp, Soft Matter **8**, 7480 (2012).

DY 55.13 Thu 15:00 P1A

Experimental Study of the Bottleneck in Fully Developed Turbulence using LDV — •Torben Neumann[1,2], Gholamhossein Bagheri[2], and Eberhard Bodenschatz[1,2] — [1]Georg-August-University, Goettingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Turbulence plays an important role in many flows. The bottleneck effect is the phenomena of energy pileup in the energy spectrum of incompressible turbulence where viscous dissipation begins to act. Previous hotwire measurements in the Variable Density Turbulence Tunnel (VDTT) have shown a decrease of the bottleneck strength for high frequencies. However, the high frequencies cannot be fully explored by hotwire measurements. Therefore, the Laser Doppler Velocimetry technique (LDV) will be used to bypass the biases the hotwires might have. In order to do that, the first challenge is to design a particle dispersion system that is capable of working in a high pressure wind-tunnel and of dispersing particles in an optimal concentration for LDV measurements. The preliminary results of the LDV measurements conducted in the VDTT will be presented.

DY 55.14 Thu 15:00 P1A

Manipulation of thermo-osmotic flows in thin liquid films — •Nicola Andreas Söker and Frank Cichos — Universität Leipzig, Peter-Debey-Institut für Physik der weichen Materie

We study the creation and manipulation of flows in a micrometer sized film of water by thermo-osmotic surface flows along the confining walls. A local temperature profile is created by optically heating a gold film inducing osmotic flows along the confining walls. Chemically patterning the gold surfaces creates asymmetric flows. The progammable directed flow might be used to position sub micrometer diffusing objects e.g. to position single biopolymers in a thermo phoretic trap structure presently developed [1] in our group. To characterize the emerging flow fields metal nano particles are used as tracers [2]. We also study the interference of the thermo-osmotic flows originating from multiple heating spots at the gold film.

[1] Fränzl, Martin., Thalheim, Tobias., Adler, Juliane. et al. Thermophoretic trap for single amyloid fibril and protein aggregation studies. Nat Methods 16, 611-614 (2019)

[2] Andreas P. Bregulla, Alois Würger, Katrin Günther, Michael Mertig, and Frank Cichos Phys. Rev. Lett. 116, 188303 * Published 5 May 2016

DY 55.15 Thu 15:00 P1A

A study of metastability in hydrophobic surfaces — •Marion Silvestrini[1,2], Alberto Giacomello[2], and Carolina Brito[1] — [1]Physics department, Federal University of Rio Grande do Sul, Porto Alegre, Brazi — [2]Dipartimento di Ingegneria Meccanica e Aerospaziale, Università di Roma "La Sapienza"

The study of wetting phenomena in solids is of great interest due to the possible technological applications of hydrophobic and hydrophilic surfaces. Besides these applications, there are some fundamental open questions concerning the transition between these two wetting states. For instance, it is known that metastability is a common feature in experiments and that these metastable states are, in general, hydrophobic states. It is then important to understand what are the properties of the substrates that leads to this effect. In previous works, we have studied such phenomena using the analytical global energy approach and Monte Carlo simulations of the Cellular Potts model.

It has been shown that the final configuration depends strongly on the choice of initial wetting state of the droplet, which suggests the existence of a metastable regime in the system. To analyze systematically and understand this effect, in this work we apply a technique called Umbrella Sampling, that consist on adding a constraining term to the Hamiltonian, which drives the system to visit several specific configurations. We then use the results to calculate the free energy profile. This allows us to relate the energy barriers that lead to metastable states to the topology of the surface, which is a key point to understand the transition between CB and W states.

DY 55.16 Thu 15:00 P1A

Topological modes in hydrodynamics — •Richard Green — Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands — Instituut-Lorentz, Universiteit Leiden, 2300 RA Leiden, The Netherlands

Topological band theory has been applied in recent work to classical fluids such as geophysical waves on the Earth's surface, and flocks on curved surfaces. I review these problems and consider what general features enable topologically protected modes to be supported in such classical systems.

DY 55.17 Thu 15:00 P1A

Nonlocal interactions in strongly correlated systems — •Daria Medvedeva — Institute of Physics of the Czech Academy of Sciences, Prague 8, Czech Republic — Ural Federal University, Yekaterinburg, Russian Federation

Systems with strong electron correlations can be perfectly described by quantum lattice models, e.g. by the Hubbard model. If coordination number or spatial dimension tend to infinity, this model can be solved by the Dynamical Mean-Field Theory taking into account only local correlations. However according to recent studies [1] we can't neglect nonlocal (between lattice sites) interactions in some materials. Moreover it was found that there are strong electron correlations in the systems with *sp*- electrons [2]. Theoretical description of such systems can be obtained making use the Extended Dynamical Mean-Field Theory (EDMFT). This research was devoted to development of a numerical algorithm to solve EDMFT equations. We have developed the numerical complex based on the exact diagonalization approach. The minimal parameterization of the effective impurity model was determined for different types of interactions. Using this scheme, we considered charge and exchange nonlocal interactions influence on the electronic properties of the model system and screening of the local Coulomb interaction by nonlocal one. We described functionalized graphene structures with adsorbed F and H atom, which can be really synthesized. [1] PRB 94, 214411 (2016). PRB 94, 224418 (2016). PRL 111, 036601 (2013). PRB 74, 212507 (2006). [2] PRL 110, 166401 (2013). PRB 88, 081405(R) (2013).

DY 55.18 Thu 15:00 P1A

Acoustogalvanic rectification in Dirac and Weyl semimetals — •Habib Rostami and Pavlo Sukhachov — Nordita, KTH Royal Institute of Technology and Stockholm University, Roslagstullsbacken 23, SE-106 91 Stockholm, Sweden

In this talk, I will discuss a nonlinear mechanism to generate a direct electric current by passing acoustic wave in inversion-symmetric Dirac and Weyl semimetals. According to the similarity with the photogalvanic rectification, where a direct current is produced in a second order response to light, we called this phenomenon the acoustogalvanic effect [1]. It relies on pseudo-electromagnetic fields [2] originating from sound-induced strain. Unlike the standard acoustoelectric effect [3], which relies on the sound-induced deformation potential and the corresponding electric field, the acoustogalvanic one originates from the pseudo-electromagnetic fields, which are not subject to screening. Due to an interplay of the pseudoelectric and pseudomagnetic fields, the acoustogalvanic current shows a nontrivial dependence on the direction of the sound wave propagation. Being within the experimental reach, the effect can be utilized to explore dynamical deformations and probe the pseudo-electromagnetic fields, which are yet to be experimentally observed in Weyl and Dirac semimetals.

[1] P. O. Sukhachov and H. Rostami, arXiv:1911.04526 (2019).

[2] A. Cortijo et al. Phys. Rev. Lett. 115, 177202 (2015).

[3] R. H. Parmenter, Phys. Rev. 89, 990 (1953).

DY 56: Poster: Glasses; Granular Matter; Brownian Motion and Anomalous Diffusion

Time: Thursday 15:00–18:00 Location: P1A

DY 56.1 Thu 15:00 P1A

Stationary current in the open Bose-Hubbard chain — Anna Bychek[1], Pavel Muraev[2], Dmitrii Maksimov[1,3], and •Andrey Kolovsky[1,2] — [1]Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia — [2]Siberian Federal University, 660041 Krasnoyarsk, Russia — [3]Siberian State Aerospace University, 660014 Krasnoyarsk, Russia

We analyze stationary current of bosonic carriers in the Bose-Hubbard chain of length L where the first and the last sites of the chain are attached to reservoirs of Bose particles acting as the particle source and sink, respectively. The analysis is curried out by using the pseudoclassical approach which reduces the original quantum problem to the classical problem for L coupled nonlinear oscillators. It is shown that an increase of oscillator nonlinearity (which is determined by the strength of inter-particle interactions) results in a transition from the ballistic transport regime, where the stationary current is independent of the chain length, to the diffusive regime, where the current is inverse proportional to L.

DY 56.2 Thu 15:00 P1A

Analytical theory for predicting variations of activation energies in mixed glass former glasses — •Julian Fischer, Marco Bosi, and Philipp Maass — Fachbereich Physik, Universität Osnabrück, Germany

The mixed glass former effect manifests itself in a nonadditive behaviour of physical and chemical properties upon mixing of two or more different glass formers in ion-conducting glasses[1]. Most striking is the behaviour of conductivity activation energies. They can exhibit minima at certain mixing ratios that at room temperature lead to enhancements of ionic conductivities by several orders of magnitude compared to the respective glasses containing only one of the network formers.
We present an analytical approach for modeling the variation of conductivity activation energies $E_a(x)$ with the glass former mixing ratio x. This approach is based on the assumption that changes of the free energy landscape for the long-range ion transport are governed by changes of the concentration of glass former units[2]. Theoretical results obtained by adjustment of only one parameter are in surprisingly good agreement with experimental findings.

[1] M.D. Ingram, Phys. Chem. Glasses 28, 215 (1987).
[2] M. Schuch, C. Trott, P. Maass, RSC Adv. 1, 1370 (2011).

DY 56.3 Thu 15:00 P1A

Collective single-file transport in periodic potentials — •Dominik Lips[1], Artem Ryabov[2,3], and Philipp Maass[1] — [1]Universität Osnabrück, Germany — [2]Charles University, Prague, Czech Republic — [3]Universidade de Lisboa, Portugal

Driven lattice gases are often used to model single-file molecular transport and biological traffic. With respect to continuous space dynamics, the discrete lattice can be regarded to represent a periodic energy landscape in a coarse-grained manner. Thermally activated transitions of particles between different potential wells correspond to jumps between lattice sites, while effects on length scales smaller than the lattice constant are neglected. To study single-file transport on a lower level of coarse-graining, the Brownian asymmetric simple exclusion process (BASEP) was recently introduced [1,2]. In this BASEP, hard spheres perform a driven Brownian motion in a periodic potential under a constant drag force. Case studies with a cosine potential show that the collective dynamics depend sensitively on the ratio of the particle size and wave length of the potential. The interplay of three physical mechanisms leads to a rich variety of nonequilibrium phase transitions in open systems [1,2], and counterintuitive short uphill transitions [3]. Here, we report on new results obtained for periodic potentials with multiple minima per period and other short-range interactions.
[1] D. Lips, A. Ryabov, P. Maass, Phys. Rev. Lett. **121**, 160601 (2018).
[2] D. Lips, A. Ryabov, P. Maass, Phys. Rev. E **100**, 052121 (2019).
[3] A. Ryabov, D. Lips, P. Maass, J. Phys. Chem. C **123**, 5714 (2019).

DY 56.4 Thu 15:00 P1A

The role of initial speed in projectile impacts into light granular media — •Kai Huang[1,2], Dariel Hernadez Delfin[3], Felix Rech[1], Valentin Dichtl[1], and Raul Cruz Hidalgo[3] — [1]Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Division of Natural and Applied Sciences, Duke Kunshan University, 215306 Kunshan, Jiangsu, China — [3]Department of Physics and Applied Mathematics, University of Navarra, 31009 Pamplona, Spain

Projectile impact into a light granular material composed of expanded polypropylene (EPP) particles is investigated systematically with various impact velocities. Experimentally, the trajectory of an intruder moving inside the granular material is monitored with a recently developed microwave radar system noninvasively. Numerically, discrete element simulations together with coarse-graining techniques are employed to address both dynamics of the intruder and response of the granular bed. Our experimental and numerical results of the intruder dynamics agree with each other quantitatively and are in congruent with existing phenomenological model on granular drag. Stepping further, we explore the 'microscopic' origin of granular drag through characterizing the response of granular bed, including density, velocity and kinetic stress fields at the mean-field level. The macroscopic profiles of the granular bed ahead of the intruder decays exponentially in the co-moving system of the intruder, giving rise to a characteristic length scale on the order of intruder size.

DY 56.5 Thu 15:00 P1A

Interpreting impedance spectroscopy data by using Poisson-Nernst-Planck anomalous models — Ervin K. Lenzi[1], Luiz R. Evangelista[2], Leila Taghizadeh[3], Daniel Pasterk[3], Rafael S. Zola[4], Trifce Sandev[5,6,7], Clemens Heitzinger[3], and •Irina Petreska[7] — [1]Universidade Estadual de Ponta Grossa — [2]Universidade Estadual de Maringá — [3]Technische Universität Wien — [4]Universidade Tecnológica Federal do Paraná — [5]Macedonian Academy of Sciences and Arts — [6]University of Potsdam — [7]Ss. Cyril and Methodius University in Skopje

The information obtained from impedance spectroscopy of electrolytic cells enables comprehension of the complex diffusion phenomena in liquid/solid interfaces. In this context, we consider two implementations of the Poisson-Nernst-Planck (PNP) anomalous models of the electrical response of electrolytic cells, one built in the frameworks of the fractional calculus and the other one being an extension of the standard PNP model presented by Barsoukov and Macdonald. Both extensions may be related to an anomalous diffusion with subdiffusive characteristics through the electrical conductivity and are able to describe the experimental data. Bayesian inversion is also applied to extract the parameter of interest in the analytical formulas of impedance, using the delayed-rejection adaptive-Metropolis algorithm (DRAM) in the context of Markov-chain Monte Carlo (MCMC) algorithms to find the posterior distributions and confidence intervals.
[1] E. K. Lenzi et al., J. Phys. Chem. B 123, 7885 (2019).

DY 56.6 Thu 15:00 P1A

Diffusion in combs with stochastic resetting — •Viktor Domazetoski[1], Axel Masó-Puigdellosas[2], Trifce Sandev[1,3,4], Vicenç Méndez[2], Alexander Iomin[5], and Ljupco Kocarev[1,4] — [1]Macedonian Academy of Sciences and Arts — [2]Universitat Autónoma de Barcelona — [3]University of Potsdam — [4]Ss. Cyril and Methodius University in Skopje — [5]Technion, Haifa

Diffusion on a three dimensional xyz–comb is analyzed. Three different types of resetting are considered. These are: (i) global resetting to the initial position, (ii) resetting to the x–backbone, and (iii) resetting to the main y–fingers. Analyzing the probability density functions, their stationary distributions and the mean squared displacements, we observe different transient dynamics along the backbone in all three cases of the resetting mechanisms. The main conclusions from the analysis are as follows. The global resetting breaks the transport in all three directions, while the resetting to the backbone breaks the transport in two (y and z) directions but enhances the transport in the main x–axis. Moreover, the resetting to the z–fingers enhances the transport in the backbone and the main y–fingers, while the transport along the z–fingers is localized, when the mean squared displacement reaches a steady value. The analytical results are confirmed by numerical simulations in the framework of coupled Langevin equations for the comb structure.

DY 56.7 Thu 15:00 P1A

Unknotting of quasi-two-dimensional ferrogranular networks by in-plane homogeneous magnetic fields — Pedro A. Sanchez[1,2], Justus Miller[3], Sofia S. Kantorovich[4], and •Reinhard Richter[3] — [1]Ural Federal Univ., 51 Lenin av., Ekaterinburg, 620000, Russian Federation — [2]Inst. of Ion Beam Physics and Materials Research, H-Z Dresden-Rossendorf e.V., 01314 Dresden, Germany — [3]Experimentalphysik 5, Univ. of Bayreuth, 95440 Bayreuth, Germany — [4]Computational Physics, Univ. of Vienna, 1090 Vienna, Austria

We are exploring in experiments and computer simulations, the aggregation process in a shaken granular mixture of glass and magnetized steel beads, occuring 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]. Here we focus on the quasi-two-dimensional case, analyzing in computer simulation the effects of a magnetic field parallel to the system plane [2]. Our results evidence that the field drastically changes the structure of the forming network: chains and elongated clusters parallel to the field are favored whereas perpendicular connecting structures tend to be supressed, leading to the unknotting of the networks familiar from zero fields. By means of a field dependent orientation parameter we compare numerical and experimental results.

[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*, accepted (2019).

DY 56.8 Thu 15:00 P1A

System size scaling of a model glass under shear — •Moumita Maiti[1], Lawrence Smith[2], and Andreas Heuer[3] — [1]Institute of Physical Chemistry, UNiversity of Muenster, Muenster,Germany — [2]Institute of Physical Chemistry, UNiversity of Muenster, Muenster, Germany — [3]Institute of Physical Chemistry, UNiversity of Muenster, Muenster, Germany

We simulate a binary Lennard-Jones glass under shear for different system sizes with a very low shear rate at a temperature close to zero. We observe shear bands for larger system sizes. The tails of the Van-Hove function of such samples display a scaling with the system size with an exponent 0.5. We relate the scaling to the presence of activating shear transformation zones (STZs) and speculate about the impact of the coupling of different STZs as the source of these finite size effects. This is further corrobated by analyzing the number of fast moving particles. We anticipate a positive correlation between the number of activated STZs and the number of single particle jumps. We observe that the number of jumps per particle scales with system sizes too but with a different exponent 0.25. We discuss possible reasons for the difference of the two scaling exponents.

DY 56.9 Thu 15:00 P1A

Accurate determination of local properties in 2D particulate systems using Set Voronoi tessellation — •Simeon Völkel[1] and Kai Huang[1,2] — [1]Universität Bayreuth, Experimentalphysik V, Universitätsstraße 30, 95447 Bayreuth, Germany — [2]Duke Kunshan University, Division of Natural and Applied Sciences, No. 8 Duke Avenue, Kunshan, Jiangsu, China 215316

Using the collective behavior of a granular rod monolayer under vertical vibrations, we demonstrate the advantages of the Set Voronoi tessellation in two dimensions (2D).

The behavior of particulate systems typically depends critically on the *local* configuration of its constituents, requiring accurate measurements of properties such as bond orientational order parameters or the local volume fraction. In this regard, Voronoi tessellation is a common tool for tiling space, but is only appropriate for mono-disperse spheres. This severely limits its applicability, especially in dense systems of poly-disperse and non-spherical particles, which are commonly found in practice. To overcome this limitation, Set Voronoi was proposed which assigns points in space according to the closest particle surface (contour for the 2D case) instead of closest particle center.

We show that Set Voronoi delivers consistent results even for extreme cases, where the error in the local volume fraction obtained using classical Voronoi goes up to 100 %. Our 2D implementation can be applied directly to a variety of (quasi-)2D particulate systems of practical interest ranging from granulates to pedestrian and traffic flow systems.

DY 56.10 Thu 15:00 P1A

Superdiffusion in Kac-Zwanzig heat baths — •Paul Ledwon and Igor Sokolov — Institut für Physik, Humboldt Universität zu Berlin

We consider the Kac-Zwanzig heat bath model, an ensemble of harmonic oscillators interacting with a single distinguished particle. The model is known to allow for rigorous derivation of the generalized Langevin equation (GLE) from the underlying Hamilton dynamics in the thermodynamic limit. The memory kernel of this equation depends on the distribution of the spring constants and masses of the bath oscillators, and on their interaction strengths with the distinguished particle. Our specific focus is on the memory kernels leading to superdiffusion of the distinguished particle, in which mean squared displacement grows faster than linearly in time. We discuss restrictions on the parameters on the bath including its size necessary for effectively simulating superdiffusion, and the algorithmic implementation of the corresponding simulations.

DY 56.11 Thu 15:00 P1A

Angle of repose of granular materials: Analytical expression from Molecular Dynamic simulations — Filip Elekes and •Eric Josef Ribeiro Parteli — Department of Geosciences, University of Cologne

The angle of repose is one of the most important quantities used to characterize the packing behavior and flowability of granular materials in industrial applications, environmental sciences and planetary research. However, the dependence of this angle on particle size and gravity remains poorly understood. Here we investigate the angle of repose of granular materials by means of particle-based simulations. Our model includes contact forces as well as non-bonded attractive inter-particle forces due to van der Waals interactions. From our simulations, we obtain a mathematical expression that predicts the angle of repose θ_r of spherical particles as a function of particle size and gravity. We find excellent agreement between predicted and experimentally observed values of θ_r for the investigated values of particle diameter within the broad range between 30 μm and 1 cm. Moreover, our results shed new light into experimental observations of the angle of repose on Mars and other extra-terrestrial environments.

DY 56.12 Thu 15:00 P1A

Coexistence of fixed and active dunes from numerical simulations — Maria Determann and •Eric Josef Ribeiro Parteli — Department of Geosciences, University of Cologne

The side-by-side coexistence of fixed and active Aeolian dunes in many environmental settings of the Earth defies our understanding of dune mobility as proxy for regional climate and environmental conditions. According to this understanding, fixed dunes prevail if the characteristic vegetation cover growth rate in a given region exceeds twice the rate of surface erosion and deposition processes caused by Aeolian transport, while dunes are predicted active otherwise. Here we show, by means of numerical simulations, that coexistence between stabilized and active dunes can be explained by climate-driven oscillations in atmospheric forcing relative to stabilizing vegetation growth conditions. The underlying factor for this co-existence is the hysteresis in the stabilization process of Aeolian dunes, i.e., much stronger winds are needed to reactivate fixed dunes than the ones required to stabilize them. Our simulations reproduce regional patterns of coexisting fixed and active dunes occurring under seasonal oscillation of rainfall and wind power, without requirement of any assumption on spatial heterogeneities in soil fertitility.

DY 56.13 Thu 15:00 P1A

Athermal Jamming for particles with exponentially decreasing repulsions — •Nicolas Wohlleben and Michael Schmiedeberg — Institut für Theoretische Physik I, FAU Erlangen-Nürnberg, Germany

We study the jamming of a colloidal system where the particles interact according to a Yukawa potential, i.e., the repulsion decreases exponentially with the distance as expected for screened Coulomb interactions of charged colloids in solution. The decay occurs on a length scale given by the screening length and in addition we consider a cutoff length where the potential is set to zero in a smooth way as often used in simulation.

By determining the athermal jamming transition by trying to remove overlaps we find that the transition packing fraction only depends on the cutoff length but hardly on the screening length. We also explore the radial distribution function and again confirm the importance of the cutoff length.

The picture that emerges is that the influence of a cutoff length on

athermal jamming is superior to that of the screening length, although the screening length is expected to control the slowdown of the dynamics (i.e., the dynamical glass transition). As a consequence, athermal jamming (as defined by overlaps) and the glass transition obviously are unrelated in the considered system.

DY 56.14 Thu 15:00 P1A

Polybutadiene confined in alumina pore — •Lama Tannoury and Wolfgang Paul — Martin Luther Universität

Several studies concerning 1,4-polyutadiene (PBD) confined between graphite walls have been performed perviously. They have shown that the polymer melts experience, at close distances to the confining walls, a variation in both monomer and chain density. Furthermore, that layer also experiences a change in dynamics incorporated in the slowing down of and an extra process of relaxation. These studies are essential to the comprehension of composite materials made of polymer matrices and inorganic filler particles such as rubber tires. The latter is a composite material filled with nanoparticles. However, since previous research on PBD melts permeated by nano-sized fillers could not reach relaxation time scales accessible by MD simulations, we attempt to study a chemically realistic model of a PBD melt inside alumina and silica pores using the GROMACS package. We aim to enhance our view concerning bulk relaxation processes and any modifications they experience due to confinement.

DY 57: Poster: Statistical Physics; Critical Phenomena; Stochastic Thermodynamics; Extreme Events; Data Analytics

Time: Thursday 15:00–18:00 Location: P1C

DY 57.1 Thu 15:00 P1C

Collecting and Analysing Formulas for Non-Linear Response — •Tristan Holsten and Matthias Krüger — Georg-August-Universität, Göttingen, Germany

We study, based on a path integral approach, the non-linear responses of interacting systems perturbed by an external stimulus. To reach a better understanding of such systems, we split the perturbative part of the system's action into its time-symmetric and time-antisymmetric, entropic component. Starting from equilibrium or more general from a steady state, relations and knowledge about the interchangeability of these two components are gathered, by evaluating correlation functions. To obtain these correlation functions, we employ series expansions in the strength of perturbation as well as a time transient approach.

DY 57.2 Thu 15:00 P1C

Haldane Insulator in the 1D Nearest-Neighbor Extended Bose-Hubbard Model with a Cavity-Mediated Long-Range Interaction — •Johannes Sicks and Heiko Rieger — Theoretical Physics, Saarland University, Campus E2.6, 66123 Saarbrücken, Germany

In the one-dimensional Bose-Hubbard model with on-site and nearest-neighbor interactions, a gapped phase characterized by an exotic non-local order parameter emerges, the Haldane insulator. Bose-Hubbard models with cavity-mediated global range interactions display phase diagrams, which are very similar to those with nearest neighbor repulsive interactions, but the Haldane phase remains elusive there. Here we study the one-dimensional Bose-Hubbard model with nearest-neighbor and cavity-mediated global-range interactions and scrutinize the existence of a Haldane Insulator phase. With the help of extensive quantum Monte-Carlo simulations, we find that in the Bose-Hubbard model with only cavity-mediated global-range interactions no Haldane phase exists. For a combination of both interactions, the Haldane Insulator phase shrinks rapidly with increasing strength of the cavity-mediated global-range interactions. Thus, in spite of the otherwise very similar behavior, the mean-field like cavity-mediated interactions strongly suppress the non-local order favored by nearest neighbor repulsion in some regions of the phase diagram.

DY 57.3 Thu 15:00 P1C

Large deviations of far-from-equilibrium RNA hairpin work processes — •Peter Werner and Alexander K. Hartmann — Institut für Physik, Carl von Ossietzky Universität Oldenburg

We investigate numerically [1] the work distribution $P(W)$ of a driven unfolding and folding process of secondary structures for simple RNA hairpins [2] of varying sizes. For the simulation of the RNA dynamics, we use a standard Monte Carlo (MC) method with creation and removal of pairs in the secondary structure. We control these MC simulations by a large deviation technique [3] to reach rare realizations of work values, similar to a previous publication [4] on the work distribution of the Ising model. This allows us to reach very small probabilities as small as 10^{-100} and to apply the Jarzynski relation and to confirm the validity of Crooks' theorem for processes far from thermal equilibrium. Furthermore, by directly sampling RNA secondary structures in equilibrium, we calculate the overlap between the equilibrium structures and non-equilibrium ones which allows us to further characterize the rare events.

[1] A.K. Hartmann, *Big Practical Guide to Computer Simulations* (World Scientific, 2015).
[2] D. Collin, F. Ritort, C. Jarzynski, S.B. Smith, I. Tinoco and C. Bustamante, Nature, vol. 437, 231-234, 2005.
[3] A.K. Hartmann, Phys. Rev. E **65**, 056102 (2002).
[4] A.K. Hartmann, Phys. Rev. E **89**, 052103 (2014).

DY 57.4 Thu 15:00 P1C

Many-body Invariants for One-Dimensional Gapped Fermions with Anti-Unitary Symmetry — •Lorenz Mayer and Martin R. Zirnbauer — Universität zu Köln, Institut für theoretische Physik

Following a proposal by S. Ryu, an invariant of ground states of topological insulators and superconductors will be defined and subsequently calculated for fermionic matrix product states (fMPS). This invariant is expressed in terms of the many-body wave-function.

As the calculation rests only on very coarse features of the formalism, this thus is suitable to tighten classification results obtained within the formalism of fMPS, which are of a more algebraic nature.

DY 57.5 Thu 15:00 P1C

Segregation Phenomena of driven Model Colloids in two-dimensional confined Geometries — •Marc Isele, Kay Hofmann, Tobias Vater, Ullrich Siems, and Peter Nielaba — Universität, Konstanz, Deutschland

Brownian dynamics simulations were employed to investigate the segregation phenomena of driven model colloids in two-dimensional confined geometries. The interactions between the colloids were calculated with a repulsive screened Coulomb potential. In the first part, two sorts of spherical particles of different sizes were driven in the same direction. This setting was created since the corresponding experimental setups are supposedly easier to prepare than oppositely driven particles. A segregation occurred that is similar to the lane formation of oppositely driven colloids. In a second setup, a closer look was taken at oppositely driven particles in circular channels. Here, not only lane formation was observed but also a previously unknown effect of bands forming perpendicularly to the channel walls.

DY 57.6 Thu 15:00 P1C

Capturing large fluctuations in the dynamics of biochemical reaction networks — •Maximilian Kurjahn[1], Ander Movilla[2], and Peter Sollich[1,2] — [1]University of Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany — [2]Department of Mathematics, King's College London, Strand, London WC2R 2LS, UK

Biological systems such as gene expression and metabolism can often be described by chemical reaction networks. Their dynamics is governed by a chemical master equation that cannot be solved analytically, so approximations are necessary. Standard approaches such as the linear noise approximation predict Gaussian fluctuations into the unphysical regime of negative concentrations, particularly when small mean molecule numbers lead to large fluctuations.

We present an alternative approach that works with Poisson fluctuations and is based on a Doi-Peliti coherent state path integral representation of the dynamics. To this we apply the Plefka expansion, a systematic approximation technique from the physics of glasses.

Up to first order the standard mass action kinetics are recovered that describe the dynamics for large molecule numbers. An accurate description in the large fluctuation regime of low copy numbers is obtained by a second order Plefka expansion. The method can be taken further by constraining as order parameters not just first moments but also second moments, i.e. time correlations.

We demonstrate the approach on simple but paradigmatic reaction networks from systems biology, comparing with the results of mass action kinetics and full stochastic simulations.

DY 57.7 Thu 15:00 P1C

Machine Learning the Anderson Transition — Djénabou Bayo[1], •Andreas Honecker[1], and Rudolf Römer[1,2] — [1]Université de Cergy-Pontoise, LPTM (UMR8089 of CNRS) , F-95302 Cergy-Pontoise, France — [2]University of Warwick, Coventry, CV4 7AL, United Kingdom

The Anderson metal-insulator transition (MIT) is characterized by a transition from a delocalized to a localized state in presence of high disorder. This phenomenon has been investigated for many years and numerical studies have given valuable insight through the determination of the critical properties of the localization length, for example. Machine Learning (ML) and Deep Learning (DL) techniques are still relatively new methods when applied to physics. Recent work shows that ML/DL techniques allow to detect quantum phase transitions directly from images of computed quantum states. The 3D Anderson model is a good candidate for this kind of analysis because of relatively easy access to its quantum states close to the MIT. Here, we implement ML/DL techniques to identify the MIT and to characterize its universal properties. We employ a standard image classification strategy with a multi-layered convolutional neural network. Common ML/DL libraries such as Keras, TensorFlow and FastAI are used in our implementation. We find that a classification by disorder and a reconstructing of the phase diagram appear possible.

DY 57.8 Thu 15:00 P1C

Subharmonic oscillations in stochastic systems under periodic driving — •Lukas Oberreiter[1], Andre Cardoso Barato[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Department of Physics, University of Houston, Houston, Texas 77204, USA

Subharmonic response is a well-known phenomenon in, e.g., deterministic nonlinear dynamical systems. We investigate the conditions under which such subharmonic oscillations can persist for a long time in open systems with stochastic dynamics due to thermal fluctuations. In contrast to stochastic autonomous systems in a stationary state, for which the number of coherent oscillations is fundamentally bounded by the number of states in the underlying network [1], we demonstrate that in periodically driven systems, subharmonic oscillations can in principle remain coherent forever, even in networks with a small number of states [2]. We also show that, *inter alia*, the thermodynamic cost rises only logarithmically with the number of coherent oscillations in a model calculation. By interpreting our finite state model as a single subharmonically oscillating spin, we can construct an interacting spin system, which above a critical coupling strength subharmonically oscillates in synchrony.

[1] A. C. Barato and U. Seifert *Phys. Rev. E* **95**, 062409, (2017)
[2] L. Oberreiter, U. Seifert, and A. C. Barato *Phys. Rev. E* **100**, 012135, (2019)

DY 57.9 Thu 15:00 P1C

Long-range correlated bonds for the two-dimensional Ising spin glass: is there an ordered phase? — •Lambert Muenster, Christoph Norrenbrock, and Alexander K. Hartmann — Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, Oldenburg (Germany)

The standard short-range two-dimensional Ising spin glass does not exhibit an ordered low-temperature phase [1]. Motivated by work that was done on the random field Ising magnet [2] we investigate the two-dimensional Ising spin glass model with long-range spatially correlated bonds. The bonds are drawn from a a standard normal distribution with a two point correlation for bond-distance r that decays as $1/(r+1)^a$, $a > 0$. Whether there exists an ordered low-temperature phase is investigated via the scaling of domain wall exitations from the ground state that are induced to the system by applying different boundary conditions. By utilizing the Kasteleyn city approach [3] to numerically calculate the ground states and corresponding excited states, systems sizes up to $N = 724^2$ spins were studied.

Our results indicate that the correlation do not inflict a global ordered spin-glass phase at finite temperature.

[1] A.K. Hartmann and A.P. Young, Phys. Rev. B. **64**, 180404 (2001).
[2] B. Ahrens and A.K. Hartmann, Phys. Rev. B. **84** 144202 (2011).
[3] Creighton K. Thomas and A. Alan Middleton, Phys. Rev. B. **76**, 220406(R) (2007).

DY 57.10 Thu 15:00 P1C

Theoretical study the heat rectification via a superconducting artificial atom — •Meng Xu, Juergen Stockburger, and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, University of Ulm, 89069 Ulm, Germany

Rectification of heat transfer at nanoscales have received increasing attention in theoretical and experimental fields. Here, We theoretically studied the heat rectification via a superconducting artificial atom where a superconducting transmon qubit coupled to two strongly unequal resonators terminated by mesoscopic heat baths. In the simulations, we have combined Hierarchical equations of motion (HEOM) and tensor network (TN) methods to efficiently study this complex system dynamics.

DY 57.11 Thu 15:00 P1C

Escape from Metastable States Driven by Asymmetric Non-Gaussian Noise — •Daniel Pflüger[1], Adrian Baule[2], and Peter Sollich[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Deutschland — [2]School of Mathematical Sciences, Queen Mary University of London, United Kingdom

The escape of Brownian particles trapped in a metastable state was originally investigated by Kramers and finds numerous applications, e.g. in the Arrhenius rate formula for chemical reactions. The underlying assumption is that the escape process is driven by Gaussian white noise. For particles in granular gases or solutions of bacterial swimmers this is no longer appropriate. We therefore consider the problem of escape from a metastable state driven by the most general kind of noise process that is stationary and uncorrelated in time. Such a noise process is a combination of Gaussian white noise and Poissonian shot noise with an arbitrary amplitude distribution. We show that an analogue of Kramers' low-temperature limit can be constructed, and use this to investigate the effect of the noise statistics on the transition rates; these can be exponentially larger than in the Gaussian case. We focus in particular on the effects of asymmetry in the noise amplitude distribution, generalizing earlier work on one-side exponential noise. We also investigate applications to systems with multiple reaction coordinates, where the selection of the most likely transition path can become dependent on the noise statistics.

DY 57.12 Thu 15:00 P1C

Clarifying the Case of Zero - Temperature Coarsening — •Denis Gessert, Henrik Christiansen, and Wolfhard Janke — Institut für Theoretische Physik, Leipzig University, Germany

For coarsening to any temperature below the critical temperature of the non-conserved Ising model exponent 1/2. For the last 30 years, also including very recent work, it was not possible to clearly perform nonequilibrium simulations on GPUs with more than 1 billion spins, allowing us to finally in three spatial dimensions theory predicts a power-law growth of domains of like spins with observe this growth-law when the quench temperature was set to absolute zero. We here beyond question confirm the theory.

DY 57.13 Thu 15:00 P1C

Impurity-induced Wavefunction Scarring on curved surfaces — •Michael Kraus, Dominik Schulz, and Jamal Berakdar — Martin-Luther Universität Halle-Wittenberg, Halle (Saale), Germany

Quantum Scarring is a phenomenom where Eigenstates of a quantum chaotic system show enhanced probability along short periodic orbits. Recently, it has been shown that strong scarring occurs by perturbing quantum oscillator systems with localized impurities. [2] Among others, magnetic fields, impurity strength and their positioning can be used to control Scars. [3] Moreover, this effect is accompanied by very efficient wave-packet dynamics which opens the possibility for useful quantum-transport applications. In this work we address the influence of curvature (systems like cylinders and tori) by using the thin-layer approximation and additionally introduce Rashba-type spin-orbit coupling along the surface.

[1] E. Heller, Phys. Rev. Let. 53, (1984); [2] P. Luukko, et al., Sci. Rep. 6, 37656 (2016); [3] J. Keski-Rahkonen, et al., Phys. Rev. B

96, 094204 (2017);

DY 57.14 Thu 15:00 P1C

CFD simulation of the wind field over a terrain with sand fences: Critical spacing for the wind shear velocity — Izael Araújo Lima[1], •Eric Josef Ribeiro Parteli[2], Yaping Shao[2], José Soares Andrade Jr.[1], Hans Jürgen Herrmann[1,3], and Ascânio Dias Araújo[1] — [1]Departamento de Física, Universidade Federal do Ceará, Fortaleza, Brazil — [2]Department Geowissenschaften, Universität zu Köln, Cologne, Germany — [3]PMMH, ESPCI Paris, France

Sand fences are often erected to reduce wind speed and prevent aeolian soil erosion. However, the search for the most efficient array of fences by means of field experiments alone poses a challenging task. Here we apply Computational Fluid Dynamic simulations to investigate the three-dimensional structure of the turbulent wind field over an array of fences. We find that the area of soil associated with wind shear velocity values smaller than the minimal threshold for sand transport has two regimes, depending on the spacing L_x between the fences. When L_x is smaller than a critical value L_{xc}, the wake zones associated with each fence are inter-connected (regime A), while these wake zones appear separated from each other (regime B) when L_x exceeds this critical value of spacing. The system undergoes a second order phase transition at $L_x = L_{xc}$, with the cross-wind width of the protected zone scaling with $[1 - L_x/L_{xc}]^\beta$ in regime A, with $\beta \approx 0.32$. Our findings have implication for a better understanding of aeolian transport in the presence of sand fences, as well as to develop optimization strategies for anti-desertification measures.

DY 57.15 Thu 15:00 P1C

Graph properties of metabolic networks reveals optimization for self-preservation — •Máté Józsa and Zsolt Iosif Lázár — Babeş-Bolyai University, Cluj-Napoca, Romania

Exploring the properties of living systems is a common topic for most fields of sciences, yet there is no comprehensive theory, that describes the most basic elements. In our search for the fundamental properties of life forms, we studied the topology of metabolic networks of thousands of organisms using carefully randomized counterparts as null model. In order to identify metabolism specific graph properties the same procedure was carried out also on other types of real networks. The discovered and quantified patterns may be the corner stones of any biochemical network of living systems: fast dynamics of the chemical processes, and optimal transport, that is, efficient distribution of chemical elements over the network. The stability of these properties, that is, resistance to network failures due to environmental effects also appears to be optimized in metabolic networks. The results suggest that modularity might arise as a consequence of these simultaneous optimizations.

DY 57.16 Thu 15:00 P1C

Immune Repertoire Dynamics across the Human Lifespan — •Mario Udo Gaimann[1,2], Jonathan Desponds[3], and Andreas Mayer[1] — [1]Lewis-Sigler Institute for Integrative Genomics, Princeton University — [2]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, LMU Munich — [3]NSF-Simons Center for Quantitative Biology, Northwestern University

Adaptive immunity relies on the dynamics of cells with specific receptors. The number of cells with the same receptor, the clone size, is known to be remarkably varied. However, the dynamical processes shaping this broad distribution remain poorly understood. Here, we develop a mathematical theory of T cell dynamics across the human lifespan compatible with statistical laws revealed by immune repertoire sequencing. We demonstrate that the frequency of large clones follows power-law scaling with a reproducible exponent across cohorts that is largely independent of age. We explain the early onset of scaling through a model for the establishment of the immune memory repertoire in infancy. We then derive predictions for how fast fluctuating selection allows later recruited clones to replace those founded early and compare them to experimental observations. We find a long-lived incumbency effect suggesting that ongoing selection only slowly reshapes the initial hierarchy of clone sizes. Together, our work provides a mechanism for how dynamical processes in infancy can have a large and long-lasting influence on the adaptive immune system with implications for pathogen defense and autoimmunity.

DY 57.17 Thu 15:00 P1C

Feedback in optical microcavity arrays — •Rebecca Cizek, Jakob Kreismann, and Martina Hentschel — TU Ilmenau, Ilmenau, Germany

Arrays of coupled optical microcavities are a rich and interesting model system with a big potential for applications [1]. Their functionality relies on the mutual coupling between the individual mircoresonators. Here, we study in detail how the coupling between two asymmetric optical microresonators depends on their geometric properties like distance, orientation, cavity size and resonance detuning based on numerical wave simulations using the FDTD package MEEP. In particular, we characterize the robustness of coupling and feedback in detuned cavities that is of special importance for applications where detuning can result from fabrication imperfections.

[1] J. Kreismann, J. Kim, M. Bosch, M. Hein, S. Sinzinger, and M. Hentschel, Superdirectional light emission and emission reversal from microcavity arrays, Phys. Rev. Research 1, 033171 (2019).

DY 57.18 Thu 15:00 P1C

Ray-wave correspondence in graphene billiards with sources — •Jule Katharina Schrepfer[1], Ming-Hao Liu[2], Klaus Richter[3], and Martina Hentschel[1] — [1]TU Ilmenau, Ilmenau, Germany — [2]National Cheng Kung University, Tainan, China — [3]Universität Regensburg, Regensburg, Germany

Graphene billiards are cavities for pseudo-relativistic electrons where trapping is modified by Klein tunneling. There are similarities to optical billiards that have proven to be an interesting model system for quantum chaos in open systems. However, the possibility to tune the effective refractive index of graphene billiards by means of gate voltages makes their study particularly interesting. In the presence of sources, properly tuned gate voltages lead a distinct lensing effect that collimates electrons in a narrow area near the graphene billiard. This lensing effect is seen both in wave simulations and ray modelling with a nice correspondence throughout the midfield of the graphene cavity. The position of the focal area can be controlled not only via the source position but also via gate voltages.

DY 58: Poster: Nonlinear Dynamics; Pattern Formation; Networks; Delay Systems; Synchronization

Time: Thursday 15:00–18:00 Location: P1C

DY 58.1 Thu 15:00 P1C

Studying free energy landscapes of peptides with neural networks — •Simon Lemcke and Thomas Speck — Institute of Physics, Mainz , Germany

Molecular dynamics simulations generate high dimensional data. A recurrent challenge in computational sciences is to perform a dimensionality reduction and to identify the relevant collective variables. Here we employ EncoderMap, which is a variational autoencoder type of neural network, to perform a structure-based reduction to a low-dimensional latent space for a short peptide. We then investigate the suitability of this latent space as collective variables in terms of the free energy and the conformational dynamics.

DY 58.2 Thu 15:00 P1C

Interaction of topological localized states in excitable delayed systems — •Florian Eckel[1], Leon Munsberg[1], Julien Javaloyes[2], and Svetlana Gurevich[1] — [1]Institut fuer theoretische Physik (WWU), Muenster, Germany — [2]Universitat de les Illes Balears, Palma, Spain

We are interested in the dynamics of topological localized states (LSs) in a injection-locked semiconductor laser with a delayed feedback loop. Instead of a depth model describing the time evolution of the electrical field and carriers, a simple delayed Adler equation for the phase of the field can be derived. We explore the interaction between LSs in the delayed Adler equation and show an intricate non-reciprocal behavior.

Furthermore, we derive a reduced model for the motion of the centers of the interacting LSs and compare it to the results obtained by direct numerical simulations.

DY 58.3 Thu 15:00 P1C

Influence of time-delayed feedback on the dynamics of temporal localised structures in a passively mode-locked semiconductor laser — •Thomas Seidel[1], Julien Javaloyes[2], and Svetlana Gurevich[1,3] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Straße 9, 48149 Münster, Germany — [2]Departament de Física, Universitat de les Illes Balears, Carretera Valldemossa km 7.5, 07122 Palma, Spain — [3]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstraße 2, 48149 Münster, Germany

We are interested in the influence of the time-delayed optical feedback in the dynamics of temporal localised structures (LSs) in the output of a semiconductor laser with saturable absorber. We use a delayed differential equation model for a ring geometry where the gain medium is coupled to a saturable absorber and a narrow band optical filter. Using a combination of direct time simulations and path-continuation methods we shall show that the presence of feedback can lead to a number of interesting regimes including the generation of satellite trains on the LS's side or can induce a coherence between LSs.

DY 58.4 Thu 15:00 P1C

Dynamic phases of magnetic gears — •Stefan Hartung and Ingo Rehberg — Universität Bayreuth

We investigate the coupling of two rotating spherical magnets experimentally. Geometries in which the driven magnet is phase-locked to the driving one are so-called cogging free couplings [1]. We find that deviations from this arrangement as well as an increasing driving frequency lead towards different kinds of more complex dynamical behavior. The experimental results are compared to a model based on pure dipole-dipole interaction and are summarized in a phase diagram that gives insight into the possibilities of technical implementation of these kinds of couplings.

[1] Exploring cogging free magnetic gears; Stefan Borgers, Simeon Völkel, Wolfgang Schöpf, and Ingo Rehberg; American Journal of Physics 86, 460 (2018); https://doi.org/10.1119/1.5029823.

DY 58.5 Thu 15:00 P1C

Ultrafast soliton interaction via Raman scattering — •Alexandra Völkel and Georg Herink — Experimental Physics VIII, University Bayreuth, Germany

Recent real-time studies revealed interactions of ultrashort soliton pulses in a femtosecond oscillator., i.e. bound states at discrete temporal binding separations [1]. We investigate the impact of the non-instantaneous nonlinear response of the laser gain medium onto the interpulse dynamic coupling. Specifically, we analyze the contribution of coherent phonons driven by impulsive Raman scattering. Employing a sensitive pump-probe scheme, we characterize the response of the nonlinear refractive index in the time domain and discuss the coupling process.

[1] Herink et al., Real-time spectral interferometry probes the internal dynamics of femtosecond soliton molecules. Science, 356 (2017)

DY 58.6 Thu 15:00 P1C

Measuring the relative importance of network constituents: A perturbation-based approach — •Timo Bröhl[1,2] and Klaus Lehnertz[1,2,3] — [1]Dept. of Epileptology, University of Bonn, Bonn, Germany — [2]Helmholtz Institute for Radiation and Nuclear Physics, University of Bonn, Bonn, Germany — [3]Interdisciplinary Center for Complex Systems, University of Bonn, Bonn, Germany

Investigating complex dynamical systems with methods from network theory has become a prominent approach in diverse areas of science, ranging from physics to the neurosciences. The powerful framework of graph theory allows characterization of a network ranging from to global to the local scale. We investigate the impact of small network perturbations on importance of network constituents (nodes and edges) as accessed with various centrality concepts. Three types of perturbations are applied on the edge level of paradigmatic network topologies with varying sizes and edge densities. Results indicate a close relationship between characteristics of the applied perturbations and the importance ranking of both nodes and edges. This relationship however differs for different network topologies and depends on the applied centrality concept. Our perturbation-based approach may be advantageous to identify spurious or salient edges in networks derived from empirical data.

(This work was supported by the Deutsche Forschungsgemeinschaft; Grant No. LE660/7-1)

DY 58.7 Thu 15:00 P1C

Hidden Markov dynamics of the chaotic diffusion of dissipative solitons — •Tony Albers[1], Jaime Cisternas[2], and Günter Radons[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Facultad de Ingeniería y Ciencias Aplicadas, Universidad de los Andes, Santiago, Chile

Dissipative solitons are persistent localized solutions which are the result of a complicated balance between dispersion and nonlinear effects as well as dissipation and energy gain. These structures can show interesting dynamical behaviors such as explosions, i.e., transient enlargements of the solitons that lead to spatial displacements if the explosions are asymmetric. Due to the chaotic nature of the underlying soliton dynamics, the sequence of spatial jumps as well as the inter-explosion times seem to be random thus leading to a random-walk kind of motion [1]. In this contribution, we show that the sequence of spatial shifts of exploding dissipative solitons in a prototypical complex Ginzburg-Landau equation, known, e.g., from nonlinear optics, is governed by a hidden Markov process with continuous output densities. It captures the non-trivial decay of correlations of jump widths and symbol sequences representing the soliton motion, the statistics of anti-persistent walk episodes and the multimodal density of the jump widths. This is the first example of a physically meaningful reduction of an infinite-dimensional deterministic dynamics to one of a probabilistic finite state machine.

[1] Tony Albers, Jaime Cisternas and Günter Radons, New J. Phys. **21** 103034 (2019)

DY 58.8 Thu 15:00 P1C

Learning in Simple Heteroclinic Networks — •Maximilian Voit and Hildegard Meyer-Ortmanns — Jacobs University Bremen, Bremen, Deutschland

Heteroclinic networks provide a promising candidate attractor to generate reproducible sequential series of metastable states. From an engineering point of view it is known how to construct heteroclinic networks to achieve certain dynamics, but a data based approach for the inference of heteroclinic dynamics is still missing. We present a method by which a template system dynamically learns to mimic an input sequence of metastable states. For this purpose, the template is unidirectionally, linearly coupled to the input. At the same time, the learning dynamics causes an adaptation of the eigenvalues of the template in order to minimize the difference of template dynamics and input sequence. Thus, after the learning procedure, the trained template constitutes a model with dynamics that are most similar to the training data. We demonstrate the capabilities and possible difficulties of this method at different examples. Our approach may be applied to infer the topology and the connection strength of a heteroclinic network from data in a dynamic fashion and may serve as a model for learning in the context of winnerless competition.

DY 58.9 Thu 15:00 P1C

Simulating nano-particle networks to solve classification problems — •Marlon Becker[1], Bram de Wilde[2], Wilfred van der Wiel[2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster — [2]Faculty of EEMCS, CTIT and MESA+ Institutes for ICT Research and Nanotechnology, University of Twente

The use of Artificial Neural Networks to solve various problems is a method of rapidly growing interest in nearly all fields of modern science. Instead of simulating Neural Networks, neuromorphic computing attempts to directly build hardware structures that can be utilized for sophisticated tasks. Recently promising experimental work was published (Classification with a disordered dopant atom network in silicon (2019), Nature (in press)) that is based on nano-particle networks (such as boron doped silicon semiconductors or gold nano-particles) to solve various classification problems, including the linearly inseparable XOR and XNOR gate. To control the desired functionality, external voltages are applied to the devices. In this work different approaches to simulate these neuromorphic networks in physical models are provided. By defining fitness functions, energy-like landscapes as a function of the external voltages are obtained. Different methods to find minima of these landscapes in which the desired functionalities can be found are investigated. To further optimize the experimental devices, gen-

eral scaling behavior as well as the system scale necessary to reach the desired functionality is analyzed.

DY 58.10 Thu 15:00 P1C

Detection of defects in soft quasicrystals with neural networks — •Ali Döner and Michael Schmiedeberg — Institut für Theoretische Physik I, FAU Erlangen-Nürnberg, Germany

The aim of this work is to employ a neural network for the detection of defects in quasicystalline patterns. Quasircrystals are aperiodic, but they exhibit a longe-range order and in principle can possess any discrete rotational symmetry. We consider quasicrystalline patterns with dodecagonal symmetry as they occur most often in soft matter systems. Our goal is to detect the positions of dislocations as well as their Burgers vector. Our training as well as test data sets consist of calculated patterns with one randomly placed dislocation with one out of six distinguishable Burgers vectors. Our trained neural network is able to recognize the type of the Burgers vector perfectly. The position of the dislocation is recognized up to a mean deviation from the real position of about 0.13 of 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 58.11 Thu 15:00 P1C

Adaptively coupled phase oscillators with discontinuous plasticity rule — •Sören Christian Nagel[1], Rico Berner[1], Eckehard Schöll[1], and Serhiy Yanchuk[2] — [1]Institut für theoretische Physik TU Berlin, Berlin, Germany — [2]Institut für Mathematik TU Berlin, Berlin, Germany

Memory and the development of neuronal populations have been widely studied using discontinuous forms of spike timing-dependent synaptic plasticity (STDP). Despite the acceptance of these approaches in the field of neuroscience, very little is known about the dynamical features that are provided by the discontinuities.

For this purpose, we study a system of two coupled phase oscillators with STDP. Our analysis reveals various dynamical scenarios, namely, the appearance of a generalized fixed point as the source of in-phase synchrony, different types of limit cycles, and unexpected bifurcations due to the discontinuous STDP.

DY 58.12 Thu 15:00 P1C

Data-driven identification of sparsely observed stochastic systems — •Dimitra Maoutsa and Manfred Opper — Technical University of Berlin, Berlin, Germany

Stochastic differential equations naturally occur in many fields in science and engineering, arising often as descriptions of systems with unresolved fast degrees of freedom. Usually, the underlying deterministic dynamics (i.e. drift function) and complete path trajectories of such systems are unknown, but instead we only have discrete time state observations at hand. Existing inference methods for such systems, either consider detailed parametric drift models, or assume densely observed trajectories for non-parametric Gaussian process drift estimation. Here, we present a data-driven approach for recovering nonlinear stochastic systems from sparse state observations. By introducing a novel method for simulating stochastic bridges consistent with the observed time series state space structure, we effectively create dense sample paths required for non-parametric drift estimation. We illustrate the power of our method on a number of simulated canonical dynamical systems, demonstrating thereby its potential and accuracy compared to existing frameworks.

DY 58.13 Thu 15:00 P1C

Isospectral reductions and pretty good state transfer — Malte Röntgen[1], Nikolaos Palaiodimopoulos[2], •Christian Morfonios[1], Ioannis Brouzos[2], Maxim Pyzh[1], Fotios Diakonos[2], and Peter Schmelcher[1] — [1]Centre for Optical Quantum Technologies, University of Hamburg — [2]Department of Physics, University of Athens

Pretty good state transfer (PGST) denotes the transfer of a single site excitation with fidelity arbitrarily close to unity at a finite transfer time in a network system. It was recently shown that PGST generally arises in a network under certain conditions on its characteristic polynomial factors corresponding to eigenvectors with opposite parity on the input and target sites. We here combine this result with isospectral reductions of networks over site pairs, exploiting a dimensionally reduced form of the associated Hamiltonians to facilitate the design of PGST. We present a variety of setups thus made to support PGST and further show how, relying on the concept of compact localized states, the obtained networks can be additionally equipped with storage of input and target states.

DY 58.14 Thu 15:00 P1C

An MCMC method to determine Complex Network properties — •Oskar Pfeffer — Potsdam Institute for Climate Impact Research

We apply the Markov Chain Monte Carlo (MCMC) algorithm Metropolis Hastings to sample graphs with specific properties. The generated networks are analysed using the measures of clustering and characteristic length that are used in literature to detect small world graphs. We show that optimizing these measures in a graph do not produce typical small world graphs.

DY 58.15 Thu 15:00 P1C

Formulation of Voltage Dynamics in Complex Quantities — •Hannes Vogel[1,3] and Frank Hellmann[2] — [1]Humboldt-Universität zu Berlin, Berlin, Germany — [2]Potsdam-Institut für Klimafolgenforschung, Potsdam, Germany — [3]Stockholm University, Stockholm, Sweden

Understanding the stability of voltage dynamics in power grids is essential to the development of decentralized power networks for renewable energy sources. Current voltage dynamics models are motivated either by physics or control theory. We aim to formulate the power grid dynamics in terms of complex voltages, which combine the dynamics of rotor angle, frequency and voltage amplitude. To get a better overview of the properties of different models and to find criteria for classification, a common general formulation is needed. Indeed, such a formulation is obtained by writing the differential equations in a complex power series. Therefore the mathematical structure of the Stuart-Landau equation functions as a prototype.

DY 59: Mitgliederversammlung

1. Report of chairmen
2. Discussion about future activities
3. Elections
4. Announcements, miscellaneous

Time: Thursday 18:15–19:15 Location: ZEU 160

Duration: 60 min.

DY 60: Data analytics for dynamical systems II (Focus Session joint with DY and BP) (joint session SOE/CPP/DY)

Time: Friday 9:30–10:00 Location: GÖR 226

DY 60.1 Fri 9:30 GÖR 226

A Variational Perturbative Approach to Graph-based Multi-Agent Systems — •Dominik Linzner, Michael Schmidt, and Heinz Koeppl — TU Darmstadt, Germany

Understanding the behavior of multiple agents is a difficult task with numerous applications in the natural and social sciences. However, the number of possible configurations of such systems scales exponentially in the number of agents leaving many queries intractable – even if limiting interactions to a static interaction graph.

Variational approaches pave a principled way towards approximations of intractable distributions. Here, traditional approaches focus on directly constraining the class of variational distributions, e.g. in naïve mean-field statistical independence of all random variates is assumed. Variational perturbation theory (VPT) offers a different approach. Here, the similarity measure itself is approximated via a series expansion. A prominent example of this approach is Plefka's expansion [1,2]. The central assumption is that variables are only weakly coupled, i.e. the interaction of variables is scaled in some small perturbation parameter.

We derive a novel VPT for stochastic dynamics on static interaction graphs and use it to develop methods for different (inverse) problems such as system identification from data or optimal planning of coordination tasks.

[1] Plefka, T. (1982). Journal of Physics A, 15, 1971-1978. [2] Bachschmid-Romano et al. (2016). Journal of Physics A: Mathematical and Theoretical, 49(43), 434003-434033.

DY 60.2 Fri 9:45 GÖR 226

A differentiable programming method for quantum control — •Frank Schäfer, Michal Kloc, Christoph Bruder, and Niels Lörch — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Precise control of quantum systems is highly desirable in many current experimental setups and quantum information technologies. In quantum control, by optimization of control pulse sequences, protocols that maximize a case-specific figure of merit are obtained. To solve quantum state control problems, we treat (closed) quantum systems as differentiable programs. Within a framework that combines machine learning and the knowledge of the differential equations governing the dynamics of the physical system, we employ predictive models for optimal parameter estimation. We analyse the sensitivity of this approach against noise in the initial states and verify the robustness of the method.

DY 61: Invited Talk

Time: Friday 9:30–10:00 Location: HÜL 186

Invited Talk DY 61.1 Fri 9:30 HÜL 186

Characterizing quantum chaos through adiabatic transformations — •Anatoli Polkovnikov[1], Anushya Chandran[1], Pieter Claeys[3], Anatoly Dymarsky[4], Mohit Pandey[1], Tamiro Renzo[1], Dries Sels[2], Sho Sugiura[2], and Jonathan Wurtz[1] — [1]Department of Physics, Boston University — [2]Department of Physics, Harvard University — [3]Cavendish Laboratory at the University of Cambridge — [4]Department of Physics, University of Kentucky

I will discuss our recent progress in understanding and characterizing quantum chaos through the adiabatic gauge potential (AGP). The latter is defined as an operator generating adiabatic transformations. In particular, I will show that these generators are highly anisotropic in the coupling space defining the families of adiabatically connected Hamiltonians implying that chaos is highly directional. I will discuss the structure of the adiabatic flows along the directions with the minimal norm of the AGP and show that these flows have natural attractors corresponding to massively degenerate points. I will also discuss emerging singularities of the AGP and the corresponding many-body dark states, which can live very far from the ground state . Finally I will show that the AGP can serve as a very sensitive probe of quantum chaos.

DY 62: Critical Phenomena and Phase Transitions

Time: Friday 9:30–11:45 Location: ZEU 118

DY 62.1 Fri 9:30 ZEU 118

Quasiparticles as Detector of Topological Quantum Phase Transitions — •Sourav Manna[1], Srivatsa Nagara Srinivasa Prasanna[1], Julia Wildeboer[2], and Anne E. B. Nielsen[1] — [1]Max-Planck-Institut fur Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Department of Physics, Arizona State University, Tempe, AZ 85287, USA

Phases and phase transitions provide an important framework to understand the physics of strongly correlated quantum many-body systems. Topologically ordered phases of matter are particularly challenging in this context, because they are characterized by long-range entanglement and go beyond the Landau-Ginzburg theory. A few tools have been developed to study topological phase transitions, but the needed computations are generally demanding, they typically require the system to have particular boundary conditions, and they often provide only partial information. There is hence a high demand for developing further probes. Here, we propose to use the study of quasiparticle properties to detect phase transitions. Topologically ordered states support anyonic quasiparticles with special braiding properties and fractional charge. Being able to generate a given type of anyons in a system is a direct method to detect the topology, and the approach is independent from the choice of boundary conditions. We provide three examples, and for all of them we find that it is sufficient to study the anyon charge to detect the phase transition point. This makes the method numerically cheap.

DY 62.2 Fri 9:45 ZEU 118

Critical Exponents of the Ising Model in Three Dimensions with Long-range Correlated Site Disorder — •Stanislav Kazmin[1,2] and Wolfhard Janke[2] — [1]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany — [2]University Leipzig, Institute for Theoretical Physics, Leipzig, Germany

We study the Ising model in three dimensions with site dilution with the help of Monte Carlo techniques. The dilution is long-range correlated and the correlation function decays proportional to a power law $\propto r^{-a}$. We derive the critical exponent of the correlation length ν in dependence of a by combining different defect concentrations $0.1 \leq p_d \leq 0.4$ and by applying finite-size scaling techniques to the derivative of the logarithm of the magnetization $\partial_\beta \ln|m|$. We study a wide range of correlation exponents $1.5 \leq a \leq 3.5$ as well as the uncorrelated case $a = \infty$. Finally, we compare our results to known estimates from other works and to the conjecture of Weinrib and Halperin: $\nu = 2/a$.

DY 62.3 Fri 10:00 ZEU 118

Exchange between two phases of confined water using deuteron two-dimensional exchange NMR — •Verena Fella and Michael Vogel — Institute for Condensed Matter Physics, TU Darmstadt, Germany

Understanding the properties of water in confinement is an impor-

tant task due to its many applications in life science and technology. Nano-confinement reduces the crystallization temperature of water to lower values and enables supercooling to temperatures even below the nucleation temperature. Our previous studies [Yao et al., Langmuir (2019)], [Weigler et al., J. Phys. Chem. B (2019)] identified two dynamically distinguishable fractions of water coexisting within the pores at sufficiently low temperatures. These fractions correspond to a liquid interfacial water layer and a less mobile water phase in the pore center. We conjecture that highly distorted and unstable crystal nuclei exist under extreme confinement that exhibit reorientational dynamics with time scales intermediate to the confined liquid and to bulk ice. This leads to a complex and heterogeneous system inside the pores. One of the still open questions is the potential exchange between both water species and the time scales on which it occurs. Therefore we measure ^{2}H two-dimensional NMR spectra of water in mesoporous silica materials. This method is well suited for heterogeneous systems because it directly probes exchange processes between fast and slow subensembles [Vogel, Rössler, J. Phys. Chem. A (1998)]. By varying the temperature and mixing time of the experiment we determine the time scale of these processes.

DY 62.4 Fri 10:15 ZEU 118

Acceptance rate is a thermodynamic function in local Monte Carlo algorithms — Evgeni Burovski[1], •Wolfhard Janke[2], Maria Guskova[1], and Lev Shchur[1,3] — [1]National Research University Higher School of Economics, 101000 Moscow, Russia — [2]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [3]Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia

We study properties of Markov chain Monte Carlo simulations of classical spin models with local updates. We derive analytic expressions for the mean value of the acceptance rate of single-spin-flip algorithms (Metropolis, heat bath) for the one-dimensional Ising chain with periodic boundary conditions. For the Metropolis algorithm we find that the average acceptance rate is a linear function of energy, independent of the chain length. We further provide numerical results for the energy dependence of the average acceptance rate for the three- and four-state Potts model, and the XY model in one and two spatial dimensions. In all cases, the acceptance rate is an almost linear function of the energy in the critical region. The variance of the acceptance rate is studied as a function of the specific heat. While the specific heat develops a singularity in the vicinity of a phase transition, the variance of the acceptance rate stays finite.

DY 62.5 Fri 10:30 ZEU 118

Lindemann melting criterion in two dimensions — •Sergey Khrapak — Institut fuer Materialphysik im Weltraum, Deutsches Zentrum fuer Luft- und Raumfahrt (DLR), 82234 Wessling, Germany

It is well known that the conventional Lindemann's melting criterion is not applicable to two-dimensional (2D) solids, because long-wavelength density fluctuations cause the mean square displacement to diverge logarithmically with system size. Here it is demonstrated that the Lindemann's criterion can be re-formulated for 2D solids using statistical mechanics arguments. With this formulation the expressions for the melting temperature are essentially equivalent in three and two dimensions. Moreover, in two dimensions the Lindemann's melting criterion practically coincides with the Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young melting condition of dislocation unbinding. Examples of application are provided.

15 min. break.

DY 62.6 Fri 11:00 ZEU 118

Fermionic Criticality Out-of-Equilibrium — •Bernhard Frank — Max-Planck-Institut für Physik komplexer Systeme — Dresden

Critical Fermions, like strange metals, exhibit correlation functions with universal, anomalous power laws, which lead to deviations from Fermi liquid results both for thermodynamic and transport quantities. Coupling a massless bosonic degree of freedom to the Fermi surface provides one mechanism to create these unconventional states of matter that so far have only been studied in thermal equilibrium. However, recent experiments combine semi-conductor devices with optical cavities and therefore mandatorily require a theoretical formulation that takes into account the intrinsically driven-dissipative nature of the photon in order to understand the electronic many-body state. Based on Keldysh quantum field theory we study a simple two-dimensional model for a stange metal out-of-equilibrium. Compared to the situation in the ground state one observes increased decay rates in the low-energy sector of the fermionic spectrum as well as a violation of the thermal fluctuation dissipation relation caused by the enhanced bosonic fluctuations generated by the drive.

DY 62.7 Fri 11:15 ZEU 118

Bond-flip Monte Carlo based on exact results for the square lattice $\pm J$ Ising model — Jan Büddefeld and •Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen

We present preliminary results on a Monte Carlo method with single bond-flip dynamics for the square lattice Ising model with $\pm J$ couplings and arbitrary boundary conditions. Using a recently derived exact expression for the free energy of a system with arbitrary nearest neighbor couplings J_{ij} on the torus, we propose an efficient update scheme for the calculation of the free energy change under a bond flip. We numerically calculate the density of states of the bond ensemble and discuss advantages and disadvantages of the method.

DY 62.8 Fri 11:30 ZEU 118

Detecting hidden and composite orders in layered models via machine learning — •Wojciech Rzadkowski[1], Nicolo Defenu[2], Silvia Chiacchiera[3], Andrea Trombettoni[4], and Giacomo Bighin[1] — [1]Institute of Science and Technology Austria (IST Austria), Am Campus 1, 3400 Klosterneuburg, Austria — [2]Institut für Theoretische Physik, Universität Heidelberg, D-69120 Heidelberg, Germany — [3]Science and Technology Facilities Council (STFC/UKRI), Daresbury Laboratory,Keckwick Lane, Daresbury, Warrington WA44AD, United Kingdom — [4]CNR-IOM DEMOCRITOS Simulation Center, Via Bonomea 265, I-34136 Trieste, Italy

Recently, machine learning is applied to the study of phase diagrams of spin models. After initial success with supervised approaches, unsupervised techniques are being extensively developed.

We use an unsupervised technique to study layered spin models where composite order parameters may emerge as a consequence of the interlayerer coupling. We determine their phase diagram, applying an algorithm based on convolutional neural networks to the raw Monte Carlo data. Remarkably our technique [1] is able to characterize all the system phases also in the case of hidden order parameters, i.e. order parameters whose expression in terms of the microscopic configurations would require additional preprocessing of the data fed to the algorithm.

[1] W. Rzadkowski, N. Defenu, S. Chiacchiera, A. Trombettoni, G. Bighin, arXiv:1907.05417 (2019)

DY 63: Invited Talk

Time: Friday 9:30–10:00 Location: ZEU 160

Invited Talk DY 63.1 Fri 9:30 ZEU 160

Coarse-grained descriptions of models of cell monolayers — •Eric Bertin — LIPhy, Univ. Grenoble Alpes and CNRS, Grenoble, France

Confluent cell monolayers exhibit a rich phenomenology and lie at the core of the field of dense active matter. From a physicist standpoint, cell monolayers may be thought of as two-dimensional dense assemblies of soft, elastic units, driven by different types of active forces or events like motility forces, contractility forces, or cellular division and apoptosis. They thus appear as paradigmatic strongly interacting systems driven far from equilibrium, whose statistical description remains challenging. We discuss here several types of coarse-grained descriptions rooted in the cell-level dynamics. We first derive active continuum elastic descriptions that are well-suited to account for the effects of cell motility or of local contractile forces. Correlated large scale velocity fluctuations resulting from cell motility are favorably compared to experimental results on epithelial cell monolayers. Going

beyond elastic effects, we also discuss how cell division and apoptosis modify, on longer time scales, the non-linear rheology of confluent cell monolayers by contributing to the mechanical noise that fluidizes the system.

DY 64: Wetting and Liquids at Interfaces and Surfaces II (joint session CPP/DY/O)

Time: Friday 9:30–12:15 Location: ZEU 260

Invited Talk DY 64.1 Fri 9:30 ZEU 260

Slide electrification: charging of surfaces by moving water drops — •Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

Water drops sliding over insulating surfaces can lead to surface charging. In contrast to charging caused by friction between two solids, drop slide electrification is largely unexplored. Slide electrification has been consistently reported, but results are difficult to reproduce. One reason for the lack of quantitative understanding is that the deposition of charge is a non-equilibrium effect and depends essentially on microscopic processes at the contact line. We address both the experimental and theoretical sides of this problem. We reproducibly measure the charge gained by water drops sliding down hydrophobic surfaces. To explain these results, we theorize that some fraction of the charge in the Debye layer is transferred to the surface rather than being neutralized as the drop passes. Given that nearly every surface in our lives comes in contact with water, this water-dependent surface charging may be a ubiquitous process that we are only beginning to understand.

DY 64.2 Fri 10:00 ZEU 260

Spreading on viscoelastic solids: Are contact angles selected by Neumann's law? — Mathijs van Gorcum[1], •Stefan Karpitschka[2], Bruno Andreotti[3], and Jacco H. Snoeijer[1] — [1]Physics of Fluid Group, University of Twente, Enschede, Netherlands — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]Laboratoire de Physique Statistique, Univ. Paris-Diderot, Paris, France

The spreading of liquid drops on soft substrates is extremely slow, owing to strong viscoelastic dissipation inside the solid. A detailed understanding of the spreading dynamics has remained elusive, partly owing to the difficulty in quantifying the strong viscoelastic deformations below the contact line that determine the shape of moving wetting ridges. Here we present direct experimental visualizations of the dynamic wetting ridge, complemented with measurements of the liquid contact angle. It is observed that the wetting ridge exhibits a rotation that follows exactly the liquid angle, as was previously hypothesized [Karpitschka et al., Nat. Commun. (2015)]. This experimentally proves that, despite the contact line motion, the wetting ridge is still governed by Neumann's law. Furthermore, our experiments suggest that moving contact lines lead to a variable surface tension of the substrate. We set up a new theory that incorporates the influence of surface strain, the so-called Shuttleworth effect, for soft wetting. It includes a detailed analysis of the boundary conditions at the contact line, complemented by a dissipation analysis, which shows, again, the validity of Neumann's balance.

DY 64.3 Fri 10:15 ZEU 260

Formation of a thin film during drop merging leads to fingering instability — •Peyman Rostami[1,2] and Günter Auernhammer[1,2] — [1]Max Planck Institute for Polymer Research, 55128, Mainz, Germany — [2]Leibniz Institute of Polymer Research, 01069, Dresden, Germany

The coalescence and interaction between two drops have been the subject of intensive studies in recent years [1], due to its wide range of application and the presence in the nature.

Here, we study the merging of partially miscible drop. We deposit drops of different liquids on a substrate. Under appropriate conditions, the merging process generates an instability which resembles the Rayleigh-Plateau instability. If the liquid with higher surface activity is deposited as a second droplet. Its vapor can diffuse through the air and induce a Marangoni flow inside the already deposited droplet. This induced flow can pull a thin liquid layer over the surface , which decays into drops by a Rayleigh-Plateau instability.

We present a detailed study of this instability analyzing the onset of the instability and its characteristic length scales. Finally, a model is presented to explain the Marangoni flow induced by the gas phase. This model is validated by particle tracking.

References [1] S. Karpitschka, C. Hanske, A. Fery, and H. Riegler, Langmuir, vol. 30, no. 23, pp. 6826*6830, 2014.

DY 64.4 Fri 10:30 ZEU 260

Condensation frosting on lubricant impregnated surfaces — •Lukas Hauer[1], Lou Kondic[2], and Doris Vollmer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Mathematical Sciences, NJIT, Newark, USA

In many technical applications the formation of frost and ice displays a hazard to the steady functionality of devices. This motivates the development of new materials to tackle the reduction of icing on surfaces. Understanding the nature of frosting and icing is indispensable to this effort. While icing on surfaces is commonly studied by localized nucleation mechanisms, the formation of frost is comparable more complicated. Condensation frost is characterized by multi-step and multi-physical phenomenon. The formation of condensate droplets, percolation, and frost front propagation is an inherently stochastic process. Despite its ubiquitous nature, a quantitative model for frost growth on surfaces remains elusive. Lubricant impregnated surfaces are known for improved anti-icing properties. They experience lower ice drop adhesion and allegedly delayed surface frosting. We show that frost formation can induce immensely strong capillary forces that could result in surface damage, lubricant depletion and the loss of anti-icing properties. Laser scanning confocal microscopy enabled us to monitor the dynamic lubricant migration during condensation frosting on micro-structured surfaces. We present a model of the lubricant migration, utilizing lubrication theory. This work serves to improve understanding of lubricant dynamic during condensation frosting, providing future roadmaps towards the future design of anti-icing surfaces.

DY 64.5 Fri 10:45 ZEU 260

Dynamics of liquid droplets on switchable prestructured substrates — •Moritz Stieneker[1] and Svetlana Gurevich[1,2] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany — [2]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, D-48149 Münster, Germany

A mesoscopic continuum model is employed to model a thin, liquid film on a substrate with a spatio-temporal wettability. In particular, the effect of a switchable wettability pattern on the structure formation is analyzed for a one-dimensional case with the help of path-continuation techniques and direct numerical time simulations. It is found that if the periodic switching is introduced, the system reaction depends on the ratio between the time scale given by switching and the reaction time of the liquid. The behaviour of the contact angle during the slow and fast switching is investigated in details. Furthermore it is demonstrated that in the case of the slow switching the droplet solutions corresponding to the local minima of the free energy can be stabilized.

DY 64.6 Fri 11:00 ZEU 260

Liquid-liquid phase separation in contact with deformable surfaces — •Hansol Jeon[1,2] and Stefan Karpitschka[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August-Universität Göttingen

The capillary forces of droplets on top of soft solids deform the solid surface into sharp wetting ridges. The amplitude of the wetting ridge is governed by elasto-capillary length, the ratio of liquid surface tension to the solid's shear modulus. Previous experiments on soft wetting used large liquid-vapour surface tensions and thus were in a highly nonlinear regime regarding the response of the solid. This led to debates in the literature regarding the effects of strain dependent solid surface tensions or the dynamics of soft wetting. Liquid interfaces with small surface tensions could instead probe the linear regime of soft wetting and shed new light onto the static and dynamic behaviours of solid surface tension. Thus we investigate the liquid-immersed case of soft wetting, aiming for a control of the liquid and solid surface tensions. We tested various liquid combinations and explored a wide range of

surface tensions and substrate shear moduli, finding valid Neumann constructions in all cases.

15 min. break

DY 64.7 Fri 11:30 ZEU 260

Droplets fighting contamination — •Abhinav Naga, William Wong, Anke Kaltbeitzel, Maria D'Acunzi, Hans-Jürgen Butt, and Doris Vollmer — Max Planck Institute for Polymer Research, Mainz, Germany

Lubricated surfaces are prone to accumulating contaminants due to their sticky yet slippery nature. The presence of contaminants, such as dust and dirt particles, alters their performance. An understanding of the effect of contaminated particles on the friction of surfaces is important not only from a fundamental perspective whereby further insight can be gained of the underlying mechanisms, but also from an applied perspective to predict the effectiveness of lubricated surfaces in the presence of contaminants.

In this study, we systematically contaminate lubricated silicone surfaces (Sylgard 184) and non-lubricated surfaces with spherical glass microparticles. We place a droplet on each surface and measure the force needed to push the droplet at different speeds towards an individual microparticle. We visualise this process with laser scanning confocal microscopy, focusing on the deformation inflicted by the microparticle on the droplet and its lubricant ridge. We combine these visualisations with our force measurements to suggest a mechanism for the removal of contaminated particles from surfaces using droplets, and we outline the differences between the outcomes on the lubricated and the non-lubricated surfaces. This work will help to understand droplet dynamics on imperfect or dirty lubricated surfaces.

DY 64.8 Fri 11:45 ZEU 260

Memory effects in polymer brushes showing co-nonsolvency effects — •Simon Schubotz[1,2], Petra Uhlmann[1], Andreas Fery[1,2], Jens-Uwe Sommer[1,2], and Günter K. Auernhammer[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany — [3]Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany

Some polymer brushes show a co-nonsolvency effect: They collapse in a mixture of two good solvents at some specific mixing ratio. Previous studies focused on the response of brushes which are entirely covered by a liquid. Here, 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 demonstrate that the wetting behavior depends on the wetting history of the polymer brush.

We use Poly(N-isopropylacrylamide) (PNiPAAm) brushes and water and ethanol as good solvents. In water/ethanol mixtures, the brush thickness is a non-monotonous function of the ethanol concentration. The memory of brushes is tested by consecutively depositing drops of increasing size at the same position. Previously deposited drops induce changes in the brush that modifies the wetting behavior (advancing contact angle) of subsequent drops.

We believe that the change in the contact angels is induced by adaptation like swelling of or liquid exchange in the brush due to the drop on top.

DY 64.9 Fri 12:00 ZEU 260

Gradient dynamics model for drops spreading on polymer brushes — •Simon Hartmann and Uwe Thiele — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Deutschland

When a liquid drop spreads on an adaptive substrate the latter changes its properties what may result in an intricate coupled dynamics of drop and substrate. We present a generic mesoscale hydrodynamic model for such processes that is written as a gradient dynamics on an underlying energy functional. We specify the model details for the example of a drop spreading on a dry polymer brush. There, liquid absorption into the brush results in swelling of the brush causing changes in the brush topography and wettability. The liquid may also advance within the brush via diffusion (or wicking) resulting in coupled drop and brush dynamics. The specific model accounts for coupled spreading, absorption and wicking dynamics when the underlying energy functional incorporates capillarity, wettability and brush energy. We employ a simple version of such a model to numerically simulate a droplet spreading on a swelling brush and provide an in-depth analysis of the simulation results and some interesting quantities.

DY 65: Partial Synchronization Patterns in Neuronal Networks II (Focus Session joint with DY / SOE / BP) (joint session SOE/DY)

Time: Friday 10:00–12:00 Location: GÖR 226

DY 65.1 Fri 10:00 GÖR 226

Control of chimera states in multilayer networks of FitzHugh-Nagumo neurons — •Giulia Ruzzene and Ralph G. Andrzejak — Universitat Pompeu Fabra, Barcelona, Spain

Chimera states are a widely studied phenomenon in nonlinear science. In oscillator networks, a chimera state is defined as the coexistence of synchronous and aysnchronous groups of nodes. Many analogies have been established between chimeras and natural phenomena, especially with brain dynamics. Here we study the dynamics of a two-layer network of FitzHugh-Nagumo oscillators, which model neuronal dynamics. Chimera states have been observed in this configuration, but only a few studies also deal with the topic of control of chimeras in multilayer networks. Here we apply a control mechanism that we previously developed for chimeras in single-layer networks of phase oscillators. We study the interplay of the control method with the multilayer configuration and show the parameter regions in which the control is effective.

DY 65.2 Fri 10:30 GÖR 226

Effect of Topology upon Relay Synchronization in Triplex Neuronal Networks — •Fenja Drauschke, Iryna Omelchenko, Rico Berner, Jakub Sawicki, and Eckehard Schöll — Institute of Theoretical Physics, Technische Universität Berlin

Complex networks consisting of several interacting layers allow for remote synchronization of distant layers via an intermediate relay layer. We investigate relay synchronization in a three-layer neuronal network and study the effect of the topology of the layers upon the synchronization scenarios. Introducing random topologies either in the outer layers or in the middle (relay) layer leads to an increase of the range of inter-layer coupling strength for which the relay-synchronized state is preserved, compared with regular nonlocal coupling topologies.

DY 65.3 Fri 10:45 GÖR 226

High-order couplings in geometric complex networks of neurons — •Alejandro Tlaie[1,2,3], Inmaculada Leyva[1,2], and Irene Sendiña-Nadal[1,2] — [1]Complex Systems Group & GISC, Universidad Rey Juan Carlos, 28933 Móstoles, Madrid, Spain — [2]Center for Biomedical Technology, Universidad Politécnica de Madrid, Madrid, Spain — [3]Department of Applied Mathematics and Statistics, ETSIT Aeronáuticos, Universidad Politécnica de Madrid, 28040 Madrid, Spain

We explore the consequences of introducing higher-order interactions in a geometric complex network of Morris-Lecar neurons. We focus on the regime where traveling synchronization waves are observed from a first-neighbors-based coupling to evaluate the changes induced when higher-order dynamical interactions are included. We observe that the traveling-wave phenomenon gets enhanced by these interactions, allowing the activity to travel further in the system without generating pathological full synchronization states. This scheme could be a step toward a simple phenomenological modelization of neuroglial networks.

15 min. break

DY 65.4 Fri 11:15 GÖR 226

Multilayer structures in adaptive oscillator networks — •Rico Berner[1,2], Jakub Sawicki[1], and Eckehard Schöll[1] — [1]Institute of Theoretical Physics, Technische Universität Berlin, Germany — [2]Institute of Mathematics, Technische Universität Berlin, Germany

Dynamical systems on networks with adaptive couplings appear naturally in real-world systems such as power grid networks, social networks as well as neuronal networks. We investigate collective behaviour in a paradigmatic network of adaptively coupled phase oscillators. The coupling topology of the network changes slowly depending on the dynamics of the oscillators on an all-to-all coupled background. We show that such a system gives rise to numerous complex dynamics, including relative equilibria and hierarchical multicluster states. Parameter regimes of high multistability are found. An analytic treatment for equilibria as well as multicluster states reveals that existence and stability are significantly influenced by the slow-fast time separation. Interactions between different clusters are further studied numerically and analytically in the framework of multiplex networks. Our results allow for the interpretation of equilibria as functional units in multicluster structures. The results contribute to the understanding of mechanisms for self-organized pattern formation in adaptive networks, such as the emergence of multilayer structure in neural systems and their interaction.

DY 65.5 Fri 11:30 GÖR 226

Hierarchical clusters in adaptive networks with random topology — •Simon Vock[1], Rico Berner[1,2], Eckehard Schöll[1], and Serhiy Yanchuk[2] — [1]Institute of Theoretical Physics, Technische Universität Berlin — [2]Institute of Mathematics, Technische Universität Berlin

Networks of adaptively coupled oscillators show certain synchronization phenomena, such as multi-cluster states or traveling-wave states. While the emergence of these self-organised structures has been previously studied on all-to-all coupled networks, the type of connections and underlying network structure play an important role in the formation of these partially synchronized states. This work extends the investigations towards more complex networks, analysing the influence of random network topologies and changing adaption functions.

DY 65.6 Fri 11:45 GÖR 226

Hierarchical frequency clusters in adaptive networks of phase oscillators — •Jan Fialkowski[1], Rico Berner[1,2], Serhiy Yanchuk[2], and Eckehard Schöll[1] — [1]Institute of Theoretical Physics, Technische Universität Berlin — [2]Institute of Mathematics, Technische Universität Berlin

Adaptive dynamical networks appear in various real-world systems. In this talk, we explain the basic mechanism behind the pattern formation in adaptive networks by considering a simple phenomenological phase oscillator model. Frequency synchronization is shown to be the key phenomenon for the emergence of hierarchical modular network structures. A particular class of phase clusters, called double antipodal clusters, are presented and shown to play an important role in the organization of the high dimensional dynamics. In the end, we also examine the importance of different timescales in the adaptive and oscillatory dynamics.

DY 66: Many-body Quantum Dynamics II

Time: Friday 10:00–12:00 Location: HÜL 186

DY 66.1 Fri 10:00 HÜL 186

Light Induced Electron Superconductivity with Driven Optical Cavity — •Ahana Chakraborty and Francesco Piazza — Max Planck Institute for Physics of Complex Systems, Dresden, Germany

In a recent work, Schlawin et. al. [PRL, 122, 133602 (2019)] studied the possibility to induce superconductivity via cavity-mediated electron-electron interactions. This cavity-induced 'Amperean' pairing, which involves electrons propagating in the same direction, with total centre-of-mass momentum on the Fermi surface is estimated to lead to superconductivity in the low kelvin-regime for GaAs using realistic cavity parameters. In our work, we investigate the possibility of stabilising the superconducting state at even higher temperatures by driving the optical cavity. The effect of loss of photons as well as incoherent pump is incorporated by non- equilibrium field theoretic techniques, which also allow us to explore beyond the weak coupling regime of the electrons and the cavity.

DY 66.2 Fri 10:15 HÜL 186

Quantum Many-Body Scars in Doubly Modulated Optical Lattices — •Hongzheng Zhao[1], Joseph Vovrosh[1], Florian Mintert[1], and Johannes Knolle[1,2] — [1]Blackett Laboratory, Imperial College London, London, United Kingdom — [2]Department of Physics, Technische Universitt Mnchen, Garching, Germany

The concept of quantum many-body scars has recently been introduced to explain the weak ergodicity breaking experimentally observed in a Rydberg atom platform. There, exceptionally long coherent oscillations are observed for quenches from a set of special initial states. Such scared eigenstates, which are concentrated in a small fragment of the total Hilbert space, have been discovered theoretically in a number of spin and fermionic models. Here, we propose a simple setup to generate quantum many-body scars in a doubly modulated Bose-Hubbard system which can be readily implemented in cold atomic gases. In the high frequency limit, we show that the dynamics is governed by density assisted tunneling. We find the optimal driving parameters for the kinetically constrained hopping which leads to small isolated subspaces of scared eigenstates. We discuss the experimental signatures and analyze the transition to fully thermalizing behavior as a function of driving frequency.

DY 66.3 Fri 10:30 HÜL 186

Higher-order and fractional discrete time crystals in clean long-range interacting systems — •Andrea Pizzi[1], Johannes Knolle[2,3,4], and Andreas Nunnenkamp[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [2]Department of Physics, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [4]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

Discrete time crystals are periodically driven systems characterized by a response with periodicity nT, with T the period of the drive and $n > 1$. Typically, n is an integer and bounded from above by the dimension of the local (or single particle) Hilbert space, the most prominent example being spin-1/2 systems with n restricted to 2. Here we show that a clean spin-1/2 system in the presence of long-range interactions and transverse field can sustain a huge variety of different 'higher-order' discrete time crystals with integer and, surprisingly, even fractional $n > 2$. We characterize these non-equilibrium phases of matter thoroughly using a combination of exact diagonalization, semiclassical methods, and spin-wave approximations, which enable us to establish their stability in the presence of competing long- and short-range interactions. Remarkably, these phases emerge in a model with continous driving and time-independent interactions, convenient for experimental implementations with ultracold atoms or trapped ions.

DY 66.4 Fri 10:45 HÜL 186

Unitary long-time dynamics with quantum renormalization groups and Artificial Neural Networks — •Heiko Burau and Markus Heyl — Max Planck Institut für Physik komplexer Systeme, Dresden, Germany

The exponential growth of complexity in quantum mechanics limits, in general, the simulation of non-equilibrium dynamics in large closed systems to short or intermediate time scales. In this work we combine quantum renormalization group approaches with deep artificial neural networks (ANNs) for the description of the real-time evolution in strongly disordered quantum matter. We find that this allows us to accurately compute the long-time dynamics of many-body localized systems. Concretely, we use this approach to describe the spatioemporal buildup of many-body localized spin glass order in random Ising models.

DY 66.5 Fri 11:00 HÜL 186

Reinforcement Learning for Digital Quantum Simulation — •Adrien Bolens and Markus Heyl — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Digital quantum simulations (DQS) are one of the most appealing applications of a quantum computer. In theory, the unitary time-

evolution of any spin-type Hamiltonian can be encoded in a quantum computer with arbitrary precision. In practice, however, unitary gates entangling different qubits are an important source of error. We use tailored reinforcement learning techniques to optimally generate DQS of collective quantum spin systems, such as the long-range Ising model and the XX model. We show that for a fixed number of entangling quantum gates, the DQS error found is systematically lower than the Trotter error, and decay much more slowly with the system size. In addition, our method let us generate efficient DQS even for models without a well-defined Trotterization in the quantum simulator. We discuss the implications of our algorithm for the implementation of DQS in trapped-ion quantum simulators.

DY 66.6 Fri 11:15 HÜL 186

Local correlations in dual kicked models — •Daniel Waltner[1], Boris Gutkin[2], Petr Braun[1], Maram Akila[3], and Thomas Guhr[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany — [2]Department of Applied Mathematics, Holon Institute of Technology, 58102 Holon, Israel — [3]Fraunhofer-Institutszentrum Schloss Birlinghoven, Schloss Birlinghoven, 53754 Sankt Augustin

Recent studies [1] have demonstrated that two-point correlations of local operators in unitary-dual circuit lattices are restricted to light cone edges. We show that for a wide class of dual kicked chain systems, built upon a pair of complex Hadamard matrices, the l-point correlators of strictly local, traceless operators vanish identically in the thermodynamic limit. On the other hand, non-local operators, generically, exhibit nontrivial correlations along the light cone edges. We obtain an explicit, analytic form of two-point correlators for operators supported at pairs of adjacent chain sites.

[1] B. Bertini, P. Kos, T. Prosen, Phys. Rev. Lett. **123**, 210601 (2019).

DY 66.7 Fri 11:30 HÜL 186

Quantum scars of bosons with correlated hopping — •Ana Hudomal[1], Ivana Vasić[1], Nicolas Regnault[2,3], and Zlatko Papić[4] — [1]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Serbia — [2]Joseph Henry Laboratories and Department of Physics, Princeton University, USA — [3]Laboratoire de Physique de l'École Normale Supérieure, ENS, CNRS, Paris, France — [4]School of Physics and Astronomy, University of Leeds, United Kingdom

Recent experiments have shown that preparing an array of Rydberg atoms in a certain initial state can lead to unusually slow thermalization and persistent density oscillations [1]. This type of non-ergodic behavior has been attributed to the existence of "quantum many-body scars", i.e., atypical eigenstates that have high overlaps with a small subset of vectors in the Hilbert space. Periodic dynamics and many-body scars are believed to originate from a "hard" kinetic constraint: due to strong interactions, no two neighbouring Rydberg atoms are both allowed to be excited. Here we propose a realization of quantum many-body scars in a 1D bosonic lattice model with a "soft" constraint: there are no restrictions on the allowed boson states, but the amplitude of a hop depends on the occupancy of the hopping site. We find that this model exhibits similar phenomenology to the Rydberg atom chain, including weakly entangled eigenstates at high energy densities and the presence of a large number of exact zero energy states [2].

[1] H. Bernien et al., Nature **551**, 579 (2017).
[2] A. Hudomal et al., arXiv:1910.09526 (2019).

DY 66.8 Fri 11:45 HÜL 186

How the energy structure of perturbations affects the relaxation of many-body quantum systems — •Lennart Dabelow and Peter Reimann — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

We investigate the response of isolated many-body quantum systems to generic perturbations. In general, such perturbations will couple states of different energies differently, but commonly the strength depends dominantly on their energy distances. Under this assumption, and in the absence of specific symmetries or macroscopic inhomogeneities, we use typicality methods to derive an integral equation relating the energy profile of the perturbation to the temporal relaxation characteristic of the perturbed system. The solution of this equation leads to a prediction for the time evolution of observables. We illustrate the general results by means of specific examples.

DY 67: Active Matter V (joint session DY/BP/CPP)

Time: Friday 10:00–11:30 Location: ZEU 160

DY 67.1 Fri 10:00 ZEU 160

A particle-field approach bridges phase separation and collective motion in active matter — •Robert Grossmann[1,2], Igor Aranson[3], and Fernando Peruani[2] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Laboratoire J.A. Dieudonné, Université Côte d'Azur, Nice, France — [3]Department of Chemistry, Pennsylvania State University, University Park (PA), United States of America

Linking seemingly disconnected realms of active matter – active phase-separation of repulsive discs and collective motion of self-propelled rods – is a major contemporary challenge. We present a theoretical framework based on the representation of active particles by smoothed continuum fields which brings the simplicity of alignment-based models, enabling an analytical analysis, together with more realistic models for self-propelled objects including their steric, repulsive interactions. We demonstrate on the basis of the collision kinetics how nonequilibrium stresses acting among self-driven, anisotropic objects hinder the emergence of motility-induced phase separation and facilitate orientational ordering. Moreover, we report that impenetrable, anisotropic rods are found to form polar, moving clusters, whereas large-scale nematic structures emerge for soft rods, notably separated by a bistable coexistence regime. Thus, the symmetry of the ordered state is not dictated by the symmetry of the interaction potential but is rather a dynamical, emergent property of active systems. This theoretical framework can represent a variety of active systems: cell tissues, bacterial colonies, cytoskeletal extracts or shaken granular media.

DY 67.2 Fri 10:15 ZEU 160

The role of inertia in active nematic turbulence — •Colin-Marius Koch and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Suspensions of active agents with nematic interactions can exhibit complex spatio-temporal dynamics such as mesoscale turbulence. Continuum descriptions for such systems are inspired by the hydrodynamic theory of liquid crystals and introduce additional effects of active stresses. The resulting equations feature an advective nonlinearity which represents inertial effects. The typically low Reynolds number of such active flows raises the question of the importance of the inertial effects. To address this question, we numerically investigate turbulent flows in a two-dimensional dense suspension of active nematic liquid crystals. We qualitatively compare numerical simulations with and without nonlinear advection of the flow field. We find that for sufficiently high activity, the simulations considering the advection term display large-scale motion not observed when excluding inertia. Performing a spectral analysis of the energy budget, we identify an inverse energy transfer to the largest scales highlighting the importance of inertial effects in this model. We additionally show that surface friction, mimicked by a linear friction term, dissipates the transported energy and slows down the large-scale motion.

DY 67.3 Fri 10:30 ZEU 160

Active Brownian particles show motility-induced spatially periodic patterns — •Samuel Grimm[1], Andreas Fischer[2], Thomas Speck[2], and Walter Zimmermann[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Physics Institute, University of Mainz, 55099 Mainz, Germany

We suggest and investigate a model for active Brownian particles, that shows motility induced pattern formation. We complement a model of motility induced phase separation (MIPS) [J. Chem. Phys. 142, 224149 (2015)] by the dynamics of auto-inducer molecules. This results in a prototype model for spatially periodic patterns under conservation constraints, here the conservation of Brownian particles. By increasing the chemotactic sensitivity of active Brownian particles a transition

from MIPS to motility induced periodic patterns takes place. They are found in a wide parameter range. Besides the phase diagrams for the onset of spatially periodic patterns also their nonlinear behavior beyond onset is investigated for selected parameter ranges.

DY 67.4 Fri 10:45 ZEU 160

The role of advection in the diffusioosmosis of an active micropump — •Gonçalo Antunes[1,2], Paolo Malgaretti[1,2], Jens Harting[3,4], and Siegfried Dietrich[1,2] — [1]MPI-IS, Stuttgart, Germany — [2]U. Stuttgart, Stuttgart, Germany — [3]HI-ERN, Forschungszentrum Jülich, Nürnberg, Germany — [4]TU/e, Eindhoven, The Netherlands

Diffusioosmosis can be exploited to fabricate active colloids that swim in a fluid/solute mixture through a self-generated inhomogeneous concentration of solute [1]. Using the same mechanism, an active channel can be fabricated such as to pump fluid in a way that is tunable via the geometry and chemistry of the channel.

In this talk, we study the flow inside an active hourglass-shaped channel. Our Lattice Boltzmann simulations are combined with a finite-difference solver for the advection-diffusion equation that determines the solute dynamics [2]. We find that even when the channel is fore-aft symmetric, advection can lead to the pumping of fluid, in analogy to the steady motion of isotropic colloids [3,4]. Furthermore, sustained oscillations are found where the magnitude of the flow oscillates with a tunable frequency. Our findings are thus relevant for those who wish to exploit surface-driven flows at small scales.

[1] J. L. Anderson, Ann. Rev. Fluid Mech. **21** 61-99 (1989) [2] T. Peter, P. Malgaretti, N. Rivas, A. Scagliarini, J. Harting, S. Dietrich, arXiv:1911.06324 (2019) [3] S. Michelin, E. Lauga, and D. Bartolo, Phys. Fluids **25** 061701 (2013) [4] P. de Buyl, A. S. Mikhailov, and R. Kapral, EPL **103** 60009 (2013)

DY 67.5 Fri 11:00 ZEU 160

Dynamical states in underdamped active matter — •Dominic Arold and Michael Schmiedeberg — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Many active matter systems are well approximated as overdamped, meaning that any inertial momentum is immediately dissipated by the environment. On the other hand, for macroscopic active systems, the time scale of inertial motion can become large enough to be relevant for the dynamics already on the single-particle level [1]. This raises the question of how collective dynamics in active matter is influenced by inertia. We propose a coarse-grained continuum model for underdamped active matter based on a dynamical density functional theory for passive systems [2]. Further, we apply the model to a system with short-range alignment of polar orientations whereas long-ranged correlations of orientational order are suppressed. Our simulations of under- and overdamped dynamics both predict a structured laning state. However, activity-induced convective flows only present in the underdamped model destabilize this state in a certain parameter regime, leading to a collective motion state which is not predicted in the overdamped limit. A turbulent transition regime between the two states is distinguished by strong density fluctuations.

[1] Scholz C et al. 2018 *Nature communications* **9** 5156
[2] Archer A J 2009 *The Journal of chemical physics* **130** 014509

DY 67.6 Fri 11:15 ZEU 160

Predictive local field theory for interacting active Brownian spheres in two spatial dimensions* — Jens Bickmann and •Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

We present a predictive local field theory for the dynamics of interacting spherical active Brownian particles in two spatial dimensions. Alongside the general theory, which includes configurational order parameters and derivatives up to infinite order, we present reduced models that are easier to apply. We show that our theory contains popular models such as Active Model B + as special cases and that it provides explicit expressions for the coefficients occurring in these models. As further outcomes, the theory yields analytical expressions for the density-dependent mean swimming speed and the spinodal corresponding to motility-induced phase separation of the particles. The analytical predictions for the spinodal are found to be in very good agreement with the results of Brownian dynamics simulations. Furthermore, the critical point predicted by our analytical results agrees excellently with recent computational results from the literature.

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DY 68: Closing Talk (joint session BP/DY/CPP)

Time: Friday 12:30–13:15 Location: HSZ 02

Invited Talk DY 68.1 Fri 12:30 HSZ 02

Physics of active droplets — •Frank Jülicher — Max Planck Institute for the Physics of Complex Systems, Dresden

Phase separation provides a general physical mechanism for the spatial organization of cells and for the compartmentalization of chemical processes. Proteins together with other molecules can condense to form liquid-like droplets that provide localized chemical environments and that can serve as micro-reactors for biochemical reactions without an enclosing membrane. The cell cytoplasm can thus be viewed as an emulsion, where phase-separated compartments organize biochemical processes in space. Droplets that carry chemical activity are active systems that maintained away from thermodynamic equilibrium by chemical energy input. I will discuss the physics of such active droplets and active emulsions and show that they exhibit unusual properties and behaviors. Examples are the arrest of coarsening and the suppression of Ostwald ripening, spontaneous droplet division and droplet positioning by concentration gradients. The physics of active droplets could play important roles in fundamental cellular processes of many organisms and could have emerged early in the evolution of life.