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Overview of Invited Talks and Sessions

(Lecture rooms BH-N 243, BH-N 334, BH-N 333, BH-N 128, EB 107, MA 001; Poster A)

Plenary Talks

PLV IV	Mon	14:00–14:45	H 0104	**Fast Parametric Interactions Between Superconducting Quantum Circuits** — •Raymond W Simmonds
PLV V	Tue	8:30– 9:15	H 0105	**Upside-Down and Inside-Out: Biomechanics of Cell Sheet Folding** — •Raymond Goldstein
PLV XI	Thu	8:30– 9:15	H 0105	**Emergent properties and functions of topological magnets** — •Yoshinori Tokura
PLV XIII	Thu	14:00–14:45	H 0104	**A significant raw material of the 21st century** — •Claudia Draxl

Invited Talks

DY 4.1	Mon	9:30–10:00	BH-N 243	**Sounds and stubbornness of active fluids.** — •Denis Bartolo, Delphine Geyer, Alexandre Morin
DY 5.1	Mon	9:30–10:00	BH-N 334	**Irreversibility and dissipation in molecular motors and kinetic networks** — •Juan MR Parrondo
DY 13.1	Mon	15:00–15:30	BH-N 334	**Diffusive Droplet Dynamics in multicomponent fluid systems** — •Detlef Lohse
DY 20.1	Tue	9:30–10:00	EB 107	**Light fields in complex media: mesoscopic physics meets wave control** — •Stefan Rotter
DY 22.1	Tue	9:30–10:00	BH-N 243	**Complex Systems in Mechanical Engineering? A paradigm shift ahead.** — •Norbert Hoffmann
DY 36.1	Wed	9:30–10:00	EB 107	**Computing quantum thermalization dynamics: from quantum chaos to emergent hydrodynamics** — •Ehud Altman
DY 36.6	Wed	11:15–11:45	EB 107	**Quantum Thermalization Dynamics: From Information Scrambling to Emergent Hydrodynamics** — •Michael Knap
DY 40.1	Wed	9:30–10:00	BH-N 243	**Measurement of the functional form of Shannon entropy by partial erasure of a bit** — •John Bechhoefer, Momčilo Gavrilov, Raphaël Chétrite
DY 41.1	Wed	9:30–10:00	BH-N 334	**From bifurcations of single sliding drops to their ensemble statistics** — •Uwe Thiele
DY 44.1	Wed	10:00–10:30	BH-N 334	**Self-organisation and positioning of sub-cellular protein clusters** — •Sean M. Murray
DY 44.5	Wed	11:30–12:00	BH-N 334	**Spatial heterogeneities shape collective behavior of the signaling amoeboid cells** — •Azam Gholami
DY 48.1	Wed	15:00–15:30	MA 001	**Network structure and dynamics: when and how multiplex really matters?** — •Vito Latora

DY 49.1	Wed	15:00–15:30	BH-N 334	**Nanorod fractionation via lyotropic liquid crystal formation, and its effect on phase diagram and gelation** — Camila Honorato-Rios, Claudius Lehr, Christina Schütz, Roland Sanctuary, Mikhail Osipov, Jörg Baller, •Jan Lagerwall
DY 55.1	Thu	9:30–10:00	EB 107	**Nuclear and electronic dynamics in ultrafast photoinduced charge separation** — •Carlo Andrea Rozzi
DY 55.2	Thu	10:00–10:30	EB 107	**Theory of pump-probe spectroscopy: Ultrafast laser engineering of ordered phases and microscopic couplings** — •Michael Sentef
DY 57.1	Thu	9:30–10:00	BH-N 243	**Anomalous Diffusion due to Crowding or External Potentials** — •Stefan U. Egelhaaf
DY 65.1	Thu	15:00–15:30	BH-N 243	**Towards a thermodynamics of active particles** — •Thomas Speck
DY 77.1	Fri	9:30–10:00	BH-N 243	**Mean field theory of ride sharing systems** — •Stephan Herminghaus
DY 78.1	Fri	9:30–10:00	BH-N 334	**Emergence of long-ranged stress correlations at the liquid to glass transition** — Manuel Maier, Annette Zippelius, •Matthias Fuchs

Invited talks of the joint symposium SYMS

See SYMS for the full program of the symposium.

SYMS 1.1	Mon	15:00–15:30	H 0105	**Stochastic numerical algorithms: from molecular dynamics to big data analytics** — •Benedict Leimkuhler
SYMS 1.2	Mon	15:30–16:00	H 0105	**A Generally-Applicable Machine-Learning Scheme for Materials and Molecules** — •Michele Ceriotti
SYMS 1.3	Mon	16:00–16:30	H 0105	**Girsanov reweighting for path ensembles and Markov state models** — •Bettina G. Keller, Luca Donati, Carsten Hartmann
SYMS 1.4	Mon	16:45–17:15	H 0105	**Liquid State Theory Meets Deep Learning and Molecular Informatics** — •Alpha Lee
SYMS 1.5	Mon	17:15–17:45	H 0105	**Computational high-throuhgput screening of drug-membrane thermodynamics** — •Tristan Bereau

Invited talks of the joint symposium SYBS

See SYBS for the full program of the symposium.

SYBS 1.1	Tue	9:30–10:00	H 0105	**Bacterial collective behaviours** — •Knut Drescher
SYBS 1.2	Tue	10:00–10:30	H 0105	**Nonlinear dynamics of beating cilia and flagella: Swimming, steering, and synchronization** — •Benjamin M. Friedrich
SYBS 1.3	Tue	10:30–11:00	H 0105	**Learning to navigate in dynamic environments: animal behavior and artificial intelligence** — •Antonio Celani
SYBS 1.4	Tue	11:15–11:45	H 0105	**Suspensions of active colloids** — •Cecile Cottin-Bizonne, Félix Ginot, Isaac Theurkauff, Christophe Ybert
SYBS 1.5	Tue	11:45–12:15	H 0105	**Spontaneous chiral symmetry breaking in active fluids** — •Jörn Dunkel

Sessions

DY 1.1–1.3	Sun	16:00–18:30	H 0104	**Tutorial: Dynamics and Fluctuations in Economic and Financial Markets (joint session SOE/DY/TUT/AKjDPG)**
DY 2.1–2.6	Mon	9:30–12:45	H 0104	**Focus Session: Recent Developments in Computational Many Body Physics (joint session TT/DY)**
DY 3.1–3.13	Mon	9:30–13:00	C 264	**Complex Fluids and Colloids I (joint session CPP/DY)**
DY 4.1–4.1	Mon	9:30–10:00	BH-N 243	**Talk D. Bartolo**
DY 5.1–5.1	Mon	9:30–10:00	BH-N 334	**Talk J. Parrondo**
DY 6.1–6.10	Mon	10:00–12:45	EB 107	**Dynamics in many-body systems: interference, equilibration and localization I (joint session DY/TT)**
DY 7.1–7.7	Mon	10:00–11:45	BH-N 128	**Modeling and Data Analysis**
DY 8.1–8.12	Mon	10:00–13:15	BH-N 243	**Active Matter I (joint session DY/CPP/BP)**
DY 9.1–9.13	Mon	10:00–13:30	BH-N 334	**Statistical Physics far from Thermal Equilibrium**
DY 10.1–10.10	Mon	10:00–12:45	BH-N 333	**Statistical Physics I (General)**
DY 11.1–11.4	Mon	12:00–13:00	BH-N 128	**Energy Systems (joint session DY/SOE)**

DY 12.1–12.7	Mon	15:00–17:00	H 2013	**Focus Session: Statistical Physics-Based Methods in Molecular Evolution - organized by Alexander Schug and Martin Weigt (joint session BP/DY)**
DY 13.1–13.1	Mon	15:00–15:30	BH-N 334	**Talk D. Lohse**
DY 14.1–14.9	Mon	15:30–17:45	EB 107	**Dynamics in many-body systems: interference, equilibration and localization II (joint session DY/TT)**
DY 15.1–15.8	Mon	15:30–17:30	BH-N 128	**Nonlinear Dynamics, Synchronization, Chaos I**
DY 16.1–16.12	Mon	15:30–18:45	BH-N 243	**Active Matter II (joint session DY/CPP/BP)**
DY 17.1–17.14	Mon	15:30–19:15	BH-N 334	**Focus: Droplets (joint session DY/CPP)**
DY 18.1–18.6	Mon	15:30–17:00	BH-N 333	**Critical Phenomena and Phase Transitions**
DY 19.1–19.3	Mon	17:30–18:15	BH-N 333	**Extreme Events**
DY 20.1–20.1	Tue	9:30–10:00	EB 107	**Talk S. Rotter**
DY 21.1–21.8	Tue	9:30–11:45	C 264	**Complex Fluids and Colloids II (joint session CPP/DY)**
DY 22.1–22.1	Tue	9:30–10:00	BH-N 243	**Talk H. Hoffmann**
DY 23.1–23.8	Tue	10:00–12:15	EB 107	**Quantum Chaos**
DY 24.1–24.4	Tue	10:00–11:00	BH-N 128	**Complex Systems**
DY 25.1–25.11	Tue	10:00–13:00	BH-N 243	**Statistical Physics II (General)**
DY 26.1–26.6	Tue	11:00–12:30	BH-N 334	**Condensed Matter Simulations augmented by Advanced Statistical Methodologies I (joint session DY/CPP)**
DY 27.1–27.6	Tue	11:15–12:45	BH-N 128	**Microfluidics**
DY 28.1–28.3	Tue	12:30–13:15	MA 001	**Evolutionary Game Theory (joint SOE/BP/DY) (joint session SOE/DY/BP)**
DY 29.1–29.7	Tue	14:00–15:45	EB 107	**Particulate Matter: From microscopic interactions to collective motion (joint session DY/CPP)**
DY 30.1–30.7	Tue	14:00–16:00	PC 203	**Modeling and Simulation of Soft Matter I (joint session CPP/DY)**
DY 31.1–31.5	Tue	14:00–15:15	BH-N 128	**Condensed Matter Simulations augmented by Advanced Statistical Methodologies II (joint session DY/CPP)**
DY 32.1–32.7	Tue	14:00–15:45	BH-N 243	**Microswimmers I (joint session DY/BP/CPP)**
DY 33.1–33.8	Tue	14:00–16:00	BH-N 334	**Delay and Feedback Dynamics**
DY 34.1–34.5	Tue	14:00–15:15	BH-N 333	**Nonlinear Stochastic Systems**
DY 35.1–35.12	Wed	9:30–13:00	H 3010	**Nonequilibrium Quantum Many-Body Systems I (joint session TT/DY)**
DY 36.1–36.8	Wed	9:30–12:15	EB 107	**Focus: Chaos and Correlation in Quantum Matter (joint session DY/TT)**
DY 37.1–37.11	Wed	9:30–12:15	MA 001	**Networks: From Topology to Dynamics (joint session SOE/DY/BP) (joint session SOE/CPP/BP/DY)**
DY 38.1–38.8	Wed	9:30–12:00	C 230	**Modeling and Simulation of Soft Matter II (joint session CPP/DY)**
DY 39.1–39.12	Wed	9:30–13:00	C 264	**Wetting, Microfluidics and Confined Liquids I (joint session CPP/DY)**
DY 40.1–40.1	Wed	9:30–10:00	BH-N 243	**Talk J. Bechhoefer**
DY 41.1–41.1	Wed	9:30–10:00	BH-N 334	**Talk U. Thiele**
DY 42.1–42.10	Wed	10:00–12:45	BH-N 128	**Turbulence**
DY 43.1–43.13	Wed	10:00–13:45	BH-N 243	**Stochastic thermodynamics and information processing**
DY 44.1–44.9	Wed	10:00–13:00	BH-N 334	**Pattern Formation I**
DY 45.1–45.13	Wed	10:00–13:30	BH-N 333	**Statistical Physics in Biological Systems (joint session DY/BP)**
DY 46.1–46.9	Wed	15:00–17:30	H 1028	**Microswimmers (joint session BP/CPP/DY)**
DY 47.1–47.12	Wed	15:00–18:30	H 3010	**Nonequilibrium Quantum Many-Body Systems II (joint session TT/DY)**
DY 48.1–48.1	Wed	15:00–15:30	MA 001	**Talk V. Latora (joint session DY/SOE)**
DY 49.1–49.1	Wed	15:00–15:30	BH-N 334	**Talk J. Lagerwall**
DY 50.1–50.10	Wed	15:30–18:15	EB 107	**Quantum Dynamics, Decoherence and Quantum Information (joint session DY/TT)**
DY 51.1–51.9	Wed	15:30–18:00	MA 001	**Networks: From Topology to Dynamics (joint session DY/SOE)**
DY 52.1–52.12	Wed	15:30–18:45	BH-N 243	**Active Matter III (joint session DY/CPP/BP)**
DY 53.1–53.14	Wed	15:30–19:15	BH-N 334	**Complex Fluids and Soft Matter (joint session DY/ CPP / BP)**

DY 54.1–54.12	Thu	9:30–13:00	H 2013	**Statistical Physics of Biological Systems I (joint session BP/DY)**
DY 55.1–55.6	Thu	9:30–11:30	EB 107	**Focus: Emergent phenomena in driven quantum many-body systems (joint session DY/TT)**
DY 56.1–56.9	Thu	9:30–13:15	MA 001	**Complex Contagion Phenomena I (Focus Session, joint SOE/DY/BP/SNPD) (joint session SOE/DY/BP)**
DY 57.1–57.1	Thu	9:30–10:00	BH-N 243	**Talk S. Egelhaaf**
DY 58.1–58.11	Thu	10:00–13:00	BH-N 128	**Chimera states: symmetry-breaking in dynamical networks (joint session DY/SOE)**
DY 59.1–59.12	Thu	10:00–13:15	BH-N 243	**Microswimmers II (joint session DY/CPP/BP)**
DY 60.1–60.12	Thu	10:00–13:15	BH-N 334	**Anomalous Diffusion (joint session DY/BP)**
DY 61.1–61.11	Thu	10:00–13:00	BH-N 333	**Granular Matter / Contact Dynamics (joint session DY/CPP)**
DY 62.1–62.3	Thu	12:00–12:45	EB 107	**Coherent Quantum Dynamics (joint session DY/TT)**
DY 63.1–63.8	Thu	15:00–17:15	H 2013	**Statistical Physics of Biological Systems II (joint session BP/DY)**
DY 64.1–64.5	Thu	15:00–16:15	MA 001	**Traffic Dynamics, Urban and Regional Systems (joint session SOE/DY)**
DY 65.1–65.1	Thu	15:00–15:30	BH-N 243	**Talk T. Speck**
DY 66.1–66.20	Thu	15:30–18:00	Poster A	**Poster: Stat. Phys. (Gen., Critical Phen., Biol.)**
DY 67.1–67.17	Thu	15:30–18:00	Poster A	**Poster: Active Matter, Microswimmers**
DY 68.1–68.23	Thu	15:30–18:00	Poster A	**Poster: Complex Fluids, Glasses, Granular**
DY 69.1–69.18	Thu	15:30–18:00	Poster A	**Poster: Quantum Systems**
DY 70.1–70.25	Thu	15:30–18:00	Poster A	**Poster: Flows, Patterns, Delay, Reaction Diffusion**
DY 71.1–71.15	Thu	15:30–18:00	Poster A	**Poster: Noneq. Stat. Phys., Stoch. Thermo, Brownian Dyn.**
DY 72.1–72.16	Thu	15:30–18:00	Poster A	**Poster: Stoch. and Nonl. Dy., Modeling, Compl. Sys.**
DY 73.1–73.11	Thu	15:30–18:00	Poster A	**Poster: Networks, Chimera, Energy Systems**
DY 74	Thu	18:15–18:45	BH-N 243	**Annual General Meeting**
DY 75.1–75.10	Fri	9:30–12:00	H 1058	**Active Matter (joint session BP/CPP/DY)**
DY 76.1–76.13	Fri	9:30–13:15	MA 001	**Complex Contagion Phenomena II (Focus Session, joint SOE/DY/BP/SNPD) (joint session SOE/DY/BP)**
DY 77.1–77.1	Fri	9:30–10:00	BH-N 243	**Talk S. Herminghaus**
DY 78.1–78.1	Fri	9:30–10:00	BH-N 334	**Talk M. Fuchs**
DY 79.1–79.8	Fri	10:00–12:15	EB 107	**The Physics of Power-Grids – Fluctuations, Synchronization and Network Structures (joint session DY/SOE)**
DY 80.1–80.5	Fri	10:00–11:15	BH-N 128	**Brownian Motion and Transport**
DY 81.1–81.9	Fri	10:00–12:30	BH-N 243	**Nonlinear Dynamics, Synchronization, Chaos II**
DY 82.1–82.10	Fri	10:00–12:45	BH-N 334	**Glasses and Glass Transition (joint session DY/CPP)**
DY 83.1–83.8	Fri	10:00–12:15	BH-N 333	**Pattern Formation II**

Annual General Meeting of the Dynamics and Statistical Physics Division

Donnerstag, 15. März 18:15–19:15 BH-N 243

- Bericht
- Verschiedenes

DY 1: Tutorial: Dynamics and Fluctuations in Economic and Financial Markets (joint session SOE/DY/TUT/AKjDPG)

Financial and economic markets display nontrivial fluctuation statistics that called attention among physicists. Methods from statistical physics have demonstrated to be able to derive stylized facts from microscopic models, to extract networks from data, and to relate multivariate economic time series to the underlying mechanisms.

Time: Sunday 16:00–18:30 Location: H 0104

Tutorial DY 1.1 Sun 16:00 H 0104

Market microstructure: dynamics of the stock markets — •Thomas Guhr — Fakultät für Physik, Universität Duisburg-Essen

At first sight, stock prices look like random walks. Indeed, Brownian motion models and related stochastic processes do a good job in describing some of the features which are empirically found in financial data. This is consistent with Fama's celebrated Efficient Market Hypothesis (EMH) which states that price changes are unpredictable. However, the closer one looks, the less reliable are those schematic models. This is so, because the way how the trading proceeds in time, i.e. the rules imposed and the ensuing dynamics, is largely ignored. Traders submit their buy and sell orders to the order book, whose content is made available to all market participants. The order flow eventually leads in a highly complex fashion to the realized prices.

Market microstructure is a quickly growing field in which economists, physicists, data scientists and mathematicians try to clarify these dynamical processes. An appealing feature, particularly for physicists, is the wealth of data available for analysis and subsequent model building. I am going to present large-scale data analysis to identify non-Markovian features. Fundamental economic reasoning as in the EMH favors Markovian models in which prices develop (apart from a deterministic drift) without memory. Sizeable memory effects could be exploited to make profit. I will present large-scale data analyses which show that there are various non-Markovian effects due to the highly complex market dynamics. Thus, there are limits to market efficiency which, furthermore, can be quantitatively identified.

Tutorial DY 1.2 Sun 16:50 H 0104

Maximum-entropy models in economics and finance — •Tiziano Squartini — IMT School for Advanced Studies Lucca, P.zza San Francesco 19, 55100 Lucca (IT)

Entropy-maximization represents the unifying concept underlying the definition of a number of methods which are now part of the discipline known as "network theory". Despite the perfect generality of this approach, a particularly fruitful application of it has been observed in disciplines like economics and finance. This tutorial will be devoted to illustrate the methodological aspects of the aforementioned approach, with particular emphasis on the definition of null models. The latter can be employed in a number of applications, ranging from pattern detection to network reconstruction: examples will be provided of both, by taking as case studies real-world systems, as the World Trade Web and the Dutch Interbank Network. The aforementioned framework also allows one to properly model fluctuations: the latter can be interpreted as errors affecting the estimation of the quantities of interest and strongly depend on the kind of constraints defining the maximization procedure. In order to illustrate how different reconstruction algorithms perform, a comparison of proposed approaches on the aforementioned real-world systems will be also carried out.

Tutorial DY 1.3 Sun 17:40 H 0104

350 years of puzzles in economics – and a solution. — •Ole Peters — London Mathematical Laboratory — Santa Fe Institute

In 1654 Fermat and Pascal puzzled over a gambling problem and invented probability theory. Three years later, Huygens declared that random quantities and their expectation values are "the same thing." Economics was the first adopter of the budding theory and to this day maintains much of the spirit of Huygens's early proclamation. Problems arising from this view of randomness have led to numerous puzzles in economic theory and beyond. An early example is the St. Petersburg paradox of 1713, a recent example is the insurance puzzle in general competitive equilibrium theory.

Economics has responded to these puzzles largely with labels. Humans are labelled irrational or risk averse.

An alternative treatment emerged from physics, where randomness entered in the 1850s with the development of statistical mechanics. Here, the question of ergodicity arose: are expectation values indicative of temporal behavior? The insight that in many cases an expectation value does not reflect the dynamics can be used to resolve the class of economics puzzles I will discuss. It leads to an alternative economic formalism that makes testable predictions. It can answer economic questions by assessing systemic stability where previously only moral assessments were available.

More at https://ergodicityeconomics.com/lecture-notes/

DY 2: Focus Session: Recent Developments in Computational Many Body Physics (joint session TT/DY)

This focus session provides an overview of recent achievements and new directions in the domain of computational many body physics. Numerical simulations provide invaluable insights in fermion quantum criticality, many body localization as well as in coupled fermion-boson systems. Tensor networks offer immense possibilities to tackle problems in and out of equilibrium. Finally, new directions such as machine learning and quantum computations will greatly impact the field. All these themes and methods will be discussed by the invited speakers.

Organization: Fakher F. Assaad, Universität Würzburg; Reinhard Noack, Philipps-Universität Marburg

Time: Monday 9:30–12:45 Location: H 0104

Invited Talk DY 2.1 Mon 9:30 H 0104

Revealing Fermionic Quantum Criticality from New Monte Carlo Techniques — •Zi Yang Meng — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

In this talk, I will present recent developments in the numerical investigations of fermionic quantum criticality in the form of Fermi surfaces coupled to various critical bosonic fluctuations. The thence obtain itinerant quantum critical points reveal rich and fundamental physics that has immediate impact on both theoretical and experimental investigations in the correlated electrons systems such as Cu- and Ir-based superconductors, heavy-fermion systems as well as the interacting topological state of matter and phase transitions. These developments are made possible due to the insightful model design as well as the timely algorithmic developments in the Monte Carlo techniques.

Invited Talk DY 2.2 Mon 10:00 H 0104

Computational Approaches to Many-Body Localization — •David J. Luitz — Physik Department T42, Technische Universität München, Germany

In the past decade, enormous progress has been made in the under-

standing of the phenomenon of many-body localization, a dynamical phase of matter in strongly disordered interacting quantum systems far from equilibrium. In particular, the understanding of the phase transition from an extended phase at weak disorder to a localized phase at strong disorder relies heavily on state of the art numerical studies. The numerically accessible system sizes have recently been increased substantially by the introduction of advanced exact numerical techniques: Exact sparse diagonalization as well as matrix product state (MPS) techniques permit the calculation of highly excited eigenstates of the system, whereas exact Krylov space time evolution methods and MPS time evolution methods can be used to study the nonequilibrium dynamics in generic many-body systems. I will give a short survey of current exact numerical techniques (cf [1] for a detailed discussion) to study the MBL phase as well as the transition regime and highlight some results obtained by these approaches.
[1] D. J. Luitz, Y. Bar Lev, Annalen der Physik 529, 1600350 (2017)

Invited Talk DY 2.3 Mon 10:30 H 0104
Tensor Network Techniques and Dynamical Systems — Nicola Pancotti[1], Michael Knapp[2], David Huse[3], Mari Carmen Banuls[1], and •Ignacio Cirac[1] — [1]Max-Planck Institut für Quantenoptic, Garching, Germany — [2]Technical University of Munich, Garching, Germany — [3]University of Princeton, Princeton, US

Tensor networks can be used to efficiently describe the equilibrium properties of many-body quantum systems with local interactions. However, they fail to describe their dynamics, at least for long times. In this talk we will present several methods based on tensor networks to extract dynamical properties of one dimensional spin chains. In particular, we will show how one can construct matrix product operators that quasi commute with the system Hamiltonian, and how this is related to the thermalization process.

15 min. break.

Invited Talk DY 2.4 Mon 11:15 H 0104
Digital Quantum Simulation — •Bela Bauer — Station Q, Microsoft Research, Santa Barbara, CA 93106-6105, USA

Recent improvements in the control of quantum systems make it appear feasible to build a quantum computer within a decade. One of the most promising applications for a quantum computer is the simulation of quantum systems that have thus far eluded numerical simulation on conventional supercomputers. In this talk, I will review the relevant models of quantum computation and survey some potential applications for a small quantum computer. I will then focus on the particular case of simulating complex materials. We show that this important and challenging problem can be tackled using a hybrid quantum-classical algorithm that incorporates the power of a small quantum computer into a framework of classical embedding algorithms.

Invited Talk DY 2.5 Mon 11:45 H 0104
Quantum Monte Carlo Simulation of Coupled Fermion-Boson Systems — Manuel Weber, Fakher Assaad, and •Martin Hohenadler — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

Problems of fermions coupled to bosonic degrees of freedom can be found in a variety of contexts in condensed matter physics. The bosons may represent, for example, quantum lattice, spin, or orbital fluctuations. Numerical simulations of such problems are challenging because of the bosonic Hilbert space, the different time scales for the fermion and boson dynamics, and the absence of efficient sampling methods for the bosons. In this talk, recent advances in quantum Monte Carlo simulations are presented. By integrating out the bosons, the original problem can be reformulated in terms of fermions with a retarded interaction. The latter can be simulated efficiently by continuous-time quantum Monte Carlo methods. Especially in combination with global updates, simulations can be carried out on system sizes currently inaccessible by any other method. Applications to be presented include the problem of competing electron-phonon couplings as well as charge-density-wave transitions in one and two dimensions.

Invited Talk DY 2.6 Mon 12:15 H 0104
Machine Learning Methods for Quantum Many-Body Physics — •Giuseppe Carleo — ETH Zurich, Institute for Theoretical Physics Wolfgang-Pauli-Str. 27 8093 Zurich - Switzerland

Machine-learning-based approaches are being increasingly adopted in a wide variety of domains, and very recently their effectiveness has been demonstrated also for many-body physics [1-4]. In this talk I will present recent applications to quantum physics.

First, I will discuss how a systematic machine learning of the many-body wave-function can be realized. This goal has been achieved in [1], introducing a variational representation of quantum states based on artificial neural networks. In conjunction with Monte Carlo schemes, this representation can be used to study both ground-state and unitary dynamics, with controlled accuracy. Moreover, I will show how a similar representation can be used to perform efficient Quantum State Tomography on highly-entangled states [5], previously inaccessible to state-of-the art tomographic approaches.

I will then briefly discuss, recent developments in quantum information theory, concerning the high representational power of neural-network quantum states.
[1] Carleo, Troyer, Science 355, 602 (2017).
[2] Carrasquilla, Melko, Nature Physics 13, 431 (2017).
[3] Wang, Physical Review B 94, 195105 (2016).
[4] van Nieuwenburg, Liu, Huber, Nature Physics 13, 435 (2017).
[5] Torlai, Mazzola, Carrasquilla, Troyer, Melko, Carleo, arXiv: 1703.05334.

DY 3: Complex Fluids and Colloids I (joint session CPP/DY)

Time: Monday 9:30–13:00 Location: C 264

DY 3.1 Mon 9:30 C 264
Brownian motion of a microbead coated with a temperature-responsive polymer brush layer — •David van Duinen, Dominik Pilat, Hans-Jürgen Butt, and Rüdiger Berger — Max Planck Institute for Polymer Research, Mainz, Deutschland

We report on a simple method that allows investigating the mechanical contact between a planar surface and a microbead that is covered with a thin stimuli-responsive polymer brush. The brush consists of linear poly(N-isopropylacrylamide) (PNIPAM), which has a lower critical solution temperature (LCST). Below the LCST, the brush is hydrated and extended. In contrast, above the LCST the polymer collapses; this system can be described using a spring model, which is stiffer in the collapsed state than in the hydrated state. Similarly, we have investigated the effect of cononsolvency on the mechanical contact.

This method allows the following and checking of the characteristics of thin polymer films upon exposure to stimuli. The method is simple, and provides information that is otherwise hard to obtain.

DY 3.2 Mon 9:45 C 264
Polymer mediated interactions between colloids immersed in a polymer blend — •Alexander Chervanyov — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

We analytically study the polymer mediated (PM) interactions between colloids immersed in a polymer blend. By making use of standard methods of the liquid state theory we have found out a novel mechanism of the PM interactions caused by non-uniformities in the local composition of the polymer blend induced by the colloids. The relative significance of the contributions to the PM interaction potential due to the finite compressibility of the polymer blend and its compositional non-uniformity is found to drastically depend on the polymer-to-colloid size ratio. In the protein limit of relatively small colloids, the mechanism due to the compositional non-uniformity, specific to polymer blends, is shown to play a dominant role in the PM interactions.

DY 3.3 Mon 10:00 C 264
Spontaneous symmetry breaking of charge-regulated surfaces — •Arghya Majee[1], Markus Bier[1], and Rudolf Podgornik[2] — [1]MPI for Intelligent Systems, Stuttgart & University of Stuttgart, Germany — [2]J. Stefan Institute, Ljubljana & University of Ljubljana, Slovenia

The interaction between two chemically identical charge-regulated sur-

faces is studied using the classical density functional theory. In contrast to common expectations and assumptions, under certain realistic conditions we find a spontaneous emergence of disparate charge densities on the two surfaces [1]. The surface charge densities can differ not only in their magnitude, but quite unexpectedly, even in their sign, implying that the electrostatic interaction between the two chemically identical surfaces can be attractive instead of repulsive. Moreover, an initial symmetry with equal charge densities on both surfaces can also be broken spontaneously upon decreasing the separation between the two surfaces. These findings are fundamental for the understanding of the forces between colloidal objects and, in particular, they are bound to strongly influence the present picture of protein interaction.

Reference:

[1] A. Majee, M. Bier, and R. Podgornik, arXiv: 1709.05005 (2017).

DY 3.4 Mon 10:15 C 264

PFA-PEG particles: A colloidal model system for the investigation of phase diagrams of PEGylated drug carrier systems — •Marcel Werner[1,2], Judith Ruland[2], Nils von Seggern[1], Moritz Tappe[1], Melanie Wernet[2], Gabriela Schmidt[2], and Eckhard Bartsch[1,2] — [1]Department of Macromolecular Chemistry, University of Freiburg, Freiburg im Breisgau, Germany — [2]Department of Physical Chemistry, University of Freiburg, Freiburg im Breisgau, Germany

Pegylated particles like proteins, peptides and lipid- or polymer-based nanoparticles are known as potential drug delivery systems (DDS) or as nano drug carriers (NDC) [1]. Current research deals with e.g. completely new systems [2], shape effects [3] or the influence of the PEG density on the biocompatibility [4]. However, the phase behaviour of the DDS is not really covered. In an attempt to close this gap we synthesised a new model system, consisting of a highly fluorinated core and a sterically stabilizing PEG-shell [5]. With these particles and different light scattering techniques as well as other complementary techniques such as microscopy and rheology, we gained first insights into the phase behaviour of PEGylated particles. Our findings can lead to higher concentrated carrier systems without unwanted inter particle interference and new formylations e.g. gels or cremes.

[1] T. M. Allen et al., Science, 2004, 303, 1818. [2] E. Ruiz-Hernandez et al., Polym. Chem., 2014, 5, 1674. [3] Y. Li et al., Nanoscale, 2015, 40, 16631. [4] J. L. Perry et al., Nano Lett., 2012, 12, 5304. [5] D. Burger et al., Colloids Surf. A: Physico. Eng. Aspects, 2014, 442, 123.

DY 3.5 Mon 10:30 C 264

Interactions in Protein Solutions in the Vicinity of the Gas-Liquid Binodal — •Jan Hansen[1], Florian Platten[1], Jannik Nedergaard Pedersen[2], Jan Skov Pedersen[2], and Stefan U. Egelhaaf[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Department of Chemistry & iNANO, Aarhus University, Denmark

Intermolecular interactions in protein solution depend on a delicate balance of electrostatic, van der Waals and hydrophobic interactions, hydration and other specific contributions. Under certain conditions, short-ranged attractions dominate. Then, proteins can be described as adhesive hard spheres, i.e. their equilibrium phase diagram contains a solubility line below which the metastable gas-liquid binodal is submerged. Here, we examine in how far effective interaction models from colloid science can help to rationalize the phase behavior and interactions of protein solutions in the vicinity of the gas-liquid binodal. For different solution compositions, binodals have been determined by cloud-point measurements, yielding estimates of the critical temperature T_c. The effective structure factor of protein solutions has been determined for various protein concentrations and temperatures by small-angle X-ray scattering. The data is well described by a one-parameter fit based on Baxter's model, from which the second virial coefficient B_2 is inferred. If plotted as a function of temperature normalized by T_c, the values of B_2 follow a universal behaviour for various solution conditions, as suggested by the extended law of corresponding states.

DY 3.6 Mon 10:45 C 264

Behavior under shear of solutions of bovine serum albumin and trivalent cations — •Stefano Da Vela[1], Miriam Siebenbürger[2], Alessio Zaccone[3], Fajun Zhang[1], Matthias Ballauff[2,4], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, University of Tübingen, Tübingen, Germany — [2]Helmholtz Zentrum für Materialien und Energie, Berlin, Germany — [3]Dept. of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge, UK — [4]Department of Physics, Humboldt-University, Berlin, Germany

Trivalent cations such as Y(III) and La(III) have been shown to induce a rich phase behavior in aqueous solutions of acidic proteins. Thanks to the specific association of the cations with the negatively charged groups on the protein surface, these systems feature directional, patchy interactions. Here we show how shear stress can trigger aggregation in solutions of the acidic protein bovine serum albumin (BSA) in the presence of La(III). The trivalent cation renders the system unstable at high shear rates and the solutions become turbid. Simultaneously a low wavevector upturn develops in small-angle neutron scattering profiles. We discuss the findings in relations to the available theoretical models. As directionality and anisotropy of the interaction are common in proteins, a better understanding of the role of patchiness for shear-induced aggregation is important for many biotechnological operations such as filtration, stirring, filling of containers, and pumping.

DY 3.7 Mon 11:00 C 264

Unification of Lower and Upper Critical Solution Temperature Transitions in Aqueous Protein Solutions — •Nafisa Begam, Stefano Da Vela, Fajun Zhang, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen

Phase separation in aqueous protein solution is of primary interest in the field of many biological and chemical processes. In particular, phase separated protein solutions exhibiting lower/upper critical solution temperature (LCST/UCST) behavior have been of significant importance in the food and pharmaceutical industries. Based on theoretical calculations [1] and experimental observations, it is predicted that proteins can be designed with tunable LCST and UCST. Here, our goal is to experimentally design such aqueous protein system showing tunable LCST and UCST transitions. The UCST phase of β-Lactoglobulin - Yttrium Chloride (YCl_3) based aqueous systems at a salt concentration higher than a critical concentration, c*, has been already reported by our group [2]. However, we obtain evidence of LCST phase behavior of this system at a lower salt concentration but higher than c*. The solution becomes turbid at high temperature and clear at low temperature. Similar indication of the presence of both LCST and UCST phase behavior we get from the SAXS measurements on Bovine serum Albumin (BSA) - YCl_3 system. The findings of this study suggest a controllable dual phase of aqueous protein solution by tuning the ionic strength. [1] Jianguo Li et. al, *J. Chem. Phys.*, **128**, 235104, (2008) [2] F. Zhang et. al, *J. App. Crystal.*, **44**,755-762, (2011)

Invited Talk DY 3.8 Mon 11:15 C 264

Reconfigurable colloidal structures — •Daniela J. Kraft — Soft Matter Physics, Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics, Leiden, The Netherlands

Reconfigurability is an essential feature of functional micro- and nanomachines. One way to realize reconfigurability is to introduce microscopic hinges, that is, elements that allow rotation while conserving the relative order of their arrangement. We have developed two experimental realizations of these pivotal elements on the colloidal length scale: I will first show how the deposition of oil droplets in colloidal aggregates lubricates the contact area and thereby enables and drives the reconfiguration into uniform, compact structures. Secondly, I will introduce colloidal particles with surface-mobile DNA linkers that enable the formation of strong and specific hinging bonds. I will describe how this bond mobility affects the self-assembly pathway and demonstrate the assembly of a variety of reconfigurable structures, such as floppy lattices, colloidal polymers and flexible colloidal molecules. These novel colloidal building blocks give access to a new class of materials with great potential in shape-shifting systems, actuators and colloidal robots.

DY 3.9 Mon 11:45 C 264

Preparation of amphiphilic asymmetric patchy particles and their effect on emulsion properties — •Marco Rehosek, Akilavasan Jeganathan, and Frank Marlow — Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr/Germany

Asymmetric patchy particles (APPs) have two different functionalities on the opposing sides of such a micro- or nanoparticle. These functionalities can be of a magnetic, chemical, or optical nature. Here we study different chemical polarities. Amphiphilic APPs having hydrophobic and hydrophilic regions show interesting performance as emulsifying

agent. This effect enhances the so-called Pickering stabilization resulting in a "breathable skin" at a liquid|liquid interface.

In this work, the preparation of amphiphilic APPs and their effect on emulsions is studied. Titania&organosilane APPs were prepared via a wax-masking-symmetry breaking step. The unmasked part was modified by vapor deposition. The effect of the APPs on emulsion stability and aging effects of APP-stabilized emulsions was studied qualitatively by liquid-phase-distribution measurements. For a deeper understanding, rheological properties of the emulsions were investigated. Viscosimetry gave information on stress-dependent viscosity effects, while oscillation measurements reveal the viscoelastic properties. Long-time measurements resulted in information on aging processes in the emulsion i.e. creaming, coalescence and Ostwald ripening.

DY 3.10 Mon 12:00 C 264

On effective sphere models for self-diffusion of nonspherical particles — •Felix Roosen-Runge, Jin Suk Myung, Peter Schurtenberger, and Anna Stradner — Division of Physical Chemistry, Lund University, Sweden

Modeling diffusion of nonspherical particles presents an unsolved and considerable challenge, despite its importance for the understanding of crowding effects in biology and nanotechnology. A common approach is the mapping of nonspherical objects on effective spheres to subsequently approximate phenomena for nonspherical particles with the established predictions for spheres. Using hydrodynamic simulations, we show that this so-called effective sphere model fundamentally fails to represent the short-time self-diffusion of nonspherical particles even at low volume fractions and small to moderate nonsphericities. Based on analytical theory of hydrodynamic interactions, we discuss possible improvements for the modeling as well as the implications of our findings for studies employing effective spheres.

DY 3.11 Mon 12:15 C 264

Ultrasoft colloids under pressure driven flow — •Deepika Deepika and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany

Star-shaped polymers show a continuous change of properties from flexible linear chains to soft colloids, as the number of arms is increased. To investigate the effect of macromolecular architecture on the flow behavior, we employed computer simulations of single star polymers as well as of mixtures of star and linear polymers under dilute conditions. Hydrodynamic interactions were incorporated through the multi-particle collision dynamics (MPCD) technique, while a bead-spring model was used to describe the polymers. At rest, the polymers were distributed homogeneously in the slit channel, irrespective of the number of arms. Once flow was applied, however, we found that the stars migrated more and more towards the channel center as the number of arms increased and the polymers became more rigid. These findings are in contrast to previous findings for deformable vesicles, where the softer particles moved to the channel center. We surmise that the observed behavior for polymers is due to effective arm stretching and hydrodynamic repulsion with the channel walls. In the star-chain mixtures, we found a flow-induced separation between stars and chains, with the stars being in the center and the chains closer to the walls. The results from our study give valuable insights for designing microfluidic devices for separating particles based on their rigidity.

DY 3.12 Mon 12:30 C 264

Control of physico-chemical properties of Pickering emulsions for catalysis — •Dmitrij Stehl[1], Tobias Pogrzeba[2], Lena Hohl[3], Yuri Lvov[4], Matthias Kraume[3], Reinhard Schomäcker[2], and Regine von Klitzing[1] — [1]Festkörperphysik, TU Darmstadt, Darmstadt, Deutschland — [2]Institut für Chemie, TU Berlin, Berlin, Deutschland — [3]Prozess- und Verfahrenstechnik, TU Berlin, Berlin, Deutschland — [4]Institute for Micromanufacturing, Lousiana Tech University, Lousiana, USA

Pickering-emulsions (PEs) are particle-stabilized emulsions. Different solid nanoparticles stabilize emulsion droplets against coalescence. Halloysite nanotubes (HNT) can be used as emulsifier. These particles are multiwall, inorganic tubes with negative charges at the outer surface and positive charges at the inner surface. The length of the HNTs in this study is 800 +- 200 nm and the outer diameter is 50 nm. HNTs adsorb laterally at the water/oil interface and the energy of detachment is several 10.000 kT. Due to the anisotropy of the HNT, the behavior of the nanotubes at the interface is different from spherical particles and the stability of the respective PE is higher which is studied in detail. The effect of different parameters on the structure of the PEs is studied, like HNT surface modification and energy input by the PE-fabrication, effect of HNT concentration, salt (NaCl) concentration and pH. In this study, the hydroformylation of long chain olefins (1-Dodecene) in PEs was used as a model system. The water phase contains the homogeneous Rh-catalyst and the oil phase (1-Dodecene) is simultaneous the reactant.

DY 3.13 Mon 12:45 C 264

Crystal-fluid surface tension in the two dimensional binary hard disk mixture, a DFT study — •Shang-Chun Lin and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany

Using fundamental measure theory, we investigate phase diagrams and crystal-fluid surface tensions in additive and nonadditive two-dimensional hard disk mixtures of small and large spheres with size ratio q. In the nonadditive case, the small disks act as ideal "polymeric" depletants (Asakura-Oosawa model) and the surface tension (for small q) shows a minimum with increasing small sphere concentration. We compared to the additive case, with an interface between fluid and crystals with substitutional disorder, and find a similar behavior (for small q). For larger q, the surface tension is almost constant upon adding the small spheres. In these investigations, the fluid-solid transitions were first-order due to the assumption of a periodic unit cell in the DFT calculations. We examine the possibility of relaxing this assumption and finding a hexatic phase in fundamental measure theory.

DY 4: Talk D. Bartolo

Time: Monday 9:30–10:00 Location: BH-N 243

Invited Talk DY 4.1 Mon 9:30 BH-N 243

Sounds and stubbornness of active fluids. — •Denis Bartolo, Delphine Geyer, and Alexandre Morin — ENS de Lyon, Lyon, France

I will first show how to engineer spontaneously flowing colloidal liquids. Simply put our strategy consists in letting self-propelled colloids with velocity-alinement interactions to collide in microfluidic channels. After a short transient they self-assemble into liquids with emergent long-range orientational order which translates into spontaneous unidirectional flows. I will devote most of my talk to discussing the fluctuations and the dynamical response of these intrinsically non equilibrium materials. (i) I will show that both density and velocity fluctuations almost freely propagate along all directions and exploit these sound modes to infer the analogous of the Navies Stokes equation for polar active liquids. (ii) I will discuss the robustness of their spontaneous flows to external pressure gradients. I will evidence that (french) colloids can be collectively very resistant when one tries to waive their privilege to freely choose their direction of motion.

DY 5: Talk J. Parrondo

Time: Monday 9:30–10:00 Location: BH-N 334

Invited Talk DY 5.1 Mon 9:30 BH-N 334

Irreversibility and dissipation in molecular motors and kinetic networks — •Juan MR Parrondo — Universidad Complutense de Madrid (Spain)

I will review our past work on the quantitative connection between entropy production and irreversibility, as measured by the relative entropy between forward and backward trajectories. In the last part of the talk, I will present some recent work on the application of those ideas to the estimation of the entropy production in molecular motors and kinetic networks when the observer has only access to a restricted number of variables.

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

Time: Monday 10:00–12:45 Location: EB 107

DY 6.1 Mon 10:00 EB 107

Post-Ehrenfest many-body quantum interferences far-out-of-equilibrium many-body systems — Steve Tomsovic[1,4], Denis Ullmo[2], Peter Schlagheck[3], •Juan-Diego Urbina[4], and Klaus Richter[4] — [1]Washington State University, USA — [2]Universite Paris Sud, France — [3]University of Liege, Belgium — [4]University of Regensburg, Germany

Many-body quantum dynamics in isolated systems far from equilibrium generate interferences beyond the Ehrenfest time where quantum and classical expectation values diverge, with recent interest in the role these interferences play in the spreading of quantum information across the many degrees of freedom[1]. We have developed a semiclassical theory which properly incorporates such quantum interference effects and showed that, for mesoscopically populated Bose-Hubbard systems, it captures post-Ehrenfest quantum phenomena very accurately even to the point to alllow for high-precision many-body spectroscopy [2].

We present here a description of this novel approach and point out how it can be used to improve the heavily used truncated Wigner method [3] by incorporating exact degenaracies of classical actions responsible of robust many-body interference effects.

[1] S. H. Shenker and D. Stanford, JHEP 3, 67 (2014).
[2] S. Tomsovic, P. Schlagheck, D. Ullmo, J. D. Urbina, and K. Richter arXiv 1711.04693 (2017).
[3] A. Sinatra, C. Lobo, and Y. Castin, J. Phys. B: Atom. Molec. Opt. Phys. 35, 3599 (2002).

DY 6.2 Mon 10:15 EB 107

Signatures of indistinguishability in bosonic many-body dynamics — Tobias Brünner[1], Gabriel Dufour[1,2], •Alberto Rodríguez[1], and Andreas Buchleitner[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104, Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität Freiburg, Albertstraße 19, D-79104 Freiburg, Germany

Many-body interference occurs as a fundamental process during the evolution of a quantum system consisting of two or more indistinguishable particles. The (measurable) consequences of this interference, as a function of the particles' mutual indistinguishability, was studied for non-interacting photons transmitted through beam-splitter arrays. However, the role of many-body interference in the dynamics of interacting particles, e.g. cold atoms in optical lattices, had so far remained unclear. We identify a quantifier of the particles' mutual indistinguishability attuned to time-continuously evolving systems of (interacting) particles, which predicts the dynamical behaviour of observables influenced by genuine few-body interference. Our measure allows a systematic exploration of the role of many-body interference in the weakly and strongly interacting regimes.

DY 6.3 Mon 10:30 EB 107

Trajectory-based approaches for simulating nonequilibrium dynamics in open quantum systems — •Shunsuke Sato[1], Aaron Kelly[2], and Angel Rubio[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, DE — [2]Dalhousie University, Halifax, Canada

We present our recently developed trajectory-based quantum dynamics approach for treating nonequilibrium phenomena in electron-phonon systems. Based on a simple extension of mean field theory, this new approach leads to simulation scheme that uses a statistical ensemble of coupled trajectory pairs. The time-evolution of each pair is governed by the Euler-Lagrange variational principle. This method yields mean field theory in the limit that the trajectories are orthogonal, and in the limit that they completely overlap. Although trajectories are only coupled to a single partner, this method shows a substantial improvement over mean field theory in capturing quantum coherence in the nuclear dynamics as well as electron-nuclear correlation. The performance of our coupled trajectory method is particularly favourable in nonadiabatic systems, as it retains quantitative accuracy well beyond the perturbative electron-phonon coupling regimes of the spin-boson model, and the Holstein polaron model.

Furthermore, when utilized in tandem with the Nakajima-Zwanzig-Mori generalized quantum master equation formalism, this hybrid trajectory-based master equation approach provides an attractive route forward to a fully ab initio description of relaxation processes, such as thermalization, in condensed phase systems.

DY 6.4 Mon 10:45 EB 107

Energy transport in the driven disordered XYZ chain — •Maximilian Schulz[1,2], Scott Taylor[2], Chris Hooley[2], and Antonello Scardicchio[3,4] — [1]Max Planck Institut für Physik komplexer Systeme — [2]University of St Andrews — [3]Abdus Salam ICTP — [4]INFN, Sezione di Trieste

The delocalized region preceding the many-body localization (MBL) transition is currently receiving a significant amount of attention due to apparent deviations from typical diffusive transport. The XXZ spin chain has been shown to exhibit subdiffusive spin transport at intermediate disorder strengths, and the nature of energy transport close to the MBL transition is still a matter of debate.

We present results of a combined time-evolving block decimation and exact diagonalization study of energy currents in the disordered XYZ spin chain on the delocalized side of the MBL transition. The significance of this choice of model is that its clean hydrodynamics involves only energy currents, whereas the XXZ model has both energy and spin currents. This allows us to explore the question of how the nature of the delocalized phase depends on the hydrodynamic properties of the underlying clean model.

DY 6.5 Mon 11:00 EB 107

Construction of exact constants of motion and effective models for many-body localized systems — •Marcel Goihl, Marek Gluza, Christian Krumnow, and Jens Eisert — Dahlem Center for Complex Quantum Systems, Freie Universitat Berlin, 14195 Berlin, Germany

One of the defining features of many-body localization is the presence of extensively many quasi-local conserved quantities. These constants of motion constitute a corner-stone to an intuitive understanding of much of the phenomenology of many-body localized systems arising from effective Hamiltonians. They may be seen as local magnetization operators smeared out by a quasi-local unitary. However, to accurately identify such constants of motion remains a challenging problem. Current numerical constructions often capture the conserved operators only approximately or trade desirable properties such as exactly commuting with the Hamiltonian against each other, restricting a conclusive understanding of many-body localization. In this talk, we use methods from the theory of quantum many-body systems out of equilibrium to establish a new approach for finding a complete set of exact constants of motion which are in addition by construction guaranteed

to represent Pauli-z operators. By this we are for the first time able to construct and investigate the proposed effective Hamiltonian using exact diagonalization. Hence, our work provides an important tool expected to further boost inquiries into the breakdown of transport due to quenched disorder.

15 min. break

DY 6.6 Mon 11:30 EB 107

Non-Ergodic Dynamics in Many-Body Systems — Carlo Danieli and •Sergej Flach — Center for Theoretical Physics of Complex Systems, Institute for Basic Sciences, Daejeon, Korea

Integrable models are characterized by a set of preserved actions. Close to the limits, the nonintegrable perturbations span a coupling network in action space which can be short or long ranged. The equilibrium dynamics of a system close to such limits is sensitive to the network type. Long range networks enforce ergodicity with large but finite relaxation time scales at a finite distance to the integrable limit. Short range networks lead to a loss of ergodicity at a finite distance from the limit. We demonstrate this by choosing observables which turn conserved actions at the limit. Off the limit, and fixing their value to the proper statistical average, they define manifolds in the phase space of an ergodic and equipartitioned many-body system. A typical trajectory pierces such manifolds infinitely often as time goes to infinity. Close to the integrable limit, the dynamics yields a power-law distribution of the excursion times off the manifolds. The exponent is used as a measure of distance from a potential nonergodic regime. We analyse several cases: the Fermi Pasta Ulam chain in the limit of small energies (long range network), and the Klein-Gordon, Discrete Gross Pitaevskii and coupled rotor lattices in the limit of large energies (short range network).

DY 6.7 Mon 11:45 EB 107

memory effects in the strongly anharmonic FPUT model — •Graziano Amati[1], Hugues Meyer[2], and Tanja Schilling[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Research Unit in Engineering Science, Université du Luxembourg, L-4364 Esch-sur-Alzette, Luxembourg

The Fermi-Pasta-Ulam-Tsingou (FPUT) Problem represents an intriguing challenge in Modern Physics. In its original formulation, it questions whether or not a Dynamical System can reach thermalization if a small anharmonicity is added to an integrable system, under specific out-of-equilibrium initial conditions. The problem was originally raised by the apparent lack of energy spreading between the normal modes of a one-dimensional chain of particles with a small anharmonicity, in case the energy at the initial time is given to the lowest frequencies of the system.

In the present work, we consider a one-dimensional chain of many particles with a strongly anharmonic interaction potential. The model is initialized at canonical equilibrium, and we take as a relevant variable the Fourier Transform of the density of particles for a tagged degree of freedom. The time correlation function of this observable exhibits an interesting non-ergodic behavior due to a temperature-driven 'FPU-like' dynamical localization, that corresponds to a nontrivial memory profile.

Via a novel coarse-graining technique, we are able to reconstruct the dynamics of the memory, and to show that the exhibited non-ergodicity can be rephrased via the memory kernel of the process.

DY 6.8 Mon 12:00 EB 107

Dynamical quantum phase transitions in the particle-antiparticle production of a lattice gauge theory — •Yi-Ping Huang and Markus Heyl — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

Particle-antiparticle production in the presence of a static classical electric field, known as the Schwinger mechanism, represents a central physical phenomenon in gauge theories. How the particle production is affected in the quantum limit, where the backaction onto the electric field becomes essential, remains a major challenge. In this work, we study particle-antiparticle production in the quantum quench dynamics after a strong coupling of the bare particles to dynamical gauge field in a quantum link model. We find that for a strong coupling the system experiences dynamical quantum phase transitions (DQPTs) where the vacuum persistence probability (Loschmidt echo) develops non-analytic behavior at critical times. As opposed to the Schwinger mechanism, where matter fields are suddenly coupled to a classical electric field, we observe that the dynamics of the vacuum persistence probability and therefore the DQPTs cannot be understood using the classical picture of particle production. Instead, a quantum dynamical pattern emerges from the strongly coupled matter fields and dynamical gauge fields. We discuss how these findings can be experimentally observed in quantum simulators such as trapped ions.

DY 6.9 Mon 12:15 EB 107

Critical quench dynamics of random quantum spin chains — •Gergö Roosz[1,2], Yu-Cheng Lin[3], and Ferenc Igloi[2] — [1]Technische Universität Dresden — [2]MTA Wigner RCP, Hungary — [3]Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan

By means of free fermionic techniques combined with multiple precision arithmetic we study the time evolution of the average magnetization, $\overline{m}(t)$, of the random transverse-field Ising chain after global quenches. We observe different relaxation behaviors for quenches starting from different initial states to the critical point. Starting from a fully ordered initial state, the relaxation is logarithmically slow described by $\overline{m}(t) \sim \ln^a t$, and in a finite sample of length L the average magnetization saturates at a size-dependent plateau $\overline{m}_p(L) \sim L^{-b}$; here the two exponents satisfy the relation $b/a = \psi = 1/2$. Starting from a fully disordered initial state, the magnetization saturates to an asymptotic value $\overline{m}_p(L) \sim L^{-b'}$, with $b' \approx 1.5$. For both quenching protocols, finite-size scaling is satisfied in terms of the scaled variable $\ln t/L^{\psi}$. Furthermore, the distribution of long-time limiting values of the magnetization shows that the typical and the average values scale differently and the average is governed by rare events. The non-equilibrium dynamical behavior of the magnetization is explained through semi-classical theory.

DY 6.10 Mon 12:30 EB 107

Many-Body Localization in the Central Spin Model — •Hetterich Daniel[1], Yao Norman[2], and Trauzettel Björn[1] — [1]Institut für Theoretische Physik, Universität Würzburg, D-97074 W\"urzburg, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA

The periodic Heisenberg chain model obeys signatures of many-body localization (MBL) that persist the insertion of a central spin, which interacts with all other spins of the periodic chain. To support this statement, we present numerical results for the level repulsion of eigenvalues and for the growth of entanglement entropy of subsystems. We discuss why under which conditions the central spin destroys the localized phase. Finally, we show that local observables that measure the central spin only serve as a MBL detector.

DY 7: Modeling and Data Analysis

Time: Monday 10:00–11:45 Location: BH-N 128

DY 7.1 Mon 10:00 BH-N 128

MD simulations on martensitic transformations in iron-palladium — •Alexander Holm[1,2] and Stefan G. Mayr[1,2] — [1]Leibniz Institute of Surface Engineering (IOM), Leipzig — [2]Division of Surface Physics, Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, University of Leipzig

We report about molecular dynamics (MD) simulation studies on martensitic transitions in iron-palladium (Fe_7Pd_3) shape memory alloys, mentioning custom-designed embedded atom method (EAM) potentials based on density functional theory (DFT) calculations. Upon application of an uniaxial compressive strain to the simulation cell it was found that the transformation from a face centered cubic crystal-lattice-configuration to a body centered tetragonal configuration occurs, exhibiting orientation variants which can be connected to the structural phenomenon of twinning, which is a prerequisite for the shape memory effect in Fe_7Pd_3.

The focus of this presentation will lie on the structural properties of the martensitic phase transition, regarding transformation paths and the introduction of a new method to determine structural changing incidents from a series of radial distribution functions, the *RDF-Separation-Function*.

DY 7.2 Mon 10:15 BH-N 128

Monte Carlo Simulations of Poly(3-hexylthiophene) aggregation — •Jonathan Gross and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig,

Poly(3-hexylthiophene) (P3HT) is a semiconducting polymer that has applications in organic photovoltaics. It is widely used as a semiconducting layer in organic thin film field effect transistors (FETs) and solar cells. We found that a recently developed coarse-grained model [1] of P3HT, is suitable and able to reproduce not only fully atomistic simulations, but also experimental results [2, 3, 4]. On the basis of those single-chain studies, we now take the next step and look at aggregation of a few polymers, to gain an understanding of the fundamental processes that happen during the crystallization of P3HT. With replica-exchange (parallel tempering) simulations we investigate a system of a few short P3HT chains in the presence of a Au(001) surface and without a substrate.

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[4] M. Ivanov, J. Gross, and W. Janke, Eur. Phys. J. Special Topics 226 (2017) 667.

DY 7.3 Mon 10:30 BH-N 128

Temporal and spatial characteristics of electron cascades triggered by X-ray photons in LiF — •Vladimir Lipp[1], Nikita Medvedev[2], and Beata Ziaja[1,3] — [1]CFEL at DESY, Hamburg, Germany — [2]Institute of Physics and Institute of Plasma Physics, Academy of Science of Czech Republic, Prague, Czechia — [3]Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland

Low-fluence X-ray irradiation of alkali halides may cause long-living lattice defects called color centers. It is assumed that their spatial distribution reflects the X-ray beam shape and, therefore, may serve as an efficient diagnostic tool for the spatial pulse profile [1]. The color centers may be created via exciton decay mechanism; excitons are created when self-trapped valence holes catch free electrons, both produced by an intense X-ray pulse. However, X-ray-induced energetic photoelectrons trigger secondary electron cascades, which may strongly influence the final distribution of the valence holes before their self-trapping, and thereby of the color centers. Our in-house classical Monte-Carlo simulation tool XCascade-3D [2] follows the electron cascades in time and space. It provides distributions of the electrons and holes in various X-ray-irradiated materials, including alkali halides. For the study case of LiF, we present the corresponding calculations which enable to establish a connection between the experimentally measured distribution of the X-ray-induced color centers in LiF and the spatial shape of the X-ray beam – with potential experimental applications. References: [1] Pikuz, Faenov, Matsuoka et al., Scientific Reports 5, 17713 (2015). [2] Lipp, Medvedev, Ziaja, Proc. SPIE 10236, 102360H (2017).

DY 7.4 Mon 10:45 BH-N 128

Phase field modeling of diffusion-limited precipitation in multi-component Ni-based superalloys — •Markus Holzinger, Michael Fleck, and Uwe Glatzel — Metals and Alloys , University Bayreuth, Germany

We develop a phase-field model for the simulation of phase transformations in metallic multi-component alloys (Ni-based superalloys) with industry-relevant chemical complexity. This model is built to take into account thermodiffusion, elastic effects and inhomogeneities. The thermodynamic formulation is validated by comparisons to respective CALPHAD equilibrium calculations using the commercial program ThermoCalc. Furthermore, an elastic term is included in the model to account for the misfit stresses as well as elastic inhomogeneities between the two considered phases. We consider the coarsening kinetics of γ'-precipitates in single crystalline Ni-based cast-alloys. Here we show the results of a elastic strain simulation. We also discuss the results in comparison with experiments.

DY 7.5 Mon 11:00 BH-N 128

Breathing with the beating of the heart: A machine-learner's approach to ECG-derived respiratory signal estimation — •Stephan Bialonski[1], Daniel Vorberg[2], and Justus Schwabedal[3] — [1]Center for Advancing Electronics Dresden (cfaed), TU Dresden — [2]Max-Planck-Institute for the Physics of Complex Systems, Dresden — [3]Department of Biomedical Informatics, Emory University School of Medicine, Atlanta

We investigated how machine learning models can be used to extract knowledge from biophysical systems. As a test case, we studied the challenge to derive respiratory information from electrocardiographic (ECG) signals, a long-standing problem in sleep research. We identified two well-known coupling mechanisms by analyzing a long short-term memory (LSTM) architecture that we fitted to predict respiratory information from ECG signals. These mechanisms couple heart beat dynamics and respiration and comprise of a physiological coupling (respiratory sinus arrhythmia) as well as a physical coupling that is related to the position of measurement electrodes relative to the heart. We verified these results by modelling the coupling mechanisms and studying the resulting patterns in our LSTM architecture.

DY 7.6 Mon 11:15 BH-N 128

Profile likelihood based analyses of infectious disease models — •Christian Tönsing[1], Jens Timmer[1,2,3,4], and Clemens Kreutz[1,2,4] — [1]Institute of Physics, University of Freiburg, Freiburg im Breisgau, Germany — [2]Freiburg Center of Data Analysis and Modeling (FDM), University of Freiburg, Freiburg im Breisgau, Germany — [3]BIOSS Centre for Biological Signalling Studies, University of Freiburg, Freiburg im Breisgau, Germany — [4]Center for Biosystems Analysis (ZBSA), University of Freiburg, Freiburg im Breisgau, Germany

Ordinary differential equation (ODE) models are frequently applied to describe the dynamics of epidemics. In this work, we use such models of infectious diseases for the estimation of a priori unknown model parameters and their uncertainties from the information contained in recorded data of infected individuals. A deterministic multistart optimization approach is applied for parameter estimation. Moreover, we introduce profile likelihood-based uncertainty analyses and check the identifiability of a simple SIR model with data from an influenza outbreak at an English boarding school in 1978. Furthermore, a complex ODE model for vector-borne diseases with data from the Zika virus (ZIKV) outbreak in Colombia in 2015/16 is used for data-based model reduction utilizing likelihood profiles.

DY 7.7 Mon 11:30 BH-N 128

Modelling of non-Gaussian stochastic processes with memory — •Katja Polotzek and Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Many real world phenomena such as wind speeds and rainfall amounts do not follow a Gaussian distribution. Among other shapes events might occur in an asymmetric or one-sidedly bounded manner. We obtain models for such situations by applying nonlinear transforma-

tions to Gaussian processes. By an appropriate choice of the transformation we can not only adjust the model distribution to the empirical data but also infer properties of the model from the well understood underlying Gaussian process. In particular, we are interested in the behaviour of the autocorrelation function and the memory structure of the stochastic processes. We illustrate the method by modelling daily rainfall amounts, which exhibit indications of long-range dependence.

DY 8: Active Matter I (joint session DY/CPP/BP)

Time: Monday 10:00–13:15 Location: BH-N 243

DY 8.1 Mon 10:00 BH-N 243

Dynamics of sedimenting active particles — •Jérémy Vachier and Marco G. Mazza — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The collective motion of active particles has attracted enormous interest on account of the technological applications of artificial and biological particles. Even in the simple case of a dilute suspension solely subject to gravity, active particles show interesting behavior. While theoretical studies have addressed this problem with effective theories, a full time-dependent solution of the sedimentation problem has been neglected. Here, we present an analytical solution of the Fokker–Planck equation for the stochastic process which allows us to describe the full dynamics of active particles in three dimensions under an external force. Our results are supported by numerical calculations in which weak hydrodynamics interactions are approximated. We address three cases: active particle under gravity, confinement by reflecting barriers, and the effect of the activity of the particles on their collective motion. Finally, we compare our results with experiments and find a very good agreement.

DY 8.2 Mon 10:15 BH-N 243

Active systems learning at the microscale — •Santiago Muiños-Landin[1], Keyan Ghazi-Zahedi[2], and Frank Cichos[1] — [1]Molecular Nanophotonics. University of Leipzig. Institut for Experimental Physics I — [2]Information Theory of Cognitive Systems, Max Planck Institute for Mathematics in the Sciences

Living organisms are able to sense and process information about the environment they live in. They are also able to update this information in order to contruct solutions for real life problems such as finding food or avoiding danger. This active adaption process that in the long run drives the evolution of species is the result of a short time scale evolution of the knowledge of an organism that we know as learning. At the microscale the learning is hampered by stochasticity given that the intrinsic Brownian noise makes critical to build a feedback between stimulus and action. Here, we present a system based on a self-themophoretic microswimmer that allows the application of artifical intelligence algorithms at the microscale. Using reinforcement learning we show that even under noise conditions a system is able to learn how to optimize a simple navigation task. We study the influence of noise and the situation where multiple agents can share information to carry out specific tasks. This way we show how adaptation and intelligent collective behavior can be studied in artificial microswimmers systems.

DY 8.3 Mon 10:30 BH-N 243

Collective rotations of active particles interacting with obstacles — •Zahra Mokhtari[1], Timo Aspelmeier[2], and Annette Zippelius[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Institut für Mathematische Stochastik, Georg-August-Universität Göttingen, Germany

We study the motion of active particles in the presence of static obstacles. We observe accumulation and crystallization of active particles around the obstacles which serve as nucleation sites, a phenomenon that is expected due to the known absorption of active particles at solid boundaries. In the limit of high activity, the crystals start to rotate spontaneously around the obstacle, resembling a rotating rigid body. We explain the occurrence of such rotations through the enhanced attraction of particles to the cluster whose orientation points along its rotational velocity as compared to those whose orientation points in the opposite direction.

DY 8.4 Mon 10:45 BH-N 243

Collective dynamics of squirmers confined to a surface by strong gravity — •Jan-Timm Kuhr, Felix Rühle, Johannes Blaschke, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenberg Str. 36, 10623 Berlin, Germany

External fields acting on microswimmers are of paramount importance for collective phenomena like bioconvection. In previous work we explored the individual [1] and collective [2] dynamics of squirmer model swimmers under moderate gravity by MPCD simulations. Here, we turn to strong gravity, where microswimmers form a single layer at the bottom surface, while interacting hydrodynamically in 3D.

We find various intriguing phenomena depending on the swimmer type (neutral, pusher, and puller) and area density: Formation of pairs, chains and other metastable bound states, but also collective swarming parallel to the surface.

Neutral squirmers at low area densities repel each other by their self-generated flow fields and thereby arrange in strongly disturbed hexagonal lattices reminiscent of 2D crystals subject to intense fluctuations. For higher densities attractive interactions become important and give rise to pair and chain formation. We characterize these distinct emergent states, compare to melting of 2D colloids, and explore the flow fields, which create hexagonal lattices.

[1] F. Rühle *et al.*, accepted at New J. Phys.
[2] J.-T. Kuhr, J. Blaschke, F. Rühle, and H. Stark, Soft Matter **13**, 7548 (2017).

DY 8.5 Mon 11:00 BH-N 243

Learning agents as a model for collective motion — •Katja Ried[1], Thomas Müller[2], and Hans J. Briegel[1,2] — [1]Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21a, 6020 Innsbruck, Austria — [2]Department of Philosophy, University of Konstanz, 78457 Konstanz, Germany

Watching a swarm of fish, birds or insects is mesmerizing, and it inevitably makes one wonder how countless independent individuals can form such a perfectly coordinated whole. A number of theoretical models attempt to answer this question by studying the collective dynamics that arise when individuals interact according to certain rules. However, these rules are often simply postulated ad hoc, and individuals are modelled as featureless points carrying them out. Naturally, such models are unlikely to provide an accurate - or even plausible - account of the individual-level behaviour that ultimately drives the swarm.

I will present a different Ansatz to this problem, wherein individuals are considered as full-fledged agents: distinct entities that can perceive certain (reasonable) features of their surroundings, endowed with a stable internal mechanism for processing these perceptions and deciding how to respond, and capable of modifying these responses as a function of their personal experience. I will illustrate this Ansatz with the example of locusts marching in a one-dimensional arena and discuss what insights agent-based models can offer to the study of collective motion.

15 min. break

DY 8.6 Mon 11:30 BH-N 243

Localized States in an Active Phase-Field-Crystal Model — •Lukas Ophaus, Johannes Kirchner, Svetlana Gurevich, and Uwe Thiele — Institut für Theoretische Physik, WWU, Münster, Germany

The Phase-Field-Crystal (PFC) model provides a simple microscopic description of the thermodynamic transition from a fluid to a crystalline state [1]. The model can be combined with the Toner-Tu theory for self-propelled particles to obtain a model for crystallization (swarm formation) in active systems [2]. Within the resulting active PFC model, resting and traveling crystals can be identified. In the linear regime, we give analytical expressions for the transitions from the liquid state to both types of crystals. In addition, we provide a general semi-analytical criterion for the onset of motion in the nonlinear regime, that corresponds to a drift-pitchfork bifurcation. Like the

passive PFC model [3], the active version describes a variety of localized states (LS) besides spatially extended crystals. In the spatially one-dimensional case we explore how the bifurcation structure (slanted homoclinic snaking) is amended by activity. Numerical continuation is applied to follow resting and traveling LS while varying the activity and mean concentration. A fold continuation allows us to determine the area of existence of different states in a two parameter plane. Finally, we look into the scattering behavior of LS through numerical time simulation. [1] M.J. Robbins et al., PRE 85, 061408 (2012). [2] A.M. Menzel and H. Löwen, PRL 110, 055702 (2013). [3] U. Thiele et al., PRE 87, 042915 (2013)

DY 8.7 Mon 11:45 BH-N 243

Turbulence and pattern formation in a minimal model for active fluids — •Martin James[1], Wouter Bos[2], and Michael Wilczek[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]LMFA, CNRS, École Centrale de Lyon, France

Continuum theories of active fluids display a fascinating range of dynamical states, including stationary patterns and turbulent phases. While the former can be tackled with classical pattern formation theory, the spatio-temporal disorder of active turbulence calls for a statistical description. In this presentation, new results on turbulence and pattern formation in a minimal continuum model for active fluids, which has been recently proposed by Wensink et al. [PNAS 109(36):14308 (2012)], will be discussed. Adopting techniques from turbulence theory, we establish a quantitative description of correlation functions and spectra for active turbulence. We furthermore report on a novel type of turbulence-driven pattern formation far beyond linear onset: the emergence of a dynamic vortex lattice state after an extended turbulent transient, which can only be explained taking into account turbulent energy transfer across scales.

DY 8.8 Mon 12:00 BH-N 243

Emergence of phytoplankton patchiness at small scales in mild turbulence — Rebekka E. Breier, Cristian C. Lalescu, Michael Wilczek, and •Marco G. Mazza — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, 37077 Göttingen

Phytoplankton often encounter turbulence in their habitat. As most toxic phytoplankton species are motile, resolving the interplay of motility and turbulence has fundamental repercussions on our understanding of their own ecology and of the entire ecosystems they inhabit. The spatial distribution of motile phytoplankton cells exhibits patchiness at distances of decimeter to millimeter scale for numerous species with different motility strategies. The explanation of this general phenomenon remains challenging. Furthermore, hydrodynamic cell-cell interactions, which grow more relevant as the density in the patches increases, have been so far ignored. Here, we combine particle simulations and continuum theory to study the emergence of patchiness in motile microorganisms in three dimensions. By addressing the combined effect of turbulent flow conditions, and spatial correlations in the particle positions, we uncover a general mechanism: when motility allows cells to cross the fluid streamlines, the typical length scale associated to the small-scale turbulence selects a characteristic cell-cell interactions scale where strong patches form. Our results shed light on the dynamical characteristics necessary for the formation of patchiness, and complement current efforts to unravel planktonic ecological interactions.

DY 8.9 Mon 12:15 BH-N 243

Critical behavior of active Brownian particles — Jonathan Tammo Siebert, •Florian Dittrich, Friederike Schmid, Kurt Binder, Thomas Speck, and Peter Virnau — Johannes Gutenberg University Mainz, Department of Physics, 55122 Mainz

We propose an improved block-density distribution method, which allows us to determine accurately the critical point of two dimensional active Brownian particles at $\mathrm{Pe}_{\mathrm{cr}} = 40(2)$, $\phi_{\mathrm{cr}} = 0.597(3)$. Based on this estimate we study the corresponding critical exponents β, γ/ν, and ν. Our results are incompatible with the 2D-Ising universality class, thus raising the fascinating question whether there exists a non-equilibrium universality class.

DY 8.10 Mon 12:30 BH-N 243

Pattern Formation and Synchronization of Disk-Shaped Circle Swimmers — •Guo-Jun Liao and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

We computationally study a generic model of disk-shaped active Brownian particles using Brownian dynamics simulation. Each particle is driven both by constant propulsion force and torque. We investigate how these two distinct propulsions combine to influence the macroscopic structure of a colloidal system. In the regime of small propulsion torque, the active colloids exhibit motility-induced clustering [1]. As the propulsion torque becomes comparable to thermal energy, the clustering phenomenon is drastically suppressed. Moreover, although all particles are intrinsically assigned to rotate counterclockwise, a novel state of clockwise vortices emerges at an optimal value of propulsion torque. We introduce a gear argument to capture the underlying mechanism of such vortices. To obtain deeper insight into the interplay between active motion and particle alignment, an additional polar interaction is then incorporated into our model. With increasing strength and range of the polar interaction, synchronization behavior is observed. Our model bears some similarity with the Kuramoto model [2], in which oscillators are actively moving over time.

[1] I. Buttinoni *et al.*, Phys. Rev. Lett. **110**, 238301 (2013)
[2] Y. Kuramoto, *Chemical Oscillations, Waves, and Turbulence*, (Springer, Berlin, 1984).

DY 8.11 Mon 12:45 BH-N 243

Pair Creation in Insect Swarms — •Dan Gorbonos and Nir Gov — Weizmann Institute, Rehovot, Israel

The macroscopic emergent behavior of social animal groups is thought to arise from the local interactions between individuals. We proposed a model of acoustic interaction within insect swarms that resemble gravitational attraction. Unlike gravity, the interactions between the insects are adaptive. Sensory mechanisms in biology, from cells to humans, have the property of adaptivity, whereby the sensitivity of the signal produced by the sensor is adapted to the overall amplitude of the signal. Adaptivity reduces the sensitivity in the presence of strong background stimulus, while increasing it when the background is weak. We find that in particular adaptivity is responsible for pairwise interaction that are characterized by higher-frequency nearly harmonic oscillations conducted by two synchronized insects. By comparison, the capture of pairs under normal gravity is extremely rare. We show that such pairs are created in simulations of the "adaptive gravity" model and compare them with pairs that were found in measurements of laboratory midge swarms. In addition we show similarities in density distributions between the simulations and laboratory measurements.

DY 8.12 Mon 13:00 BH-N 243

Dynamically Generated Patterns in Dense Suspensions of Active Filaments — •Prathyusha Kokkoorakunnel Ramankutty[1], Silke Henkes[2], and Rastko Sknepnek[3] — [1]Max Planck Institute of Physics of Complex Systems, Dresden Germany — [2]University of Aberdeen, United Kingdom — [3]University of Dundee, United Kingdom

We use Langevin dynamics simulations to study dynamical behaviour of a dense planar layer of active semi-flexible filaments. Using the strength of active force and the thermal persistence length as parameters, we map a detailed phase diagram and identify several non-equilibrium phases in this system. In addition to a slowly flowing melt phase, we observe that for sufficiently high activity, collective flow accompanied by signatures of local polar and nematic order appears in the system. This state is also characterised by strong density fluctuations. Furthermore, we identify an activity- driven cross-over from this state of coherently flowing bundles of filaments to a phase with no global flow, formed by individual filaments coiled into rotating spirals. This suggests a mechanism where the system responds to activity by changing the shape of active agents, an effect with no analog in systems of active particles without internal degrees of freedom

DY 9: Statistical Physics far from Thermal Equilibrium

Time: Monday 10:00–13:30 Location: BH-N 334

DY 9.1 Mon 10:00 BH-N 334

An electronic Maxwell demon in the coherent strong-coupling regime — •Gernot Schaller[1], Javier Cerrillo[1], Geort Engelhardt[1], and Philipp Strasberg[2] — [1]Institut für Theoretische Physik, TU Berlin — [2]Physics and Materials Science Research Unit, Uni Luxembourg

We consider feedback control on a single electron transistor. Monitoring the occupation of the dot, conditional control operations can be interpreted as the action of a Maxwell demon. This can generate a current against a potential bias, producing electric power from information. While this is well-explored in the weak-coupling limit and has recently been implemented [1], we can address the strong-coupling regime with a collective mapping [2]. A continuous projective measurement of the central dot would lead to a complete suppression of electronic transport due to the quantum Zeno effect [3]. However, a microscopic model implements a weak measurement, which allows for closure of the control loop without inducing complete transport blockade [4]. In the weak-coupling regime, the energy flows associated with the feedback loop are negligible, and the information gained in the measurement bounds the generated electric power. In contrast, in the strong coupling limit, the protocol requires more energy than electric power produced, removing Maxwell's demon.

[1] K. Chida *et al.*, Nat. Comm. **8**, 15310 (2017).
[2] P. Strasberg *et al.*, arXiv:1711.08914.
[3] G. Engelhardt and G. Schaller, arXiv:1710.06306.
[4] G. Schaller *et al.*, arXiv:1711.00706.

DY 9.2 Mon 10:15 BH-N 334

Qubit absorption refrigerator at strong coupling — Anqui Mu[1], Bijay Kumar Agarwalla[2], •Gernot Schaller[3], and Dvira Segal[1] — [1]Dept. of Chemistry, University of Toronto — [2]Dept. of Physics, Indian Inst. of Science Education and Research — [3]Institut f. Theoretische Physik, TU Berlin

We demonstrate that a quantum absorption refrigerator can be realized from the smallest quantum system, a qubit, by coupling it in a non-additive (strong) manner to three heat baths. This function is un-attainable for the qubit model under the weak system-bath coupling limit, when the dissipation is additive. We obtain then closed expressions for the cooling window and refrigeration efficiency, as well as bounds for the maximal cooling efficiency and the efficiency at maximal power. Our results agree with macroscopic designs and with three-level models for quantum absorption refrigerators, which are based on the weak system-bath coupling assumption. Our work demonstrates that strongly-coupled quantum machines can exhibit function that is un-attainable under the weak system-bath coupling assumption.

[1] A. Mu *et al.*, NJP in press, arXiv:1709.02835.

DY 9.3 Mon 10:30 BH-N 334

Energy efficient quantum machines — •Obinna Abah[1] and Eric Lutz[2] — [1]Centre for Theoretical Atomic, Molecular and Optical Physics, Queen's University Belfast, United Kingdom. — [2]Department of Physics, University of Erlangen-Nuremberg, Germany.

We investigate the performance of a quantum thermal machine operating in finite time based on shortcut-to-adiabaticity techniques. We compute efficiency and power for a paradigmatic harmonic quantum Otto engine by taking the energetic cost of the shortcut driving explicitly into account. We demonstrate that shortcut-to-adiabaticity machines outperform conventional ones for fast cycles. We further derive generic upper bounds on both quantities, valid for any heat engine cycle, using the notion of quantum speed limit for driven systems. We establish that these quantum bounds are tighter than those stemming from the second law of thermodynamics.

Reference: Obinna Abah and Eric Lutz, EPL 118, 40005 (2017).

DY 9.4 Mon 10:45 BH-N 334

Diverging, but negligible power at Carnot efficiency: theory and experiment — •Viktor Holubec[1,2] and Artem Ryabov[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Brüderstraße 15, 04103 Leipzig, Germany — [2]Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, V Holešovičkách 2, 18000 Praha, Czech Republic

We discuss the possibility of reaching the Carnot efficiency by heat engines (HEs) out of quasi-static conditions at nonzero power output. We focus on several models widely used to describe the performance of actual HEs. These models comprise quantum thermoelectric devices, linear irreversible HEs, minimally nonlinear irreversible HEs, HEs working in the regime of low dissipation, over-damped stochastic HEs and an under-damped stochastic HE. Although some of these HEs can reach the Carnot efficiency at nonzero and even diverging power, the magnitude of this power is always negligible compared to the maximum power attainable in these systems. We provide conditions for attaining the Carnot efficiency in the individual models and explain practical aspects connected with reaching the Carnot efficiency at large power output. Furthermore, we show how our findings can be tested in practice using a standard Brownian HE realizable with available micromanipulation techniques.

DY 9.5 Mon 11:00 BH-N 334

Quantum heat engines and laser cooling: A study beyond the weak coupling and Markovian approximations — •Sebastian Restrepo[1], Javier Cerrillo[1], Philipp Strasberg[2], and Gernot Schaller[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Complex Systems and Statistical Mechanics, University of Luxembourg, Luxembourg

We study a periodically driven thermal machine beyond the weak coupling and Markovian approximations by combining a collective coordinate mapping with Floquet theory and full counting statistics. We identify a collective degree of freedom in the reservoir that is included as part of an enlarged supersystem to take strong coupling and non-Markovian effects into account. The periodicity of our extended model is exploited using Floquet theory to obtain a master equation with full counting statistics methods permitting a thermodynamic analysis. The formalism is applied to a thermal machine consisting of a driven two-level system coupled to two reservoirs at different temperatures with one of the couplings considered time-dependent. In the weak-coupling regime, the setup can switch between the operational modes of a heat engine or a refrigerator directly. As the coupling is increased, we identify four different operation regimes and see the eventual disappearance of the refrigerator. We observe that the efficiency and coefficient of performance decrease for stronger couplings. Taking the limit of a single reservoir, our model is able to replicate the setup of state preparation in laser cooling of trapped ions.

DY 9.6 Mon 11:15 BH-N 334

Singularity in large deviations of work in quantum quenches — •Pietro Rotondo, Jiri Minar, Igor Lesanovsky, Juan P. Garrahan, and Matteo Marcuzzi — University of Nottingham, School of Physics and Astronomy, University Park NG7 2RD

We investigate the large deviations of the work performed in a quantum quench across two different phases separated by a quantum critical point. We analyse the Dicke model as a paradigmatic example, and employ an approximate description, valid in each phase in the thermodynamic limit, which reduces it to a set of two harmonic oscillators. We identify large deviations forms for the corresponding Loschmidt amplitude and its conjugate functional, the distribution of the work. We then compare these findings with the predictions of a recently-proposed classification scheme put forward in [Phys. Rev. Lett. 109, 250602 (2012)]. For certain values of the parameters, we highlight a regime going beyond the ones listed in this classification. In these cases, the rate function exhibits a non-analytical point, a strong indication of the presence of an out-of-equilibrium phase transition in the functional describing the rare fluctuations of the work.

DY 9.7 Mon 11:30 BH-N 334

Correlational latent heat by nonlocal quantum kinetic theory — •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 — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The nonlocal kinetic equation unifies the achievements of the transport in dense quantum gases with the Landau theory of quasiclassical transport in Fermi systems. Large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors [1]. The

remaining corrections are expressed in terms of shifts in space and time that characterize the non-locality of the scattering process [2]. In this way quantum transport is possible to recast into a quasi-classical picture [3]. The balance equations for the density, momentum, energy and entropy include besides quasiparticle also the correlated two-particle contributions beyond the Landau theory [4]. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy. For Maxwellian particles a sign change of the latent heat is reported at a universal ratio of scattering length to the thermal De Broglie wavelength. This is interpreted as a change from correlational heating to cooling. [1] Ann. Phys. 294 (2001) 135, [2] Phys. Rev. C 59 (1999) 3052, [3] "'Interacting Systems far from Equilibrium -Quantum Kinetic Theory"', Oxford University Press, (2017), ISBN 9780198797241, [4] Phys. Rev. E 96 (2017) 032106

15 min. break

DY 9.8 Mon 12:00 BH-N 334

Thermodynamic signatures of shear-induced transitions in confined colloidal suspensions in shear flow — •Sascha Gerloff and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Colloidal suspensions under the combined influence of shear flow and strong spatial confinement display a rich non-equilibrium behavior [1]. One intriguing question is how these dynamical transitions are reflected by macroscopic quantities, such as the shear stress and thermodynamic functions. Here, we perform overdamped *Brownian* dynamic (BD) simulations of charged colloids under shear flow confined to a narrow slitpore. In equilibrium, the colloids organize in crystalline layers, whose in-plane structure depends on the slitpore width [2]. Applying shear flow introduces new types of structural transitions driven by the collective motion of the colloids [1]. We investigate the work- and heat rate, as well as the entropy production related to different steady states. These quantities are calculated from particle trajectories in the spirit of stochastic thermodynamics [3]. We find that transitions between different steady states are reflected in these thermodynamic quantities. In particular, the work- and heat rates are closely related to the shear stress, which characterizes the rheological response of the system.

[1] S. Gerloff and S. H. L. Klapp, *Phys. Rev. E* **94**, 062605 (2016).
[2] A. Fortini and M. Dijkstra, *J. Phys. Condens. Matter* **18**, L371 (2006).
[3] T. Speck and U. Seifert, *Phys. Rev. E* **79**, 178302 (2009).

DY 9.9 Mon 12:15 BH-N 334

Oscillating Modes of Driven Colloids in Overdamped Systems — •Johannes Berner[1], Boris Müller[2,3], Juan Ruben Gomez-Solano[1], Matthias Krüger[2,3], and Clemens Bechinger[1] — [1]Physics Department, University of Konstanz, 78457 Konstanz, Germany — [2]4th Institute for Theoretical Physics, University of Stuttgart, 70569 Stuttgart, Germany — [3]Max Planck Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

Microscopic particles suspended in liquids are the prime example of an overdamped system because viscous forces dominate over inertial effects. Apart from their use as model systems, they receive considerable attention as sensitive probes from which forces on molecular scales can be inferred. The interpretation of such experiments rests on the assumption, that, even if the particles are driven, the liquid remains in equilibrium, and all modes are overdamped. Here, we experimentally demonstrate that this is no longer valid when a particle is forced through a viscoelastic fluid. Even at small driving velocities where Stokes law remains valid, we observe particle oscillations with periods up to several tens of seconds. We attribute these to non-equilibrium fluctuations of the fluid, which are excited by the particle's motion. The observed oscillatory dynamics is in quantitative agreement with an overdamped Langevin equation with negative friction-memory term and which is equivalent to the motion of a stochastically driven underdamped oscillator. This fundamentally new oscillatory mode has considerable implications on how molecular forces are determined by colloidal probe particles under natural viscoelastic conditions.

DY 9.10 Mon 12:30 BH-N 334

On the generalized generalized Langevin equation : a non-stationary approach of the Mori-Zwanzig formalism — •Hugues Meyer[1], Thomas Voigtmann[2], and Tanja Schilling[3] — [1]Université du Luxembourg, Esch-sur-Alzette, Luxemburg — [2]Albert-Ludwigs-Universität, Freiburg-im-Breisgau, Germany — [3]DLR, Köln, Germany

As a researcher in statistical physics, one may often be interested in reducing the complexity of a many-particle system to the study of a set of relevant observables (for instance, the system could be a polymer melt and the aim could be to develop a rheological model). This procedure is called coarse-graining as soon as the timescale of these variables is much larger than the microscopic timescale. A systematic way to derive an equation of motion for these observables from the microscopic dynamics is known for some time as the Mori-Zwanzig formalism and leads to the generalized Langevin equation. In contrast, if the dynamics is not stationary, it is not a priori clear which form the equation of motion for an averaged observable has. We adapt this formalism to derive the equation of motion for a non-equilibrium trajectory-averaged observable as well as for its non-stationary autocorrelation function. We also derive a fluctuation-dissipation-like relation which relates the memory kernel and the autocorrelation function of the fluctuating force. In addition, we show how to relate the Taylor expansion of the memory kernel to experimental data, thus allowing to construct the equation of motion from direct measurements. We finally illustrate this method on various simple examples.

DY 9.11 Mon 12:45 BH-N 334

Investigating the Reaction Dynamics for a Thermally Coupled System with a Rank-1 Saddle Potential — •Robin Bardakcioglu, Philippe Schraft, Johannes Reiff, Martin Tschöpe, Matthias Feldmaier, Jörg Main, and Günter Wunner — 1. Institut für Theoretische Physik, Universität Stuttgart, Germany

Transition State Theory provides an atomistic approach to the calculation and prediction of chemical reaction rates. By analyzing classical equations of motion for a molecular system, one can determine the reactant and product regions in phase space. With the use of an invariant manifold approach, we can find recrossing-free dividing surfaces between these regions, which allow us to determine the reaction rate for an open, time-dependently driven system. We use these methods to investigate the reaction dynamics of a system subject to Langevin dynamics, i.e. thermal noise.

DY 9.12 Mon 13:00 BH-N 334

Localized Deposition - Controlling cluster growth far from thermal equilibrium — •Thomas Martynec, Benedikt Hartung, and Sabine H.L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Thin-film growth by means of molecular beam epitaxy (MBE) is a typical example of non-equilibrium growth and a powerful method to produce devices for various technological applications [1-2]. Initially, particles are deposited at constant rate F on an empty lattice where these monomers freely diffuse until they meet other free particles on the lattice to form clusters. Nucleation events are randomly distributed on the lattice and one can only control the number of nucleation events (by varying temperature T and adsorption rate F) but not the location. This can be circumvented by using a stencil (or shadow) mask of linear size l [3-4]. Varying the size l, the particle flux F and the temperature T allows to spatially control nucleation events and the shape of clusters. We perform kinetic Monte-Carlo (KMC) simulations with spatially localized flux and identify three different growth modes that also emerge in experiments [4-5].

[1] S. Liu et al., npj 2D Materials and Applications **1**, 30 (2017)
[2] Parkes et al., Sci Rep. **3**, 2220 (2013)
[3] H. Yun et al., Sci Rep. **5**, 10220 (2015)
[4] P. Fesenko et al., Cryst. Growth Des. **16**, 4694 (2016)
[5] T. Martynec, B. Hartung, and S. H. L. Klapp, in preparation

DY 9.13 Mon 13:15 BH-N 334

Effective thermodynamics for a marginal observer — •Matteo Polettini and Massimiliano Esposito — Physics and Materials Science Research Unit, University of Luxembourg, Campus Limpertsberg, 162a avenue de la Faiencerie, L-1511 Luxembourg (Luxembourg)

Thermodynamics often presumes that the observer has complete information about the system she or he deals with: no parasitic current, exact evaluation of the forces needed to drive the system out of equilibrium. However, most often the observer only measures marginal information. How is she or he to make consistent thermodynamic claims? Disregarding sources of dissipation might lead to bold claims,

such as the possibility of perpetuum mobile. We show that it is nevertheless possible to produce an effective description that does not dispense with the fundamentals of thermodynamics: the 2nd Law, the Fluctuation-Dissipation paradigm, and the more recent and encompassing Fluctuation Theorem.

DY 10: Statistical Physics I (General)

Time: Monday 10:00–12:45 Location: BH-N 333

DY 10.1 Mon 10:00 BH-N 333

Scaling behavior of self-avoiding walks on critical percolation clusters in two to seven dimensions from exact enumeration — •Wolfhard Janke and Niklas Fricke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We study the scaling behavior of self-avoiding walks on critical percolation clusters by means of a recently developed exact enumeration method, which can handle walks of several thousand steps. We had previously presented results for the two- and three-dimensional cases; here we take a wider perspective and vary the system's dimensions up to $D = 7$, beyond the supposed upper critical dimension of $D_{\mathrm{uc}} = 6$. These results may serve as a check of analytical predictions and help understand how the medium's fractal structure impacts on the walks' scaling behavior. For the physically relevant, smaller dimensions, the scaling exponent ν for the end-to-end distance turns out to be smaller than previously thought and appears to be the same on the backbones as on full clusters. For the number of conformations, the "partition function", we find strong evidence against the widely assumed scaling law and propose an alternative, which perfectly fits our data.

[1] N. Fricke and W. Janke, Phys. Rev. Lett. **113**, 255701 (2014).
[2] N. Fricke and W. Janke, J. Phys. A **50**, 264002 (2017).

DY 10.2 Mon 10:15 BH-N 333

High precision free energy-distribution of directed polymers in random media — •Alexander K. Hartmann[1], Pierre Le Doussal[2], Satya N. Majumdar[3], Alberto Rosso[3], and Gregory Schehr[3] — [1]Institut für Physik, Universität Oldenburg, Germany — [2]LPT, Ecole Normale Supérieure, Paris, France — [3]LPTMS, Université Paris Sud, France

We study the distribution of relative free energies H of directed polymers in disordered media coupled to a heat bath at temperature T, which is in the Kardar-Parisi-Zhang (KPZ) universality class in $1 + 1$ dimensions. We study the distribution at large and medium small temperatures, corresponding to short and medium long times in KPZ. Using a statistical mechanics-based large-deviation approach [1], the distribution can be obtained over a large range of the support, down to a probability density as small as 10^{-1000}. We compare with analytical predictions for the KPZ equation for short [2] and long times [3], respectively. For short times a very good agreement is found for $H < 0$ and a convergence is visible for $H > 0$. For large times, an asymptotic convergence in the tails is visible.

[1] A.K. Hartmann, Phys. Rev. E **65**, 056102 (2002).
[2] P. Le Doussal, S.N. Majumdar, A. Rosso, and G. Schehr, Phys. Rev. Lett. **117**, 070403 (2016).
[3] P. Sasorov, B. Meerson, and S. Prolhac, J. Stat. Mech. 2017, 063203 (2017).

DY 10.3 Mon 10:30 BH-N 333

Optimal packing of confined dipolar hard spheres — •Florian Deissenbeck[1], Hartmut Löwen[1], and Erdal Celal Oguz[2] — [1]HHU Düsseldorf, Institut für Theoretische Physik 2: Weiche Materie — [2]Tel Aviv University, School of Mechanical Engineering and The Sackler Center for Computational Molecular and Materials Science

We investigate the ground state of a classical two-dimensional system of hard-sphere dipoles confined between two hard walls. Using lattice sum minimization techniques we reveal that at fixed wall separations, a first-order transition from a vacuum to a straight one-dimensional chain of dipoles occurs upon increasing the line density. A further increase in this density yields the stability of an undulated chain with a nontrivial magnetic dipolar structure. By exploring the close-packed configurations of dipoles, which in general possess complex magnetizations, we find a novel phase structure that has a higher packing fraction than hitherto known ones. Our predictions serve as a guideline for experiments with granular dipolar and magnetic colloidal suspensions confined in slit-like geometry.

DY 10.4 Mon 10:45 BH-N 333

A new perspective on laser-induced freezing and reentrant melting — •Alexander Kraft and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

Laser-induced freezing (LIF) of a two-dimensional colloidal system describes the phenomenon in which a one-dimensional interfering laser beam pattern can induce a liquid-crystal freezing transition [1]. In this contribution, we propose a new perspective of the microscopic origin of LIF. Using free minimization techniques within density functional theory for a model system subjected to two different substrate potentials, we show that there is strong evidence that the increase of the light intensity is not the only reason for the occurrence of LIF, but its accompanying side-effect to increase the effective average density. In our approach, we characterize the inhomogeneous density distribution of particles in terms of two quantities: We introduce a confining length L_c to characterize the region within which a representative fraction of particles are confined and the effective average density $\bar{\rho}_{eff}$ within this region. In this way, our approach allows to make theoretical predictions for the critical value of the light intensity for the onset of LIF and allows to define a quantitative measure for the reduced registration introduced by [2] to understand reentrant melting.

[1] A. Chowdhury et al., Phys. Rev. Lett. **55**, 833 (1985)
[2] Q. H. Wei et al., Phys. Rev. Lett. **81**, 2606 (1998)
[3] L. Radzihovsky et al. Phys. Rev. E **63**, 031503 (2001)

DY 10.5 Mon 11:00 BH-N 333

Duality between relaxation and first passage in reversible Markov dynamics — •David Hartich and Aljaz Godec — Mathematical Biophysics Group, Max-Planck-Institute for Biophysical Chemistry (Göttingen)

The first passage time characterizes the time until a stochastic process reaches a given threshold for the first time, e.g. the first instance a molecule reaches its target, or the first crossing of an energetic barrier. Complementary to first passage time statistics are well known relaxation processes. Until now an explicit connection between a first passage process and a relaxation process, albeit sought for, remained elusive.

Here, we prove a duality between them in the form of a spectral interlacing enabling us to explicitly determine the full first passage time distribution in terms of a simple relaxation process. To illustrate our theory we analyze diffusion in a triple-well potential, and express the first passage time statistics in terms of relaxation eigenmodes. Finally, we highlight the relevance of our theory by studying first passage kinetics in the so-called few-encounter limit dominated by the fastest reactive trajectories. Our results are relevant for gene regulation processes and the triggering of certain neurodegenerative diseases.

15 min. break

DY 10.6 Mon 11:30 BH-N 333

Linear Programming and Cutting Planes for Ground States and Excited States of the Traveling Salesperson Problem — •Hendrik Schawe[1], Jitesh Jha[2], and Alexander K. Hartmann[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Manipal Institute of Technology

The Traveling Salesperson problem asks for the shortest cyclic tour visiting a set of cities given their pairwise distances and belongs to the NP-hard complexity class, which means that all NP problems, like spin glass groundstate, can be mapped to it.

We look at excited states to explore the energy landscape in detail. The linear programming approach offers capable tools to find excited states fulfilling very specific requirements. This allows us, e.g., to find the second shortest tour or the tour most different to the optimal tour within some allowed excitation ϵ, e.g., 1% longer than the optimum. We are especially interested whether the energy landscape is complex,

i.e., shows signatures of replica symmetry breaking in analogy to spin glasses.

DY 10.7 Mon 11:45 BH-N 333

Langevin equations for reaction-diffusion processes — Federico Benitez[1,2], •Charlie Duclut[3], Hugues Chaté[4,5,3], Bertrand Delamotte[3], Ivan Dornic[4,3], and Miguel A. Muñoz[6] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Physikalisches Institut, Universität Bern, Sidlerstr. 5, 3012 Bern, Switzerland — [3]Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR7600, UPMC-Sorbonne Universités, 75252 Paris Cedex 05, France — [4]Service de Physique de l'Etat Condensé, CEA, CNRS, Université Paris-Saclay, CEA-Saclay, 91191 Gif-sur-Yvette, France — [5]Beijing Computational Science Research Center, Beijing 100094, China — [6]Instituto de Física Teórica y Computacional Carlos I, Facultad de Ciencias, Universidad de Granada, 18071 Granada, Spain

For reaction-diffusion processes with at most bimolecular reactants, we derive well-behaved, numerically-tractable, exact Langevin equations that govern a stochastic variable related to the response field in field theory. Using *duality* relations, we show how the particle number and other quantities of interest can be computed. Our work clarifies long-standing conceptual issues encountered in field theoretical approaches and paves the way to systematic numerical and theoretical analyses of reaction-diffusion problems.

DY 10.8 Mon 12:00 BH-N 333

Random distributions: what doping densities enable entangling gates to be formed in silicon? — •Eleanor Crane[1], Andrew Fisher[1], Thomas Crane[2,3], Ben Murdin[4], and Neil Curson[1] — [1]London Centre for Nanotechnology, University College London, London WC1H 0AH, UK — [2]ENS Paris, 45 Rue d'Ulm, 75005 Paris, France — [3]Université Sorbonne Paris Cité, Université Paris Diderot - Paris VII, 5 Rue Thomas Mann, 75013 Paris, France — [4]Advanced Technology Institute, University of Surrey, Guildford, GU2 7XH, United Kingdom

Entangling the quantum states of impurity atoms in condensed matter is a crucial step towards the creation of a solid state quantum computer. In a whole range of experiments aiming at this, atoms need to be spaced by specific spatial distances. This is also the case in the Stoneham Fisher Greenland scheme [1] for which we determine the density of entangling gates in a randomly doped multi-species silicon sample. We use Poisson point processes, for which we also show a number of properties, and verify our results using a Monte Carlo simulation. These methods are of general interest for Poisson point processes and the fields which use them as models of random physical phenomena.

[1] Stoneham A M, Fisher A J and Greenland P T, 2003, J. Phys.: Condens. Matter 15 L447*L451

DY 10.9 Mon 12:15 BH-N 333

Expanding the effective action around non-Gaussian theories — •Tobias Kühn[1] and Moritz Helias[1,2] — [1]Inst. of Neurosc. and Medicine (INM-6), Inst. for Advanced Simulation (IAS-6) and JARA BRAIN Inst. I, Jülich Research Centre, Germany — [2]Department of Physics, Faculty 1, RWTH Aachen University, Aachen, Germany

The effective action or Gibbs Free Energy is the central quantity to study phase transitions and is at the core of effective theories constructed, for example, by the renormalization group. It is known that only one-line-irreducible Feynman diagrams contribute in the case that the theory, about which one expands, is Gaussian. We introduce a generalized notion of one-line-irreducibility: diagrams that remain connected after detaching a single leg of an interaction vertex. We show that the effective action decomposes into diagrams that are either irreducible in this more general sense or belong to a second class of diagrams that has no analogue in Gaussian theories [Kühn & Helias 2017, arXiv:1711.05599]. The presented method allows the efficient diagrammatic perturbative computation of the effective action around any exactly solvable problem. We illustrate this method by application to the (classical) Ising model expanded in the coupling strength. This reproduces the Plefka expansion [Plefka 1982], including the TAP-correction [Thouless et al. 1977] to mean-field theory. We find that the diagrammatic formulation considerably simplifies the calculation compared to existing techniques [Takayama & Nakanishi 1997, Georges & Yedidia 1991]. Supported by the Helmholtz foundation (VH-NG-1028, SMHB); EU Grant 604102 (HBP).

DY 10.10 Mon 12:30 BH-N 333

Scaling of density fluctuations and hyperuniformity in one-dimensional substitution tilings — •Erdal C. Oğuz[1,4], Joshua E. S. Socolar[2], Paul J. Steinhardt[3], and Salvatore Torquato[4] — [1]School of Mechanical Engineering and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel — [2]Department of Physics, Duke University, Durham, NC 27708 — [3]Princeton Center for Theoretical Science and Department of Physics, Princeton University, Princeton, NJ 08544 — [4]Department of Chemistry, Princeton University, Princeton, 08540

Substitution tilings include periodic, quasiperiodic, limit periodic, and other self-similar structures generated by iterated subdivision and rescaling of a finite set of tiles. We study the scaling of density fluctuations associated with a broad class of substitution rules in one dimension. We show that a simple, heuristic argument for the rate of decay of the integrated Fourier intensity $Z(k)$ at small values of the wavenumber k correctly predicts the scaling of the variance $\sigma^2(R)$ in the number of points contained in intervals of length $2R$. The exponent α, defined by $Z \sim k^{\alpha+1}$, is determined by the ratio of the second largest and largest eigenvalues of the substitution matrix and can vary between -1 and 3, where $\alpha > 0$ implies a hyperuniform distribution of tile vertices. The hyperuniform class includes tilings that are periodic, quasiperiodic, or limit periodic, including a new class of limit-periodic tilings for which Z approaches zero faster than any power law. Tilings with singular continuous diffraction spectra may be hyperuniform or may exhibit stronger fluctuations than a Poisson system.

DY 11: Energy Systems (joint session DY/SOE)

Time: Monday 12:00–13:00 Location: BH-N 128

DY 11.1 Mon 12:00 BH-N 128

Energy recuperation system for skip trucks — •Robin Masser, Karsten Schwalbe, and Karl Heinz Hoffmann — Chemnitz University of Technology, Chemnitz, Germany

When braking with conventional brake discs, kinetic energy is converted into heat that is released to the environment. The reduction of the energy made unusable in this process has been in the focus of research during the last decades. Following this goal, our work aims to reduce the fuel consumption of commercial vehicles, in particular of skip trucks. Therefore, a module consisting of a hydraulic pump driven by the cardan shaft and a bladder accumulator is installed to store and reuse energy. The stored energy may then be used to operate auxiliary units, to support the thermal management and as additional propulsion. This system consisting of the hydraulic components, the cooling circuit as well as pressure and heat losses is modeled applying endoreversible thermodynamics. Based on this model, system parameters and control strategies can be optimized in terms of power and efficiency. The resulting fuel and operational cost savings are estimated evaluating recorded urban driving data.

DY 11.2 Mon 12:15 BH-N 128

Scaling of transmission capacities in coarse-grained renewable electricity networks — •Mirko Schäfer[1], Simon Bugge Siggaard[2], Kun Zhu[1], Chris Risager Poulsen[2], and Martin Greiner[1] — [1]Department of Engineering, Aarhus University, Denmark — [2]Department of Physics and Astronomy, Aarhus University, Denmark

Network models of large-scale electricity systems feature only a limited spatial resolution, either due to lack of data or in order to reduce the complexity of the problem with respect to numerical calculations. In such cases, both the network topology, the load and the generation patterns below a given spatial scale are aggregated into representative nodes. This coarse-graining affects power flows and thus the resulting transmission needs of the system. We derive analytical scaling laws for measures of network transmission capacity and cost in coarse-grained

renewable electricity networks. For the cost measure only a very weak scaling with the spatial resolution of the system is found. The analytical results are shown to describe the scaling of the transmission infrastructure measures for a simplified, but data-driven and spatially detailed model of the European electricity system with a high share of fluctuating renewable generation.

DY 11.3 Mon 12:30 BH-N 128

Frequency fluctuations and dynamically induced cascading failures in power grids — •Benjamin Schäfer[1,2], Dirk Witthaut[3,4], Christian Beck[5], Kazuyuki Aihara[6], Marc Timme[1,2], and Vito Latora[5,7] — [1]Chair for Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute for Theoretical Physics, Technical University of Dresden, 01062 Dresden, Germany — [2]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [3]Forschungszentrum Jülich, Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE), 52428 Jülich, Germany — [4]Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany — [5]School of Mathematical Sciences, Queen Mary University of London, London E1 4NS, United Kingdom — [6]Institute of Industrial Science, The University of Tokyo, Meguro-ku, Tokyo, Japan — [7]Dipartimento di Fisica ed Astronomia, Università di Catania and INFN, I-95123 Catania, Italy

Reliable functioning of infrastructure networks is essential for our modern society. Cascading failures are the cause of most large-scale network outages while small fluctuations dominate the grid on a daily basis. In this talk, we demonstrate the importance of transient dynamics when investigating cascades in power grids. Furthermore, we analyze power grid frequency fluctuations based on measurements from several continents, explaining heavy tails and revealing the impact of trading.

DY 11.4 Mon 12:45 BH-N 128

Flow-tracing and nodal cost allocation in a heterogeneous highly renewable European electricity network — Bo Tranberg[1], Leon Schwenk-Nebbe[2], Mirko Schäfer[1], Jonas Hörsch[3], and •Martin Greiner[1] — [1]Department of Engineering, Aarhus University — [2]DONG Energy — [3]Frankfurt Institute for Advanced Studies

For a cost efficient design of a future renewable European electricity system, the placement of renewable generation capacity will seek to exploit locations with good resource quality, that is for instance onshore wind in countries bordering the North Sea and solar PV in South European countries. Regions with less favorable renewable generation conditions benefit from this remote capacity by importing the respective electricity as power flows through the transmission grid. The resulting intricate pattern of imports and exports represents a challenge for the analysis of system costs on the level of individual countries. Using a flow-tracing technique, we introduce flow-based nodal levelized costs of electricity (LCOE) which allow to incorporate capital and operational costs associated with the usage of generation capacity located outside the respective country under consideration. This concept and a complementary allocation of transmission infrastructure costs is applied to a simplified model of an interconnected highly renewable European electricity system. We observe that cooperation between the European countries in a heterogeneous system layout does not only reduce the system-wide LCOE, but also the flow-based nodal LCOEs for every country individually.

DY 12: Focus Session: Statistical Physics-Based Methods in Molecular Evolution - organized by Alexander Schug and Martin Weigt (joint session BP/DY)

Time: Monday 15:00–17:00 Location: H 2013

Invited Talk DY 12.1 Mon 15:00 H 2013

Evolution of quantitative traits and non-equilibrium matrix ensembles — Simone Pompei, Torsten Held, and •Michael Lässig — Institute for Theoretical Physics, University of Cologne

Evolution affects molecular quantitative phenotypes, such as stability, binding affinities, and metabolic activities of cellular proteins. Linking sequence data to phenotypic and functional changes remains a critical gap in our understanding of evolutionary processes. In this talk, we present new methods to infer *a priori* unknown quantitative phenotypes from their correlation signature in time-resolved sequence data, using non-equilibrium statistical mechanics and random matrix theory. We use these methods to map the phenotypic evolution of the human influenza virus.

DY 12.2 Mon 15:30 H 2013

Big Data in Structural Biology: Predicting Protein and RNA Structures by inferring residue co-evolution — •Alexander Schug — John von Neumann Institute for Computing, Jülich Supercomputer Centre, Forschungszentrum Jülich

To gain any detailed understanding of biomolecular function, one needs to know their structure. The structural characterization of many important biomolecules and their complexes remains experimentally challenging. Novel statistical tools based on statistical physics such as Direct Coupling Analysis (DCA) take advantage of the explosive growth of sequential databases and trace residue co-evolution to infer secondary and tertiary contacts for proteins [1] and RNAs [2]. These contacts can be exploited as spatial constraints in structure prediction methods leading to excellent quality predictions [1,2,3]. Going beyond anecdotal cases of a few protein families, we have applied our methods to a systematic large-scale study of nearly 2000 PFAM protein families of homo-oligomeric proteins [4]. Also, we can apply DCA to infer mutational landscapes by capturing epistatic couplings between residues and can assess the dependence of mutational effects on the sequence context where they appear [5].

[1] Weigt M et al., PNAS (2009); F. Morcos et al., PNAS (2011)
[2] E. De Leonardis et al., NAR (2015)
[3] Schug A et al., PNAS (2009); Dago A et al., PNAS (2012)
[4] G. Uguzzoni et al., PNAS (2017)
[5] M. Figliuzzi et al., MBE (2016)

DY 12.3 Mon 15:45 H 2013

Coevolution based inference of allosteric architectures — •Barbara Bravi[1], Carolina Brito[2], Riccardo Ravasio[1], and Matthieu Wyart[1] — [1]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [2]Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil

We analyze maximum entropy approaches to infer the functional design of elastic materials exhibiting allostery, i.e. the property of highly specific responses to ligand binding at a distant active site. To guide and inform protocols of de novo drug design, it is fundamental to understand what architectures underlie such a transmission of information and whether their features can be predicted from sequence data alone. We consider the functional designs of in silico evolved allosteric architectures which propagate efficiently energy (including shear, hinge, twist) or strain (resulting in a less-constrained trumpet-shaped region between the allosteric and the active site). We show that maximum entropy approaches, built to capture statistical properties such as conservation and correlations, can provide predictive information on the cost of single and double mutations while their performance at reproducing the original allosteric fitness is strongly design-dependent. We benchmark existing maximum entropy inference methods on these computationally evolved functional architectures and we propose an improved framework accounting for a multiplicity of co-evolutionary factors which is aimed at disentagling allostery-based correlations from extrinsic ones.

DY 12.4 Mon 16:00 H 2013

Architecture of allosteric materials — Carolina Brito[1], Solange Flatt[2], •Riccardo Ravasio[2], Matthieu Wyart[2], and Le Yan[3] — [1]Universidad Federal do Rio Grande do Sul, CP 15051, 91501-970 Porto Alegre RS, Brazil — [2]Ecole Polytechnique Federale de Lausanne, CH-1015, Lausanne, Switzerland — [3]Kavli Institute for Theoretical Physics, Santa Barbara, CA 93106, USA

Allosteric proteins transmit a mechanical signal induced by binding a ligand. However, understanding the nature of the information transmitted and the architectures optimising such transmission remains a

challenge. We show using an in-silico evolution scheme and theoretical arguments that architectures optimised to be cooperative, which propagate efficiently energy, qualitatively differ from previously investigated materials optimised to propagate strain. Although we observe a large diversity of functioning cooperative architectures — including shear, hinge and twist designs, they all obey the same principle of nearly displaying a mechanism, i.e. an extended zero mode with a predicted optimal frequency. Overall, our approach leads to a natural explanation for several observations in allosteric proteins, and suggests a path to discover new ones. On this line, we study the extended soft modes of hessians defined from 46 couples of proteins for which the active and inactive structures are available and compare them with the aforementioned principle. Moreover, the set of architectures that are evolved through the in-silico scheme defines a well controlled ground where to benchmark the results of co-evolutionary methods, usually applied to protein sequences.

DY 12.5 Mon 16:15 H 2013

Direct Coupling Analysis on the genome scale — •Erik Aurel — Royal Institute of Technology in Stockholm, Sweden

Direct Coupling Analysis (DCA) is a powerful tool to find pair-wise dependencies in large biological data sets. It amounts to inferring coefficients in a probabilistic model in an exponential family, and then using the largest such inferred coefficients as predictors for the dependencies of interest. A main success story has been predicting spatially proximate residues in protein structures from sequence data.

From a population genetics point of view DCA should be viewed as inferring epistasis, synergistic effects on fitness, from samples. I will discuss applications of DCA to the genome scale in bacteria and how that allows to find unexpected (and expected) dependencies between genes in trans i.e. that are not close on the genome.

This is joint work with many people, most recently with Chen-Yi Gao and Hai-Jun Zhou, available as arXiv:1710.04819.

DY 12.6 Mon 16:30 H 2013

Interprotein coevolution: bridging scales from residues to genomes — Giancarlo Croce[1], Thomas Gueudre[2], Hendrik Szurmant[3], Matteo Figliuzzi[1], and •Martin Weigt[1] — [1]Université Pierre & Marie Curie, Sorbonne Université, Paris, France — [2]Human Genetics Foundation, Turin, Italy — [3]Western University of Health Sciences, Los Angeles, USA

Interacting proteins coevolve at multiple but interconnected scales, from the residue-residue over the protein-protein up to the family-family level. The recent accumulation of enormous amounts of sequence data allows for the development of novel, data-driven computational approaches. Notably, these approaches can bridge scales within a single statistical framework [1,2], which is built upon idea from the inverse statistical physics [3,4]. While being currently applied mostly to isolated problems on single scales, their immense potential for an evolutionary informed, structural systems biology is steadily emerging.

[1] H. Szurmant and M. Weigt, Current Opinion in Structural Biology 50, 26-32 (2017).

[2] G. Croce, T. Gueudre, MV Ruiz Cuevas, H. Szurmant, M. Figliuzzi, M. Weigt, submitted (2017).

[3] S. Cocco, C. Feinauer, M. Figliuzzi, R. Monasson, M. Weigt, Rep. Prog. Phys. (2017), https://doi.org/10.1088/1361-6633/aa9965.

[4] H. Chau Nguyen, Riccardo Zecchina, Johannes Berg, Advances in Physics, 66 (3), 197-261 (2017)

DY 12.7 Mon 16:45 H 2013

The evolutionary consequences of population spread on curved surfaces — Daniel A. Beller[1], Kim M. J. Alards[2], Ricardo A. Mosna[3], Federico Toschi[2], and •Wolfram Möbius[4] — [1]Brown University, Providence, RI, USA — [2]TU Eindhoven, Eindhoven, The Netherlands — [3]Universidade Estadual de Campinas, Campinas, SP, Brazil — [4]University of Exeter, Exeter, United Kingdom

We investigate the evolutionary dynamics of populations growing and expanding on curved surfaces. Using a combination of individual-based simulations and theory we characterize the effect of individual features (cones and spherical caps) on the shape of the population front and the genetic composition of an expanding population. We find that, on sufficiently large scales, geodesics allow us to describe both population and evolutionary dynamics quantitatively. Using these findings, we characterize the consequences of large-scale surface roughness on genetic diversity and compare to the case of heterogeneous but flat environments.

DY 13: Talk D. Lohse

Time: Monday 15:00–15:30 Location: BH-N 334

Invited Talk DY 13.1 Mon 15:00 BH-N 334

Diffusive Droplet Dynamics in multicomponent fluid systems — •Detlef Lohse — Physics of Fluids, University of Twente, The Netherlands

Liquid-liquid extraction - the transfer of a solute from one solvent to another - is one of the core processes in chemical technology and analysis. To be able to control & optimize the extraction processes, it is crucial to quantitatively understand the diffusive droplet dynamics in such multicomponent fluid systems. This is essential not only for modern liquid-liquid extraction processes for diagnostics & microanalysis, for droplet microfluidics, or in the paint & coating industry, but on larger scales also in the remediation industry, in chemical technology, or in food processing.

Taking examples from daily life, in this talk I will report on our efforts to come to a quantitative understanding of diffusive droplet dynamics on multiple scales, in order to bridge the gap from modern fluid dynamics to process-technology and colloidal & interfacial science, from nano/microscopic and purely diffusively governed droplets to macroscopic ones and from single droplets to multiple and multicomponent droplets.

One of these examples is the evaporation of droplets of ternary mixtures such as the Greek drink Ouzo (a transparent mixture of water, ethanol, and anise oil). The evaporation process can trigger a phase transition and the nucleation of microdroplets of anis oil. We find and explain four life phases of the evaporating ouzo droplet, illustrating the richness of such phenomena.

DY 14: Dynamics in many-body systems: interference, equilibration and localization II (joint session DY/TT)

Time: Monday 15:30–17:45 Location: EB 107

DY 14.1 Mon 15:30 EB 107

Finite-size effects in canonical and grand-canonical quantum Monte Carlo simulations for fermions — Zhenjiu Wang, Fakher F. Assaad, and •Francesco Parisen Toldin — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We introduce a quantum Monte Carlo method at finite temperature for interacting fermionic models in the canonical ensemble, where the conservation of the particle number is enforced. Although general thermodynamic arguments ensure the equivalence of the canonical and the grand-canonical ensembles in the thermodynamic limit, their approach to the infinite-volume limit is distinctively different. Observables computed in the canonical ensemble generically display a finite-size correction proportional to the inverse volume, whereas in the grand-canonical ensemble the approach is exponential in the ratio of the linear size over the correlation length. We verify these predictions by quantum Monte Carlo simulations of the Hubbard model in one and two dimensions in the grand-canonical and the canonical ensemble. We prove an exact formula for the finite-size part of the free energy density, energy density and other observables in the canonical ensemble and relate this correction to a susceptibility computed in the corresponding grand-canonical ensemble. This result is confirmed by an exact computation of the one-dimensional classical Ising model in the canonical ensemble, which for classical models corresponds to the so-called fixed-magnetization ensemble. Our method is useful for simulating finite systems which are not coupled to a particle bath, such as in nuclear or cold atom physics.

DY 14.2 Mon 15:45 EB 107

Coupling of hydrodynamic fluctuations to diffusive modes in a one-dimensional current-carrying wire — •Philipp Weiss, Marcel Gievers, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

Closed systems with conservation laws approach thermal equilibrium only algebraically slowly after a sudden perturbation. The reason is that the built-up of equilibrium fluctuations is tied to the diffusive transport of the conserved quantities which results in hydrodynamic long-time tails. A similar behavior is expected for a current-carrying wire, coupled to leads which serve as source and sink of electrons. Here, fluctuation corrections near the connections decay slowly in space along the wire. Though tailored to transport problems, the Boltzmann equation predicts exponentially fast relaxation indicating that the Boltzmann description omits crucial processes. This can be cured *ad hoc* by adding collision noise which gives rise to a stochastic Boltzmann-Langevin equation. However, the full equation is hard to solve and approximation schemes are needed when investigating a specific system.

We propose a "noisy relaxation time approximation" which satisfies the conservation laws and provides a properly correlated noise term. We examine this novel tool using the example of the one-dimensional current-carrying wire: Can we observe the expected long-distance tails? How does our approximation compare to the real dynamics? And to which extent can we control it?

DY 14.3 Mon 16:00 EB 107

Photo-carrier relaxation of correlated band insulators — •Nagamalleswara Rao Dasari[1] and Martin Eckstein[2] — [1]Friedrich-Alexander Universitat Erlangen-Nurnberg, Erlangen, Germany. — [2]Friedrich-Alexander Universitat Erlangen-Nurnberg, Erlangen, Germany.

Ionic band insulators are characterized by charge gap, which is given by staggered Ionic potential (Δ). Electronic correlations (U) in these insulators screens the charge gap and makes it smaller than the spin gap. Such correlated band insulators are realized by using simplest model Hamiltonian, i.e., Ionic Hubbard model. In this work, we have studied Ionic Hubbard model in the weak coupling limit by using non-equilibrium dynamical mean-field theory and iterated perturbation theory as an impurity solver. We find that photo-excited correlated band insulators thermalize rapidly when local coulomb interaction is greater than or equal to staggered Ionic potential ($U>=\Delta$). However, in the opposite case where $U<\Delta$, photo-excited system relaxes to a non-thermal steady state, and we did not see the thermalization of this state in our simulation time.

DY 14.4 Mon 16:15 EB 107

Resonant thermalization of periodically driven strongly correlated electrons — •Francesco Peronaci, Marco Schiró, and Olivier Parcollet — Institut de Physique Théorique (IPhT), Gif-sur-Yvette, France

We study the dynamics of the Fermi-Hubbard model driven by a time-periodic modulation of the interaction within nonequilibrium Dynamical Mean-Field Theory. For moderate interaction, we find clear evidence of thermalization to a genuine infinite-temperature state with no residual oscillations. Quite differently, in the strongly correlated regime, we find a quasi-stationary extremely long-lived state with oscillations synchronized with the drive (Floquet prethermalization). Remarkably, the nature of this state dramatically changes upon tuning the drive frequency. In particular, we show the existence of a critical frequency at which the system rapidly thermalizes despite the large interaction. We characterize this resonant thermalization and provide an analytical understanding in terms of a break down of the periodic Schrieffer-Wolff transformation.

DY 14.5 Mon 16:30 EB 107

Dynamical Typicality for initial states with a preset measurement statistics of several commuting observables — •Ben Niklas Balz and Peter Reimann — Fakultät für Physik, Universität Bielefeld, Germany

We consider all pure or mixed states of a quantum many-body system which exhibit the same, arbitrary but fixed measurement outcome statistics for several commuting observables. Taking those states as initial conditions, which are then propagated by the pertinent Schrödinger or von Neumann equation up to some later time point, and invoking a few additional, fairly weak and realistic assumptions, we show that most of them still entail very similar expectation values for any given observable. This finding thus corroborates the widespread observation that few macroscopic features are sufficient to ensure the reproducibility of experimental measurements despite many unknown and uncontrollable microscopic details of the system.

DY 14.6 Mon 16:45 EB 107

Formation of Few-Electron-Complexes — •Hubert Klar — Univ. Freiburg

Systems of 2,3 or 4 electrons in the field of a nucleus are shown to posses unstable equilibrium configurations. The many-body potential energy surface has in such configurations saddle points. AS model we study a saddle point with only one fragmentation direction, and show that the diffraction of an electron wave from the corresponding potential ridge manifests itself as a novel fictitious force being temporarily attractive between electrons. Moreover that force deforms the static potential surface and predicts an energy gap. Our theory extends and translates Wannier classical ionization theory into quantum mechanics. In contrast to Cooper pairs our electronic binding mechanisme stems entirely from correlation rather than fom lattice vibrations.

DY 14.7 Mon 17:00 EB 107

Dynamic Analysis of a Scissors Structure — •Yuta Hama[1], Ichiro Ario[1], Kotaro Adachi[1], and Yuki Chikahiro[2] — [1]Hiroshima University, Higashi-hiroshima, Japan — [2]Shinsyu University, Nagano, Japan

The paper presents a new type of deployable and/or folding bridge, which can be quickly constructed in case of damages after a natural disaster. The concept of the bridge is based on the application of scissor-type mechanism, which provides its rapid deployment. The presented research reviews fundamental numerical and experimental results for the full-sized scissors structure. Experimental testing included strain and acceleration measurements in free and forced loading conditions. From these results, it was possible to estimate basic dynamic characteristics of the bridge. Besides, in order to provide a basis for development of new construction methods under gravity. This dynamic research allows for a better and safer design of the movable and foldable full-scale scissors type of bridge.

DY 14.8 Mon 17:15 EB 107

Dynamics in the ergodic phase of the many-body localization transition for a periodically driven system — •Talía L. M. Lezama[1], Soumya Bera[2], and Jens H. Bardarson[3] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India — [3]Department of Physics, KTH Royal Institute of Technology, Stockholm, SE-106 91 Sweden

Closed disordered interacting quantum systems can experience a many-body localization phase transition when tuning the disorder strength around its critical value. Recent studies have shown that the ergodic phase is not a common metallic phase but that it rather exhibits non-trivial mechanisms (mainly Griffiths effects) foregoing the many-body localized phase. Those mechanisms have been described in terms of dynamical quantities such as autocorrelation functions, return probability, entanglement entropy and imbalance, to mention some. Here, we study the dynamics of a Floquet model of many-body localization, focussing on the dynamical regimes on the ergodic side of the transition.

DY 14.9 Mon 17:30 EB 107

Characterizing time-irreversibility in disordered fermionic systems by the effect of local perturbations — •Giuseppe De Tomasi[1], Frank Pollmann[2], Markus Heyl[1], Shreya Vardhan[3], and Eric Heller[4] — [1]MPIPKS, Dresden, Germany — [2]TMU, Munich, Germany — [3]MIT, Cambridge, USA — [4]Harvard, Cambridge, USA

We study the effects of local perturbations on the dynamics of disordered fermionic systems in order to characterize time-irreversibility. We focus on three different systems, the non-interacting Anderson and Aubry-André-Harper (AAH-) models, and the interacting spinless disordered t-V chain. First, we consider the effect on the full many-body wave-functions by measuring the Loschmidt echo (LE). We show that in the extended/ergodic phase the LE decays exponentially fast with time, while in the localized phase the decay is algebraic. We demonstrate that the exponent of the decay of the LE in the localized phase diverges proportionally to the single-particle localization length as we approach the metal-insulator transition in the AAH model. Second, we probe different phases of disordered systems by studying the time expectation value of local observables evolved with two Hamiltonians that differ by a spatially local perturbation. Remarkably, we find that many-body localized systems could lose memory of the initial state in the long-time limit, in contrast to the non-interacting localized phase where some memory is always preserved.

DY 15: Nonlinear Dynamics, Synchronization, Chaos I

Time: Monday 15:30–17:30 Location: BH-N 128

DY 15.1 Mon 15:30 BH-N 128

Ubiquity of macroscopic chaos in balanced networks of spiking neurons — •Alessandro Torcini[1], Ekkehard Ullner[2], and Antonio Politi[2] — [1]Laboratoire de Physique Théorique et Modélisation Université de Cergy-Pontoise - 2 avenue Adolphe Chauvin, Pontoise 95302 Cergy-Pontoise cedex, Île-de-France, France — [2]Institute for Complex Systems and Mathematical Biology and Department of Physics (SUPA), Old Aberdeen, Aberdeen AB24 3UE, UK

We revisit the behavior of a prototypical model of balanced activity in networks of spiking neurons. A detailed study of an appropriate thermodynamic limit for fixed density of connections shows that, when inhibition prevails, the asymptotic regime is characterized by a self-sustained irregular, macroscopic (collective) dynamics rather than being asynchronous. This holds true even for very small coupling strengths. A relationship with the collective chaos observed in standard (unbalanced) heterogeneous networks is also put forward and the role played by clustered states discussed.

DY 15.2 Mon 15:45 BH-N 128

Partial synchronisation in yeast cell populations — André Weber[1], Werner Zuschratter[1], and •Marcus J. B. Hauser[2] — [1]Leibniz-Institut für Neurobiologie Magdeburg, Germany — [2]Institut für Biometrie und Medizinische Informatik, Otto-von-Guericke-Universität Magdeburg, Germany

The mechanism of the transition between synchronised and desynchronised behaviour of intact yeast cells of the strain *Saccharomyces carlsbergenis* was investigated. In cell colonies of intermediate cell density, all cells remain oscillatory, in addition, a partially synchronised and a desynchronised state are accessible for experimental studies. In the partially synchronised state, the mean oscillatory period is shorter than that of the cells in a desynchronised state. Thus, synhronisation occurs due to entrainment to cells that oscillate more rapidly. This is typical for synchronisations due to phase advancement. However, the cells do not synchronise completely, as the distribution of the oscillatory frequencies only narrows but does not collapse to a single frequency. The desynchronisation is characterised by a broadening of the distribution of oscillation frequencies of the cells. Chimera states, i.e., the coexistence of a synchronised and a desynchronised parts of the population, could not be observed.

DY 15.3 Mon 16:00 BH-N 128

Synchronization in systems with linear, yet nonreciprocal interactions — •Christoph Räth, Michael Haslauer, and Ingo Laut — DLR, Institut für Materialphysik im Weltraum, Münchner Str. 20, 82234 Wessling

Synchronization of oscillatory subsystems is a widespread phenomenon in science. It is argued that the presence of nonlinearities is a necessary prerequisite for synchronization. Here, we study synchronization in complex plasmas consisting of microparticles in addition to the plasma. The particles can form 2D crystalline structures. They can melt via mode-coupling instability (MCI), which is a consequence of the effective nonreciprocal interactions. Synchronized particle motion during MCI-melting of 2D plasma crystal was reported in [1]. To disentangle the effects of nonlinearity and nonreciprocity on the emergence of synchronization, we solved numerically the nonlinear and the linearized system. Analyzing the synchronization with a new order parameter [2] reveals that a linearized version of the interaction model exhibits the same synchronization patterns as the full, nonlinear one. Further, theoretical considerations show that nonreciprocal interactions among particles generally provide a mechanism for the selection of dominant wave modes causing the system to show synchronized motion. Thus, we demonstrate numerically and analytically that also linear systems can synchronize and that the nonreciprocity of the interaction is the more decisive property for a n-body system to synchronize [3].

[1] L. Couëdel et al., Phys. Rev. E, 89, 053108 (2014) [2] I. Laut et al., EPL, 110, 65001 (2015) [3] C. Räth et al. (in preparation)

DY 15.4 Mon 16:15 BH-N 128

Synchronization of Viscoelastically Coupled Excitable Oscillators with Excitation-Contraction Coupling — •Florian Spreckelsen[1,2], Ulrich Parlitz[1,2,4], and Stefan Luther[1,2,3,4,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Germany — [3]University Medical Center Göttingen (UMG), Institute of Pharmacology and Toxicology, Göttingen, Germany — [4]DZHK (German Center for Cardiovascular Research), Partner Site Göttingen, Germany — [5]Department of Physics and Department of Bioengineering, Northeastern University, Boston, USA

Viscoelastically coupled excitable oscillators are used to model individually beating spatially separated cardiomyocytes surrounded by an extra-cellular matrix (ECM) of collagen. This corresponds to the early states in the development of engineered heart muscle (EHM). Synchronization of the beating of the cardiomyocytes is necessary for functioning of EHM. We investigate how mechanical coupling via the ECM can synchronize two excitable oscillators with excitation contraction coupling and electromechanical feedback and how this synchronization depends on the rheological properties of the ECM.

DY 15.5 Mon 16:30 BH-N 128

Synchronization of excitation waves in excitable media using low-pass filtered signals. — •Baltasar Rüchardt[1], Jochen Bröcker[4], 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

Excitable media are spatially extended systems with diffusion-like local transport in at least one variable. They respond strongly in this variable if it is pertubated above a threshold. They are suitable for modelling the electric activity in the heart muscle.

In this contribution we demonstrate that it is possible to synchronize two systems of excitable media by means of a uni-directional coupling with spatially low-pass filtered signals. The resulting ability of reconstructing the full spatio-temporal dynamics from a sequence of blurred images is crucial for recovering dynamical information in cardiac experiments using multichannel ECG measurements and synchronization based data assimilation methods.

DY 15.6 Mon 16:45 BH-N 128

Synchronization of high dimensional systems using an ensemble approximation of the inverse linearized delay coordinates map — Flavia R. Pinheiro[1], Peter Jan van Leeuwen[1], and •Ulrich Parlitz[2] — [1]Dept. of Meteorology, University of Reading, UK and the National Centre for Earth Observation (NCEO) — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen

Synchronization of uni-directly coupled systems can be significantly improved by using delay reconstruction of states in the coupling term [1], [2]. This approach, however, requires the computation and (pseudo) inversion of the Jacobian matrix of the delay coordinates map which is for high dimensional systems computationally extremely expensive. As an alternative, we present a method for approximating the required Jacobian matrix using an ensemble approach [3]. The feasibility and efficacy of this coupling scheme is demonstrated for D-dimensional Lorenz-96 systems with D ranging from 20 to 1000. With its capability to achieve synchronization of high dimensional systems this approach may serve as a building block of novel data assimilation schemes (nonlinear particle filters) [3].

[1] D. Rey et al.. Phys. Lett. A. 378, 869-873 (2014) DOI: 10.1016/j.physleta.2014.01.027
[2] D. Rey et al., Phys. Rev. E. 90: 062916 (2014) DOI: 10.1103/PhysRevE.90.062916
[3] F. R. Pinheiro, P. J. van Leeuwen, and U. Parlitz, to appear in Q. J. R. Meteorol. Soc., DOI: 10.1002/qj.3204

DY 15.7 Mon 17:00 BH-N 128

A bifurcation approach to the synchronization of coupled van der Pol oscillators — •Jorge Galan — Applied Mathematics. University of Sevilla

The van der Pol Oscillator is the canonical example of a planar limit cycle and has been extensively studied in the dynamical system community. Its coupled version has become the basic model of nonlinear dynamical system undergoing mutual synchronization.

We investigate the parameter dependence of the solutions of

$$\ddot{x} - (\lambda_1 - x^2)\dot{x} + x + \beta x^3 + \mu(\dot{x} - \dot{y}) = 0\,,$$
$$\ddot{y} - (\lambda_2 - y^2)\dot{y} + (1+\delta)y + \beta y^3 + \mu(\dot{y} - \dot{x}) = 0.$$

The basic tool for our study has been continuation of the unique equilibrium point of the system; the origin. The appearance of Hopf bifurcations accounts for the regions where oscillations are present. The families of periodic orbits have been followed as the parameters are varied with special attention to the bifurcations and resonances and their relation to synchronization. In particular, we have tried to clarify the presence of a special synchronization regime on an infinitely long band in parameter space between oscillator death and the quasiperiodic area. We present partial bifurcation diagrams both for the van der Pol ($\beta = 0$) and Duffing-van der Pol ($\beta \neq 0$) scenarios.

The structure of the synchronization regions in the parameter space is organized around curves of limit point bifurcations of periodic orbit where isolas are formed and a special curve where a tangency condition with a appropriate Poincare section is present.

DY 15.8 Mon 17:15 BH-N 128

Generalized synchronization of a population of semiconductor lasers in some-to-all coupling configuration — •Axel Dolcemascolo[1], Francesco Marino[2], Romain Veltz[3], and Stéphane Barland[1] — [1]Université de Nice, CNRS, Institut Non Linéaire de Nice, Sophia Antipolis, France — [2]Dipartimento di Fisica, Università di Firenze, INFN, Sezione di Firenze, Italy — [3]Inria Sophia Antipolis, MathNeuro Team, Sophia Antipolis, France

Synchronization between different oscillators occurs in many natural and technological systems, from cardiac pacemaker cells to electronic components or coupled lasers. Here we explore a system of around 500 lasers arranged in an array, which are coupled together with an opto-electronic coupling, where the intensity of the emitted light (after continuous component removal and a saturable nonlinear function) controls the current used to drive collectively all the lasers. The coupling is of some-to-all type, where an arbitrary set of the devices is coupled with the whole population.

The particular case of just one coupled laser has already been studied in *Chaotic spiking ...* by Kais Al-Naimee et al., New J. Phys. 11 (2009), where it has been shown that one single laser can produce a sequence of slow chaotic spiking as a result of an incomplete homoclinic scenario to a saddle-focus. Here we study experimentally the different types of dynamics that emerge when changing the set of feedback lasers while also keeping constant the feedback strength, and the emergence of chaos and synchronization when changing control parameters such as the coupling strength and the operating point of the whole array.

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

Time: Monday 15:30–18:45 Location: BH-N 243

DY 16.1 Mon 15:30 BH-N 243

Run-and-Tumble-like Motion of Synthetic Microswimmers in Viscoelastic Media — •Celia Lozano, J. Ruben Gomez-Solano, and Clemens Bechinger — Fachbereich Physik, Universität Konstanz, Konstanz D-78457, Germany

Run-and-tumble (RNT) motion is a prominent locomotion strategy employed by many living microorganisms. It is characterized by straight swimming intervals (runs), which are interrupted by sudden reorientation events (tumbles). In contrast, directional changes of synthetic microswimmers (active particles, APs) are caused by rotational diffusion, which is superimposed with their translational motion and, thus, leads to rather continuous and slow particle reorientations. Here we demonstrate that APs can also perform a swimming motion where translational and orientational changes are disentangled, similar to RNT. In our system, such motion is realized by a viscoelastic solvent and a periodic modulation of the self-propulsion velocity. Experimentally, this is achieved using light-activated Janus colloids, which are illuminated by a time-dependent laser field. We observe a strong enhancement of the effective translational and rotational motion when the modulation time is comparable to the relaxation time of the viscoelastic fluid. Our findings are explained by the relaxation of the elastic stress, which builds up during the self-propulsion, and is suddenly released when the activity is turned off. In addition to a better understanding of active motion in viscoelastic surroundings, our results may suggest novel steering strategies for synthetic microswimmers in complex environments.

DY 16.2 Mon 15:45 BH-N 243

Effective viscosity of active suspensions — Levan Jibuti[1], Walter Zimmermann[1], Salima Rafai[2], and •Philippe Peyla[2] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]LIPhy, Université Grenoble Alpes and CNRS, F-38402 Grenoble, France

Micro-organisms usually can swim in their liquid environment by flagellar or ciliary beating. In this numerical work, we analyze the influence of flagellar beating on the orbits of a swimming cell in a shear flow. We also calculate the effect of the flagellar beating on the rheology of a dilute suspension of microswimmers. A three-dimensional model is proposed for Chlamydomonas Reinhardtii swimming with a breaststroke-like beating of two anterior flagella modeled by two counter-rotating fore beads. The active swimmer model reveals unusual angular orbits in a linear shear flow. This peculiar behavior has some significant consequences on the rheological properties of the suspension. We calculate Einstein's viscosity of the suspension composed of such isolated modeled microswimmers (dilute case) in a shear flow. The results show an increased intrinsic viscosity for active swimmer suspensions

in comparison to nonactive ones as well as a shear thinning behavior in accordance with our previous experimental measurements.

Effective viscosity of a suspension of flagellar-beating microswimmers: Three-dimensional modeling Levan Jibuti, Walter Zimmermann, Salima Rafaï, and Philippe Peyla Phys. Rev. E 96, 052610 (2017)

DY 16.3 Mon 16:00 BH-N 243

Self propulsion of droplets driven by an active permeating gel — •Reiner Kree and Annette Zippelius — Inst. f. Theoret. Physik, Univ. Göttingen, Friedrich-Hund. Pl. 1, 37077 Göttingen

We discuss the flow field and velocity of active droplets, which are driven by body forces residing on a rigid gel. The latter is modeled as a porous medium which gives rise to permeation forces. In the simplest model, the Brinkmann equation, the porous medium is characterized by a single length scale l, the square root of the permeability. We compute the flow fields, the translational and rotational velocity of the droplet and the energy dissipation as a function of l. We show that the model gives rise to non-monotic behaviour of the droplet velocities and the dissipated power as functions of the gel fraction. As l changes from large to small values, the properties of the medium change from a simple viscous fluid to a Darcy medium. We discuss the behaviour of flow, velocities and force densities as these limits are approched.

DY 16.4 Mon 16:15 BH-N 243

Viscotaxis: a theory for microswimmer navigation in viscosity gradients — •Benno Liebchen[1], Paul Monderkamp[1], Borge ten Hagen[2], and Hartmut Loewen[1] — [1]Institut fuer Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universitaet Duesseldorf, D-40225 Duesseldorf, Germany — [2]Physics of Fluids Group, Faculty of Science and Technology, University of Twente, 7500 AE Enschede, The Netherlands

The survival of many microorganisms, like Leptospira or Spiroplasma bacteria, which swim poorly in low-viscosity fluids, depends on their ability to navigate up viscosity gradients. While this ability, called viscotaxis, has been observed in several experiments with microorganisms, the underlying mechanism remains unclear. In the present talk, we present a simple theory for viscotaxis of self-propelled swimmers [1] in slowly varying viscosity gradients: this theory unveils specific mechanisms for viscotaxis based on a systematic imbalance of viscous forces acting on different body parts of a swimmer and allows to classify microswimmers regarding their ability to perform viscotaxis based on their body shapes. Besides shedding new light on microorganism viscotaxis, our results may be useful to design synthetic swimmers with the ability to navigate in viscosity gradients (akin to synthetic chemo- or thermotactic swimmers [2]).

[1] B. Liebchen, P. Monderkamp, B.t. Hagen and H. Löwen, in preparation.

[2] B. Liebchen, D. Marenduzzo, and M. E. Cates, Phys. Rev. Lett. 118, 268001 (2017).

DY 16.5 Mon 16:30 BH-N 243

Photo-gravitaxis in synthetic microswimmers — •William Uspal[1,2], Dhruv Singh[1], Mihail Popescu[1,2], Laurence Wilson[3], and Peer Fischer[1,4] — [1]Max-Planck-Institut für Intelligente Systeme — [2]IV. Institut für Theoretische Physik, Universität Stuttgart — [3]Department of Physics, University of York — [4]Institut für Physikalische Chemie, Universität Stuttgart

We study the dynamics of active Janus particles that self-propel in aqueous solution by light-activated catalytic decomposition of chemical "fuel." In experiments, the particles, initially sedimented at a bottom wall, exhibit wall-bound states of motion, dependent on the size of the particle, when illuminated from underneath the wall. Upon increasing the intensity of the light above a threshold value, which is also dependent on the size of the particle, the particles lift off the wall and move way from it, i.e., they exhibit a photo-gravitactic behavior similar to some planktonic microorganisms. The dependencies on the particle size are rationalized by using a theoretical model of self-phoresis that explicitly accounts for the "shadowing" effect of the opaque catalytic face of the particle. Our model allows us to unequivocally identify the photochemical activity and phototactic response as the key mechanisms beyond the observed phenomenology. Consequently, one has the means to design photo-gravitatic particles that can reversibly switch between operating near a boundary or in the volume away from the boundary by judiciously adjusting the light intensity, i.e., simply by "turning a knob".

15 min. break

DY 16.6 Mon 17:00 BH-N 243

Active Rods in a Converging Flow — •Andreas Kaiser[1], Mykhailo Potomkin[2], Leonid Berlyand[2], and Igor Aranson[1,2] — [1]Department of Biomedical Engineering, Pennsylvania State University, University Park, 16802, USA — [2]Department of Mathematics, Pennsylvania State University, University Park, 16802, USA

We consider active rodlike particles swimming in a convergent fluid flow in a trapezoid nozzle by using mathematical modeling to analyze trajectories of these particles inside the nozzle and numerical simulations to show that trajectories are strongly affected by the background fluid flow and geometry of the nozzle leading to wall accumulation and rheotaxis. We describe the non-trivial focusing of active rods depending on physical as well as geometrical parameters. It is also established that the convergent component of the background flow leads to stability of both downstream and upstream swimming at the centerline. The stability of downstream swimming enhances focusing, and the stability of upstream swimming enables rheotaxis in the bulk.

DY 16.7 Mon 17:15 BH-N 243

Guidance of self-phoretic Janus particles by chemically patterned surfaces — William Uspal[1,2], •Mihail Popescu[1,2], Mykola Tasinkevych[3], and Siegfried Dietrich[1,2] — [1]M.P.I. for Intelligent Systems, Stuttgart, Germany — [2]University of Stuttgart, Germany — [3]University of Lisbon, Portugal

Self-phoretic Janus particles move by inducing – via non-equilibrium chemical reactions occurring on their surfaces – gradients in chemical composition along the surface of the particle, as well as along any nearby boundaries. The chemical gradients along a wall can give rise to chemi-osmosis, which, in turn, drives flow in the volume of the solution and thus couples back to the particle. This response flow induced and experienced by a particle encodes information about any chemical patterning of the wall. Here, we show by analytical calculations, complemented with numerical solution, that wall-patterning by chemical steps can provide the means for docking of achieving a step-guided motion of such an active particle, and we discuss the dependence of the phenomenology on the shape (spherical or rod-like) of the particle. Furthermore, we show that such chemically active particles in general align with, and follow, spatial gradients in the surface chemistry of the wall (i.e., they exhibit thigmo-taxis).

DY 16.8 Mon 17:30 BH-N 243

Randomly shaped magnetic Micropropellers — •Felix Bachmann[1], Agnese Codutti[1,2], Klaas Bente[1], and Damien Faivre[1] — [1]Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Science Park Golm — [2]Max Planck Institute of Colloids and Interfaces, Department of Theory & Bio-Systems, Science Park Golm

Over the last decade many different actuation mechanisms for swimming at low Reynolds number have been suggested and implemented. Magnetic micropropellers are a promising example that combines remote and fuel-free actuation with precise control. Now, the realization of the envisioned, mostly medical application is the next step. Therefore, automation and additional control strategies have to be developed. In this regard, randomly shaped micropropellers offer the possibility to find and test new actuation schemes and the associated propeller shapes. We screen a pool of such randomly shaped magnetic micropropellers by applying different magnetic fields and record their swimming behavior by optical high speed microscopy, which additionally enables tomographic 3D-shape reconstructions of interesting propellers. This is the basis for their reproduction through micro- and nanofabrication and eventually facilitates the formulation of micropropeller design guidelines for special applications.

DY 16.9 Mon 17:45 BH-N 243

Active Brownian particles in a inhomogeneous activity or magnetic field — •Hidde Vuijk and Abhinav Sharma — Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, 01069 Dresden

We study spherically symmetric active particles in a spatially inhomogeneous activity or magnetic field. In both cases the particles spontaneously orient themselves, which results in an inhomogeneous distribution of particles. Using Green-Kubo approach we obtain analytical expression for the orientation of the particles. We find that the relevant equilibrium correlation function is the self-part of the Van Hove

function, which can be approximated accurately. Density does not have a linear response to the activity; however, an expression for the density is derived by using the orientation as input to dynamic density functional theory. All theoretical predictions are validated using Brownian dynamics simulations.

DY 16.10 Mon 18:00 BH-N 243

Active colloidal particles in evaporating liquid droplets — •Borge ten Hagen[1], Maziyar Jalaal[1], Hai Le The[2], Christian Diddens[1], Alvaro Marin[1], and Detlef Lohse[1,3] — [1]Physics of Fluids Group and Max Planck Center Twente, University of Twente, Enschede, The Netherlands — [2]MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands — [3]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Inspired by biological microswimmers, various types of artificial self-propelled particles have been developed and thoroughly characterized in recent years. While in most studies quiescent solvents or stationary flow fields were considered, much less is known about the behavior of synthetic microswimmers in more complicated flow environments as they often occur in biological systems under non-laboratory conditions. Here, we investigate the dynamics of self-propelling Janus particles in an evaporating droplet of hydrogen peroxide solution. The competition between the flows due to the evaporation and the active motion of the particles leads to a complex dynamical behavior. The system is analyzed using three-dimensional particle tracking measurements and numerical simulations of the nontrivial fluid flow within the evaporating droplet. It will also be discussed how the particle activity affects the coffee-ring formation in the final state of evaporation, where the orientation of the Janus particles introduces a new order parameter.

DY 16.11 Mon 18:15 BH-N 243

Active droplet model of cellular aggregates — •Hui-Shun Kuan, Frank Jülicher, and Vasily Zaburdaev — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Active systems appear in various biological contexts such as cell cytoskeleton and bacterial colonies. Such systems may exhibit phase separation, which is not governed by free energy minimization. In this talk, we use the concept of phase separation to study the formation of bacterial colonies, of N. gonorrhoeae, due to active force generation by cell appendages type IV pili. We use a hydrodynamics approach, representing bacterial colonies as active droplets, which exhibit different surface profiles and position-dependent motility gradients. In addition, the coalescence of two such droplets exhibits two time scales which cannot be understood by the surface tension and viscosity. Our theoretical description of active droplets provides means of describing bacterial colonies and can be extended to other cell types.

DY 16.12 Mon 18:30 BH-N 243

3D dynamics of synthetically assembled microtubules and motors — •Smrithika Subramani, Christian Westendorf, Eberhard Bodenschatz, and Isabella Guido — Max Planck Institute for dynamics and self-organization, Göttingen, Germany

Cytoskeletal filaments such as microtubules play a major role in cell division, organelle transport and cellular motility. These diverse biological functionalities are driven by bending, looping and buckling of microtubule (MT) filaments. In our study, we intend to gain a deeper understanding of these phenomena by synthetically reconstituting dynamic MT structures.

We hierarchically build a model active matter system using depletion-driven MT bundles and the processive motor Kinesin-1, assembled in a tetrameric complex. By hydrolyzing ATP and undergoing a conformational change, the motor complex is able to effectively 'walk' along MT bundles and generate motion in a 3D environment. Our observations include continuous sliding, bending and buckling of MT bundles into long-wavelength arcs, resembling their in vivo behaviour. By using the Fluorescence Recovery After Photobleaching (FRAP) method, we are able to analyze the MT structure distribution. A multi-plane fluorescence microscopy technique enables us to observe the bundle dynamics in 3D.

DY 17: Focus: Droplets (joint session DY/CPP)

The physics of droplets is surprisingly rich - and full of surprises. This holds for droplets in ambient gas and for droplets in other liquids. The geometric and dynamical parameters which enter are size and velocity and the material properties are density, surface tension, velocity, volatility, freezing and melting points, latent heat, viscosity, thermal conductivity,... and all this holds for both the drops and for the surrounding gas or liquid. Moreover, both droplet and surrounding can be multicomponent and phase transitions and chemical reactions. The consequence of this huge parameter space is a plethora of often very surprising phenomena - and many are technologically very important. The systematic optimization of processes involving such phenomena needs a fundamental understanding of the physics. In this session various examples are given in which the community has worked towards such an understanding, combining controlled experiments, numerical simulations, and theoretical analysis.

D. Lohse

Time: Monday 15:30–19:15 Location: BH-N 334

DY 17.1 Mon 15:30 BH-N 334

Marangoni Contraction of Evaporating Sessile Droplets of Binary Mixtures — •Stefan Karpitschka[1], Ferenc Liebig[2], and Hans Riegler[3] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen — [2]Institute of Chemistry, University of Potsdam, Karl-Liebknecht-Straße 24-25, 14476 Potsdam — [3]Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam

The evaporation of sessile droplets of mixtures is a ubiquitous natural and industrial process, relevant, e.g., for cleaning/drying of semiconductor surfaces or for ink-jet printing. For binary mixtures, the component with the higher vapor pressure will usually evaporate faster and thus deplete from the contact line region of a droplet. In general, different liquids have different surface tensions. Thus, evaporation causes surface tension gradients and Marangoni flows. Here we investigate the impact of evaporation on the wetting behavior of binary mixtures [Langmuir 33, 4682 (2017)]. We measure non-zero apparent contact angles even if both liquid components individually wet the substrate completely. Simulations show that the interplay of Marangoni flow, capillary flow, diffusive transport, and evaporative losses can establish a quasi-stationary drop profile with an apparent nonzero contact angle. In good agreement with experiments, we reveal a previously unknown universal power-law relation between the apparent contact angle and the relative undersaturation of the atmosphere, which can be inferred from the scaling analysis of the hydrodynamic-evaporative evolution equations.

DY 17.2 Mon 15:45 BH-N 334

Equilibrium versus non-equilibrium positioning of droplets — •Samuel Krüger[1,2], Christoph A. Weber[4], Jens-Uwe Sommer[2,3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Leibniz Institute of Polymer Research Dresden e.V — [3]Technische Universität Dresden, Institute of Theoretical Physics, Dresden, Germany — [4]Division of Engineering and Applied Sciences, Harvard University, Cambridge, USA

The position of droplets can be controlled by concentration gradients of a component which affect phase separation. A concentration gradient can be generated by an external potential or by boundary conditions. While systems with external potentials belong to the class of equilibrium systems, applying boundary conditions corresponds to a

non-equilibrium scenario. We aim to understand what is the difference between these two scenarios and how the positioning is affected. To this end, we consider a ternary system where two components phase separate while a third component regulates their phase separation. We use Monte-Carlo simulations to compare the positioning of droplets between the two scenarios. In both scenarios we find that the droplet is positioned toward the region of low or high regulator concentration depending on their interaction parameters. The essential differences are the set of interaction parameter where the switch of position occurs. The positioning of droplets is relevant in cells prior to cell division or applications in microfluidic devices such as aqueous computing.

DY 17.3 Mon 16:00 BH-N 334

Drying Teardrops — •Alvaro Marin[1], Stefan Karpitschka[2], Christian Diddens[3], Massimiliano Rossi[4], Christian J. Kähler[4], Diego Noguera-Marin[5], and Miguel A. Rodriguez-Valverde[5] — [1]Max Planck + University of Twente Center for Complex Fluid Dynamics, The Netherlands — [2]Max Planck Center for Dynamics and Self-Organization, Germany — [3]Physics of Fluids, University of Twente, The Netherlands — [4]Bundeswehr University Munich, Neubiberg, Germany — [5]Biocolloid and Fluid Physics group, University of Granada, Spain

Salt can be found in different forms in almost any evaporating droplet in nature, our homes and in our own tears. Dried teardrops present an amazing variety of forms, shapes and crystals (even for the same person), but they all have something in common: a ring-shaped stain. In this talk we will address a model teardrop system consisting of an evaporating water sessile droplet with sodium chloride concentrations from 1 mM up to 100 mM. With experimental measurements and numerical simulations we can show that the transport of liquid in this system differs strongly from 'sweet' evaporating water droplets: the liquid flows in the inverse direction due to strong Marangoni stresses at the surface. Such an effect has crucial consequences to the deposition of salt, its crystallization and to the formation of the ring-shaped stains. In summary, our aim is to show that other mechanisms different than the famous "coffee-stain effect" can yield ring-shaped stains in evaporating sessile droplets.

DY 17.4 Mon 16:15 BH-N 334

Protein Interactions Control Dynamics Of Liquid Compartments — •Tyler S. Harmon[1,2], Anthony A. Hyman[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Molecular Cell Biology, 01307 Dresden, Germany

Membraneless organelles form in cells due to liquid-liquid phase separation and have been implicated in a range of functions. The physical properties of these compartments are important for their function and thus should be tuned to match their intended purpose. Multiple diseases are associated with a hardening transition where these liquid compartments transition from a functional liquid-like state to an aberrant solid-like state over a long period of time. Other compartments appear to be designed to mature naturally from a liquid into a more solid compartment. Therefore, the physical mechanism controlling the liquid to solid transition is at the heart of how cells regulate and control these compartments.

We designed a three-dimensional polymer lattice model to investigate mechanisms for hardening in liquid compartments. We explore several mechanisms affecting the time dependence of protein dynamics. This allows us to test which protein properties are important for controlling the slowing of the dynamics of the liquid compartments. We analyzed the transition to a solid-like state by quantifying the time dependence of diffusion rates, density, and reversibility of dissolution. These results are a promising first step to reach a molecular picture of the hardening process.

DY 17.5 Mon 16:30 BH-N 334

Oscillatory wetting under drops impacting on a hot plates — •Kirsten Harth, Michiel A. J. van Limbeek, Chao Sun, Andrea Prosperetti, and Detlef Lohse — Physics of Fluids, Max Planck Center for Complex Fluid Dynamics and University of Twente, The Netherlands

The Leidenfrost phenomenon, where an evaporating drop levitates above a layer of its vapour on sufficiently hot plates is well-known for gently deposited drops. For impacting drops, the additional impact pressure can cause much thinner vapour layers in the nanometer range, and conventional side or bottom view imaging is incapable of detecting substrate contact. Using frustrated total internal reflection (FTIR), three main regimes were distinguished: contact, nucleate boiling at low temperatures (drop spreads in contact with substrate), Leidenfrost (film) boiling without contact and a broad transition regime. Then, the outer parts of the spreading lamella levitate, while the central region of the drop touches the substrate. However, the wetted locations and the drop's partially levitated bottom surface increasingly fluctuate with increasing temperature. Most striking are periodic waves travelling from the lamella tips toward the centre of the wetted region. We analyze and discuss this currently unresolved phenomenon.

DY 17.6 Mon 16:45 BH-N 334

Spontaneous jumping, bouncing and trampolining of hydrogel drops on a heated plate — •Doris Vollmer[1], Jonathan Pham[1], Sanghyuk Wooh[1], Tadashi Kajiya[1,2], and Hans-Jürgen Butt[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Analysis Technology Center, Fujifilm, Nakanuma, Japan

We study the dynamics of hydrogel drops, i.e. sold drops containing up to 97% of water. Using high speed video microscopy, we demonstrate that hydrogel drops, initially at rest on a surface, spontaneously jump upon rapid heating and continue to bounce with increasing amplitudes. Jumping is governed by the surface wettability, surface temperature, hydrogel elasticity, and adhesion. A combination of low adhesion impact behavior and fast water vapor formation supports continuous bouncing and trampolining. Our results illustrate how the interplay between solid and liquid characteristics of hydrogels results in intriguing dynamics, as reflected by spontaneous jumping, bouncing, trampolining, and extremely short contact times.

J.T. Pham, M. Paven, S. Wooh, T. Kajiya, H.-J. Butt, D. Vollmer, Nat. Comm., 2017, 8, 905

15 min. break

DY 17.7 Mon 17:15 BH-N 334

Droplets in moist Rayleigh-Bénard convection — Prasanth Prabhakaran, Alexei Krekhov, •Stephan Weiss, and Eberhard Bodenschatz — Max Planck Institute f. Dynamics and Self-Organisation, Göttingen, Germany

We report experiments on condensation patterns in a moist Rayleigh-Bénard convection experiment. We use Sulphur Hexaflouride (SF_6) at high pressure as the working fluid and the experiment is operated across the liquid-vapor coexistence line close and far from the critical point. A layer of liquid SF_6 forms at the warm bottom of the cell. From its surface, vapor evaporates and condenses at the cold top plate, where it forms a thin film that undergoes a Rayleigh-Taylor like instability. As a result droplets form due to pinch-off that fall back into the liquid layer. Depending on the pressure and the temperature difference between bottom and top, locations where droplet form can lie on an almost stationary hexagonal grid with a well defined wavelength. When the liquid level at the bottom plate is eliminated the droplets falling from the top plate levitate above the bottom plate due to Leidenfrost effect. Under appropriate conditions the Leidenfrost drops form large domains with multiple chimneys (multi-connected domains).

DY 17.8 Mon 17:30 BH-N 334

Growing drops on an inclined plate: Onset of sliding — •Simeon Völkel, Jonas Landgraf, and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

Liquid drops sitting on or running down an inclined plane are ubiquitous in our daily lives. Their sliding can be triggered by tilting the surface at a fixed drop volume or by increasing the drop volume at a fixed inclination angle. Here, we present experiments on the latter protocol. Therefore we employ a conventional inkjet printhead, which provides a volume resolution of 23 picoliters, high repeatability, as well as the flexibility of following the drop's development by selecting different nozzles. Based on an analysis of both top view and side view images, we explore the evolution of the drop shape in the vicinity of the depinning transition and compare our results with numerical simulations.

DY 17.9 Mon 17:45 BH-N 334

Contact angle saturation in electrowetting of nanodrops — •Nicolas Rivas and Jens Harting — Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11)

The wetting angle of a drop in contact with a substrate can be modified by applying an external electric field, a phenomenon referred to as

electrowetting. The degree of wetting most commonly increases with the applied electric field, although in many cases only until a certain angle, after which the electric field has little or no influence on the wetting properties of the drop. This limit behavior is referred to as contact angle saturation (CAS). The origin of CAS is unknown, with numerous possible explanations present in the literature. In the following work we investigate electrowetting and CAS at the nanoscale. A model is proposed that takes into account the hydrodynamics of two fluids and the diffusion of charged solutes (ions). The numerical methodology used to solve this model is presented together with validation cases. The model is used to study electrowetting of conductive sessile drops as a function of the overall ion concentration and the relative conductivity of the two fluid phases. The variations of the contact angle are consistent with previous studies. We also observe CAS in regions of low salt concentration. A mechanism for CAS is proposed based on the progressive loss of ions from the drop as the electric field increases. This is discussed in relation to previously proposed mechanisms for CAS, which in general involve physics which our model does not intend to capture.

DY 17.10 Mon 18:00 BH-N 334

Oblique Impact onto a Spherical Target — •Vignesh Thammanna Gurumurthy, Daniel Rettenmaier, Ilia V. Roisman, and Cameron Tropea — Insitute for Fluid Dynamics and Aerodynamics, Technical University of Darmstadt, Darmstadt,Germany

Drop impact onto spherical targets can be found in applications such as coating of particles in pharmaceutical products, spray encapsulation or agglomeration of particles in fluidized bed, etc. The chances of the drop impinging on the target asymmetrically are high which necessitates the understanding of its hydrodynamics. In this work, we investigate the drop impact onto spherical targets using numerical simulations. We use a modified version of volume of fluid method available in the open source code OpenFOAM for the simulations, with adaptive mesh refinement on the liquid-gas interface. Reynolds number and the off-axis distance between the target and the drop are the two parameters varied while the drop to target size ratio is kept constant. The impact is characterized by measuring the thickness of the film at the point of impact over time. Finally, an empirical correlation based on the Reynolds number for the residual film thickness will be presented.

DY 17.11 Mon 18:15 BH-N 334

Morphological evolution of microscopic dewetting droplets with slip — Tak S. Chan[1], Joshua D. McGraw[1,2], Thomas Salez[3], Ralf Seemann[1], and •Martin Brinkmann[1] — [1]Experimental Physics, D-66123 Saarland University — [2]Département de Physique, Ecole Normale Supérieure/PSL Research University, CNRS, 24 rue Lhomond, 75005 Paris, France — [3]Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI Paris, PSL Research University, Paris, France

A liquid drop sitting on a smooth substrate will contract or spread depending on the equilibrium contact angle and the initial shape of the drop. One well known example is that of drops spreading over a completely wetting surface, which follow Tanner's law. In this study, we numerically compute the dynamics of contracting microscopic droplets where the slip-length b on the substrate is comparable to the intial drop height H. As quantified by the asphericity of the drop shape, we find a cross-over between two different dynamic regimes at slip length $b \ll H$ and $b \gg H$. These findings are explained from a competition between viscous dissipation in elongational flows for $b \gg H$, friction at the substrate for $b \approx H$, and viscous dissipation in shear flows for $b \ll H$. Following the changes between the dominant dissipation mechanisms, our study not only indicates two universal rescalings of the evolution of asphericity, but also a cross–over to the quasi-static shape evolution when b is many orders of magnitude smaller than the slip length b_m where the asphericity assume its maximum value.

DY 17.12 Mon 18:30 BH-N 334

Role of hydrodynamics in chemically driven droplet division — •Rabea Seyboldt and Frank Jülicher — Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Macromolecular phase separation and droplet formation have long been proposed as key elements in the formation of protocells during the origin of life. A simple model of a protocell consists of a droplet, where droplet material is produced outside the droplet, and chemical reactions inside the droplet play the role of a simple metabolism. Our previous theoretical study showed that such chemically active droplets can have a flux-driven shape instability that leads to a symmetric droplet division. Here we study the role of hydrodynamic flows on the chemically driven droplet division. In the deformed droplet, gradients of Laplace pressure create the hydrodynamic flows that have a tendency to relax the droplet to a spherical shape. We find that despite these stabilizing flows, droplet division can still occur. We analyze the dependence of the instability on the droplet viscosity and parameters that characterize the metabolism and material production. A comparison with protein/RNA droplets suggests that the droplet division could be observable in experimental systems. This highlights the possibility that chemically driven shape instabilities could play a role for the organization of membrane-less organelles in biological cells. Additionally, our work provides a physical mechanism for the division of early protocells before the appearance of membranes.

DY 17.13 Mon 18:45 BH-N 334

Content of secondary droplets formed by drop impact onto a solid wall wetted by another liquid — •Hannah M. Kittel, Ilia V. Roisman, and Cameron Tropea — Institute of Fluid Mechanics and Aerodynamic, Technische Universität Darmstadt, 64287 Darmstadt, Germany

Drop impact onto a wetted substrate is of importance in many engineering applications, for example in a combustion chamber, during spray coating or airframe icing.. The impact outcome s determined by the inertia, viscous and capillary forces. If the drop and wall film are of different fluids, the miscibility and the interfacial forces also influence the outcome. The composition of secondary drops resulting from such an impingement, and the state of the liquid film influence significantly the mixture preparation in either the engine or the catalytic converter. In the case of non-miscible fluids, the distribution of both fluids during and after the impact is important in order to understand the mechanism behind the drop impact of different liquids.

The main focus of this experimental work is on the impact of a single drop onto a thin, horizontal wall film of dif-ferent fluids. The liquids of drop and wall film are non-miscible in order to have a phase interface between both liquids. A dye is added to the liquid of the drop in order to distinguish both phases during and after the drop impact. The composition of the secondary droplets resulting from splashing, as well as the content of the partial rebound are characterized.

DY 17.14 Mon 19:00 BH-N 334

Breakup of a stretching liquid bridge — •Sebastian Brulin, Ilia V. Roisman, and Cameron Tropea — Institute of Fluid Mechanics and Aerodynamics, Technische Universität Darmstadt, Darmstadt, Germany

Liquid bridge stretching occurs in many industrial applications like gravure printing, granulation of fine powders or fiber spinning. One industrial process where the phenomenon plays an important role is the ink transfer in gravure printing. This technique is used for the production of electrical circuits. The liquid is transferred from the printing role onto the printable substrate. During this transferring process the liquid forms a liquid bridge with the two substrates. In this work, the dynamics of a stretching liquid bridge between two solid plates, one of which moves with a constant acceleration, is studied using a high-speed video system. Experiments on fast bridge stretching and breakup were performed with the aim to measure the breakup time and the residual liquid volume at various initial gape thicknesses.

The measurements involve different non-dimensional initial gap heights (d= 0.1-0.4) for a wide range of accelerations (10 m/s2 -180 m/s2). The distilled water and water-gylcerol mixtures are used for the liquid bridge formation to investigate the effect of the viscosity and surface tension on the breakup time and breakup length. A semi-empirical model is developed in this study to predict these values.

DY 18: Critical Phenomena and Phase Transitions

Time: Monday 15:30–17:00 Location: BH-N 333

DY 18.1 Mon 15:30 BH-N 333

Heterogeneous crystal nucleation on and far away from the pre-structured seeds — •Swetlana Jungblut — Physikalische Chemie, TU Dresden

We investigate the impact of the simultaneous presence of two seeds with various structures on the process of crystal nucleation in an undercooled Lennard-Jones fluid by means of computer simulations. In the presence of seeds with face- and body-centered cubic structures, we find that decreasing the inter-seed distance enhances the probability of the crystalline clusters formed on one of the seeds to grow beyond the critical size, thus, increasing the crystal nucleation rates. In contrast, when seeds have an icosahedral structure, the crystalline clusters form mostly in the bulk. The crystal nucleation rate, however, is also determined by the distance between the seeds, pointing to a heterogeneous crystal nucleation that occurs away from the icosahedrally structured seeds.

DY 18.2 Mon 15:45 BH-N 333

The plain and layered Ising spin glasses in two dimensions — •Martin Weigel[1], Hamid Khoshbakht[1,2], Mohammad-Sadegh Vaezi[3], Gerardo Ortiz[4], and Zohar Nussinov[3] — [1]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany — [3]Department of Physics, Washington University, St. Louis, MO 63160, USA — [4]Department of Physics, Indiana University, Bloomington, IN 47405, USA

The Ising spin glass in 2D exhibits rich behavior with subtle differences in the scaling for different coupling distributions. We use combinatorial optimization methods to determine exact ground states for systems with up to $10\,000 \times 10\,000$ spins. A combination of new algorithms allow us to treat samples with fully periodic boundaries and to sample uniformly from degenerate ground states for the $\pm J$ model. To establish a unified framework for studying both discrete and continuous coupling distributions, we introduce the *binomial* spin glass. In this model, the couplings are the sum of m identically distributed Bernoulli random variables. In the continuum limit $m \to \infty$, this system reduces to the Edwards-Anderson model with Gaussian couplings, while $m = 1$ corresponds to the $\pm J$ spin glass. Using this model, we derive a rigorous bound for the degeneracy of any energy level. Studying the defect energies in this model, we uncover intriguing subtleties in the behavior of the model with respect to the order in which the thermodynamic ($N \to \infty$) and continuum ($m \to \infty$) limits are taken.

DY 18.3 Mon 16:00 BH-N 333

Disassembling Casimir scaling functions at finite aspect ratios — •Hendrik Hobrecht and Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

The finite-size scaling functions for the free energy of the two-dimensional Ising universality class are known exactly only either for finite aspect ratios at criticality due to conformal field theory (CFT), or for thin films at arbitrary temperatures. Beyond the thin films and CFT there are but a few results, namely for the torus, the open cylinder, and approaches for topologically more exotic forms like the open Möbius strip and the Klein bottle. Despite their role as potential for the critical Casimir force, even less is known in the presence of surface fields. We present a systematic calculation of the interlink between those limiting cases, implementing both symmetric (++) and asymmetric (+-) symmetry-breaking boundary conditions (BCs) on the cylinder with finite aspect ratio, as well as the often discussed Brascamp-Kunz BC. We show that the scaling limit of the latter one is indeed equal to open boundaries, as both are believed to represent Dirichlet BCs. An impressive feature of these scaling functions is the possibility to disassemble them not only into recurring bulk, surface, and finite-size contributions, but even beyond. We can distinguish different building blocks for the surfaces and surface fields, as well as for the breaking of the Z_2-symmetry and the surface tension due to imposed domain walls.

DY 18.4 Mon 16:15 BH-N 333

Analytic finite-size scaling functions in the anisotropic Ising rectangle — •Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

The partition function of the square lattice Ising model on the rectangle, with open boundary conditions in both directions, is calculated exactly for arbitrary system size $L \times M$ and temperature. We start with the dimer method of Kasteleyn, McCoy & Wu, construct a highly symmetric block transfer matrix and derive a factorization of the involved determinant, effectively decomposing the free energy of the system into two parts, $F(L,M) = F_{\text{strip}}(L,M) + F^{\text{res}}_{\text{strip}}(L,M)$, where the residual part $F^{\text{res}}_{\text{strip}}(L,M)$ contains the nontrivial finite-L contributions for fixed M. While $F^{\text{res}}_{\text{strip}}(L,M)$ becomes exponentially small for large L/M or off-critical temperatures, it leads to important finite-size effects such as the critical Casimir force near criticality.

In the finite-size scaling limit $L, M \to \infty$, $T \to T_c$, with fixed temperature scaling variable $x \propto (T/T_c - 1)M$ and fixed aspect ratio $\rho \propto L/M$, we derive exponentially fast converging series for the related universal Casimir potential and Casimir force scaling functions. At the critical point $T = T_c$ we confirm predictions from conformal field theory. The presence of corners and the related corner free energy has dramatic impact on the Casimir scaling functions and leads to a logarithmic divergence of the Casimir potential scaling function at criticality.

A. Hucht, J. Phys. A: Math. Theor. **50**, 065201 (2017), arXiv:1609.01963; **50**, 265205 (2017), arXiv:1701.08722

DY 18.5 Mon 16:30 BH-N 333

Emergence of bistability in coupled spreading dynamics — •Fakhteh Ghanbarnejad — Institute of Theoretical Physics, Technical University of Berlin

In this work, we study different coupled spreading dynamics in an evolutionary ecological framework. Spreading of pathogens, fashions, ideas, products and so on are examples of such dynamical systems. These spreading phenomena are often coupled with each other in different ways: either to strengthen or weaken each other propagation. The coupling may lead to "nucleation" and as a consequence first order phase transitions at epidemic thresholds. Also it may lead to bi-stability in a wide regime of parameters [New J. Phys. 19, 103041(2017)]. Here we present examples of such scenarios from epidemiological modelling in mean filed approximations as well as simulations results on random generated networks. We also discuss which mechanisms may cause abrupt transitions in different time scales of the system [Frontiers in Physics, V 5, P 46 (2017)].

DY 18.6 Mon 16:45 BH-N 333

cooperative elastic self-amplification in molecular materials induced by ultrafast spin state photo-switching — •Roman Bertoni[1], Marco Cammarata[1], Hervé Cailleau[1], Maciej Lorenc[1], Eric Collet[1], and Cristian Enaschescu[2] — [1]University Rennes 1, UMR UR1-CNRS 6251, Rennes, France — [2]Faculty of Physics, Alexandru Ioan Cuza University, Iasi, Romania

The field of Photo-Induced Phase transition (PIPT) is reaching dynamical material control at fundamental time scale. Amongst molecular photo-switchable materials, spin crossover crystals are archetype of molecular bi-stability. We are now able to switch and control such systems at ultrafast time scale. The ultrafast photo-switching of these materials leads to a complex multistep out-of-equilibrium dynamics spanning from local molecular process to macroscopic material changes. The initial photo-switching process occurs within one picosecond at the local molecular scale involving coherent structural dynamics [1]. At longer time scale, the material response departs from that observed in diluted molecules due to the lattice action through structural feedback. Our new results have evidenced the existence of self-amplified elastic amplification during the volume expansion of the material inducing a multiplication of the fraction of molecules by factor five [3]. Such elastically-driven cooperativity triggered by a light pulse offers a new efficient way to generate and stabilize photo-induced phases in many volume-changing materials. [1]M. Cammarata et al, Phys. Rev. Lett 113, 227402 (2014)[2]R. Bertoni et al, Nature Materials 15 606-610 (2016)

DY 19: Extreme Events

Time: Monday 17:30–18:15 Location: BH-N 333

DY 19.1 Mon 17:30 BH-N 333

Dragon-king-like extreme events in coupled bursting neurons — •Syamal Dana — Department of Mathematics, Jadavpur University, Kolkata, India

We observe dragon-king-like extreme events in two slow-fast HR bursting oscillators that are mutually communicating via three different chemical synaptic interactions, excitatory, inhibitory and a mixed type. The extreme events follow a common mechanism for all three choices of synaptic coupling: two coupled bursters emerged into antiphase synchronization (APS), either with a burst synchrony or a spiking synchrony depending upon the nature of coupling (excitatory or inhibitory). They intermittently lost stability of APS when two arbitrary spikes within the two bursting oscillations evolve into in-phase synchony. As a result, the trajectory of the error dynamics of the coupled bursters moves out of the APS manifold, which is manifested as an extreme event. Such extreme events are recurrent and outliers to a power law that is obeyed by other small to medium size events present in the dynamics and, follow the drangon-king-like distribution. This is also observed for purely diffusive and repulsive coupling in two HR neurons. We present experimental evidence of the dragon-king-like extreme events using two analog circuits of the HR model under simple linear diffusive and repulsive coupling.

DY 19.2 Mon 17:45 BH-N 333

Riddled Basins of Attraction in Systems exhibiting Extreme Events — •Arindam Saha and Ulrike Feudel — ICBM, University of Oldenburg, Germany

Extreme events are rare, recurrent and irregular events which have a large impact on the system. Due to their occurrence in a variety of physical systems including oceans, atmosphere, lasers, ecological communities and financial markets, the existing literature studies their generation mechanisms, impact and possible precursors in detail. However, none of these studies discuss the implications of a system where extreme events are exhibited in a multistable system. In this talk, we investigate the basin structure of a system where extreme events co-exist with a few other possible stable dynamics. To this end, we study a system of two identical FitzHugh-Nagumo oscillators coupled to each other by multiple delay couplings. We show that if extreme events occur in a multistable regime, the phase space may be partitioned into 'pure' and 'mixed' regions, where trajectories starting from the pure regions are certain not to exhibit extreme events; the trajectories starting from the mixed regions may or may not exhibit extreme events. By computing the uncertainty exponent using final state sensitivity method, we verify that the uncertainty exponent tends to zero, which indicates that basin corresponding to extreme events is riddled. We therefore demonstrate the existence of riddled basins of attraction in delay-coupled systems for the first time.

DY 19.3 Mon 18:00 BH-N 333

Extrem Velocity Fluctuations in Turbulence Characterised as Negative Entropy Events — Andre Fuchs[1], Nico Reinke[1], Daniel Nickelsen[2], Matthias Wächter[1], and •Joachim Peinke[1] — [1]Institute of Physics, Carl von Ossietzky University of Oldenburg, Germany — [2]Institute of Theoretical Physics, University of Stellenbosch, South Africa

The turbulent cascade is analysed with respect to the evolution process of velocity increments towards smaller scales. A general n-point description is achieved by means of Markow process in the scale. Finally we set up Fokker-Planck equation for the cascade. Based in this description entropies values S_i can be assigned to all velocity fluctuations. These fluctuating entropy values fulfil integral fluctuation theorem, claiming that $< exp(-S_i) >= 1$. As a main finding we see that negative entropies events are linked to localised extrem velocity fluctuations on small scales.

DY 20: Talk S. Rotter

Time: Tuesday 9:30–10:00 Location: EB 107

Invited Talk DY 20.1 Tue 9:30 EB 107

Light fields in complex media: mesoscopic physics meets wave control — •Stefan Rotter — TU Wien, Vienna, Austria

In my talk I will explain how insights from mesoscopic scattering theory can be used to understand and engineer the behaviour of waves in complex media [1]. In particular, I will focus on the concept of time-delay in scattering, which we recently employed to show that the mean path length of light in a medium is independent of whether this medium is transparent or opaque [2]. The concept of scattering time-delay can also be used for novel wave front shaping protocols such as for engineering transmission channels through multi-mode fibres [3] or through strongly scattering media [4,5] with an extreme spectral robustness as required in communication technology. A suitable generalisation of such ideas allows to construct wave fronts that focus on a designated target inside a disordered medium [6] with potential applications in imaging. I will conclude my talk with an outlook on the possibilities to engineer waves in non-Hermitian media with gain and loss, where completely new functionalities are currently emerging [7,8].

[1] S. Rotter and S. Gigan, Rev. Mod. Phys. 89, 015005 (17).
[2] R. Savo, et al., Science 358, 765 (17).
[3] W. Xiong, et al., PRL 117, 053901 (16) & PRX 7, 041053 (17).
[4] B. Gérardin et al., PRB 94, 014209 (16).
[5] J. Böhm, et al., arXiv:1706.08926
[6] P. Ambichl, et al., PRL 119, 033903 (17).
[7] K. G. Makris, et al., Light Sci. Appl. 6, e17035 (17).
[8] J. Doppler, et al., Nature 537, 76 (16).

DY 21: Complex Fluids and Colloids II (joint session CPP/DY)

Time: Tuesday 9:30–11:45 Location: C 264

DY 21.1 Tue 9:30 C 264

Effective Landau description of ferronematics — •Grigorii Zarubin[1,2], Markus Bier[1,2], and Siegfried Dietrich[1,2] — [1]Max Planck Institute Int. Sys. — [2]University of Stuttgart, Germany

A ferromagnetic phase of anisotropic particles suspended in a nematic liquid crystal (NLC) was predicted as early as 1970 [1]. A recent experimental realization [2] confirmed that a dilute suspension of magnetic platelets in NLC forms ferromagnetic phase which is susceptible to weak magnetic fields. In this work we develop a Landau-like description of such a suspension starting from a microscopic model. Our functional represents an expansion in powers of two spatially varying fields: i) magnetization field and ii) director field and their cross terms. Using this result we can compare our theory to the one proposed in [2], in particular we have an access to the effective coupling coefficient between magnetization and director field which provides a way to estimate coupling of the director to the surface of the single platelet experimentally.

[1] F. Brochard and P.G. de Gennes, J. Physique 31, 691 (1970).
[2] A. Mertelj, D. Lisjak, M. Drofenik and M. Copic, Nature 504, 237 (2013).

DY 21.2 Tue 9:45 C 264

Self-assembly of colloidal particles with a magnetic coating under external magnetic fields — Gabi Steinbach[1,2], Michael Schreiber[1], Dennis Nissen[3], Manfred Albrecht[3], •Ekaterina Novak[4], Pedro A. Sanchez[5], Sofia Kantorovich[4,5], Sibylle

Gemming[1,2], and Artur Erbe[2] — [1]Institute of Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Lenin Av.51 — [3]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [4]Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — [5]Computational Physics, Universität Wien, Sensengasse 8, Vienna, 1090, Austria

In recent years, in order to build tailored structures, magnetic nanoparticles and colloids that deviate from the model of a spherical particle with a dipole moment at its center were studied. Among them are dumbbells, magnetic core-shell particles, elongated ferroparticles, and colloidal particles with a magnetic cap. In this contribution, we both experimentally and numerically shows how an equilibrium state with non-collinear arrangement of the magnetic moments of colloidal particles with a magnetic cap enables the controlled self-assembly of diverse structures in two dimensions via constant and low-frequency external magnetic fields. Branched clusters of staggered chains, compact clusters, linear chains, and dispersed single particles can be formed and interconverted. The presented precise control of structure formation and reconfiguration under external fields of only a few mT open new potential for using in responsive materials for highly sensitive magnetic and optical applications.

DY 21.3 Tue 10:00 C 264

Self-assembly of magnetic filaments with different topologies — •Elena Pyanzina[1], Ekaterina Novak[1], Dmitry Rozhkov[1], Pedro Sanchez[2], and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]University of Vienna, Sensengasse 8, 1090, Wien, Austria

Semi-flexible polymer-like chains of magnetic nanoparticles permanently crosslinked with polymers (magnetic filaments) have been recently pointed as promising building blocks for the creation of sophisticated magnetoresponsive materials. Our research addresses the study of magnetic filaments with different chain conformations - simple open chains, closed rings and branched structures with "X" and "Y" junctions - inspired by the recent findings on the low temperature self-assembly of dipolar hard spheres (Kantorovich et al, PCCP, 2015). The introduction of the polymer crosslinkers to stabilise the structure of such self-assembled nanoparticle aggregates is expected to have an important impact on the properties of the system. Here we focus on low-concentration solutions, analysing in detail their self-assembly behaviour. Extensive cluster analysis allows us to compare the structures formed by these filament solutions to those observed in "conventional" magnetic fluids containing non-crosslinked nanoparticles. These results will pave the way for the development of analytical models and identify the most interesting building block candidates for the design of novel magnetoresponsive materials.

DY 21.4 Tue 10:15 C 264

Magnetic microgels in computer simulations — •Elena Minina[1,2], Pedro Sanchez[1], Christos Likos[1], and Sofia Kantorovich[1,2] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russian Federation

In this work, we study magnetic microgels – spherical colloidal particles consisting of polymer network with embedded magnetic dipolar particles – by means of molecular dynamics computer simulations. Our main focus is concentrated on how the microgels change their shape and size depending on their internal structure and magnetic component. Microgels are initially modelled as bead-spring polymer chains randomly crosslinked into a polymer network. Changing degree of crosslinking allows us to vary microgel's internal structure. This way, we consider weekly crosslinked and highly crosslinked microgels. The fraction of magnetic particles is in the range between 0.5 to 10 per cent of the total fraction of particles comprising the polymer network. Studying such systems at different strength of dipole-dipole interactions, we estimate the change of magnetic microgel in size, self-assembly of magnetic particles and the initial magnetic susceptibility. We show that an appropriate combination of magnetic component and degree of crosslinking may offer an additional way to control.

DY 21.5 Tue 10:30 C 264

Influence of rotating magnetic field on magnetic fluids with different viscosities — •Anastasia Storozhenko[1], Ralf Stannarius[2], Alexey Eremin[2], Torsten Trittel[2], and Igor Aref'ev[3] — [1]Southwest State University, 305040 Kursk, Russia — [2]Otto von Guericke University Magdeburg, 39016 Magdeburg, Germany — [3]Ivanovo Power Engineering University, 153003, Ivanovo, Russia

In an external rotating magnetic field, the magnetization of magnetic nanoparticles follows the field direction with a certain phase lag, which results in a macroscopic torque. We investigated experimentally the dependence of the torque density on the strength and frequency of the magnetic field, as well as on the viscosity of magnetic fluid.

The torque density increases with the square of the field strength; this can be explained by well-known expressions. At the same time, the magnetization direction changes slower than the external magnetic field due to the relaxation of magnetic nanoparticles. The dependence of the torque on frequency is thus complex and depends on the viscosity of magnetic fluid. We find a growth of the torque with rotation rate of the field, followed by a decay at higher rates. The torque maximum shifts with changing viscosity. This phenomenon can be related to the balance of Neel and Debye relaxation times.

This study was funded by DFG within SPP 1681, Project STA 425/36 and a DAAD Stipendium.

DY 21.6 Tue 10:45 C 264

Microfludic-SANS: Rapid screening and flow processing of complex fluids — •Carlos Lopez[1], Takaichi Watanabe[2], Marco Adamo[3], Andreas Poulos[3], Anne Martel[4], Lionel Porcar[4], and Joao Cabral[3] — [1]RWTH Aachen University — [2]Okayama University — [3]Imperial College London — [4]Institut Laue Langevin

The coupling of microfluidics and small angle neutron scattering (SANS) is demonstrated. We have developed microfluidic devices with low SANS background and high pressure resistance for the investigation of flow-induced phenomena and high throughput phase mapping of soft matter.

We study the structure of model water-surfactant-oil mixtures under extensional flow and obtain scattering profiles from 50 micron wide channels, with 1 - 300 second acquisition times. The microfluidic geometry enables the variation of both flow type and magnitude, beyond traditional rheo-SANS setups, and is well-suited for complex fluids due to the commensurability of relevant time and lengthscales.

Using an online micromixer we implement a high-throughput approach, scanning in excess of 10 SANS profiles per minute for model surfactant and colloid solutions both in continuous and multiphase (droplet) flow. We show that microfluidic approaches can reduce experimental time and sample volume and considerably improve the accuracy of contrast matching experiments.

15 min. break

DY 21.7 Tue 11:15 C 264

Biaxial Phases in binary mixtures of liquid crystals — •Robert Skutnik, Louis Lehmann, Sergej Püschel-Schlotthauer, and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Sekr. C7, Straße des 17. Juni 135, Berlin 10623, Germany

Liquid crystals are organic molecules of anisotropic shape exhibiting anisotropic interactions. In fact, because of their delocalized π electron system, they exhibit π-π stacking and align parallel with their neighbors. Generally speaking, liquid crystal molecules can be classified as prolate or oblate molecules where the π-π electrons are parallel and perpendicular to the molecular symmetry axis. Hence, the interaction of an oblate and prolate liquid crystal results in a perpendicular alignment with respect to their symmetry axes. We perform Monte Carlo simulations and model both species (i. e., prolate and oblate) by an anisotropic potential based on the well-known 12-6 Lennard-Jones potential which promotes a parallel alignment if both particles are of the same species and perpendicular alignment otherwise. Besides the isotropic phase, we observe the formation of a nematic phase in the presence of a biaxial isotropic phase and the formation of a biaxial nematic phase despite the otherwise uniaxial symmetry of molecules of both species.

DY 21.8 Tue 11:30 C 264

Polar and nematic liquid crystals on curved surface — •Axel Voigt, Simon Praetorius, Michael Nestler, Ingo Nitschke, and Sebastian Reuther — TU Dresden, Institut für Wissenschaftliches Rechnen

We consider a thin film limit of a Frank-Oseen and a Landau-de Gennes model. In the limiting process we observe a continuous transition where the normal and tangential parts of the director and the Q-tensor decouple and various intrinsic and extrinsic contributions emerge. For the derived surface models, we consider an L^2-gradient flow. The

resulting vector- or tensor-valued surface partial differential equations are numerically solved to demonstrate realizations of the tight coupling of elastic and bulk free energy with geometric properties. We further discuss extensions towards surface Ericksen-Leslie and Beris-Edwards models and active liquid crystals on curved surfaces.

DY 22: Talk H. Hoffmann

Time: Tuesday 9:30–10:00 Location: BH-N 243

Invited Talk DY 22.1 Tue 9:30 BH-N 243

Complex Systems in Mechanical Engineering? A paradigm shift ahead. — •Norbert Hoffmann — Hamburg University of Technology, Germany

For a variety of reasons, mechanical engineering systems, like aircraft, space structures, vehicles, and the like, have always been said to be designed and operated at the limit of the feasible in terms of complexity. Traditionally complexity in this context has mostly been understood in terms of optimally exploiting physical processes and other variables of design spaces. The resulting machines typically consist of many thousands of interlinked and interacting components, which are often operating in highly sophisticated time-dependent manners. Still, the majority of design paradigms in mechanical engineering are largely dominated by the concepts of static equilibrium or simple periodicity. Since the early days of the industrial revolution this approach seems to have been very successful. The price was an over-design of machines to cope with a wide envelope of complex loading and response states. It is only rather recently that the wish for further optimisation, e.g. towards truly light-weight structures, a stronger and stronger individualisation of machines, and a growing amount of machine intelligence questions the traditional approach. First findings from research, as well as from business innovations pose the question if innovative future mechanical engineering systems will also be designed and operated on the basis of truly complex dynamics.

DY 23: Quantum Chaos

Time: Tuesday 10:00–12:15 Location: EB 107

DY 23.1 Tue 10:00 EB 107

Universal two-point correlations in many-body systems: the Random Wave Model in Fock space — •Juan-Diego Urbina and Klaus Richter — Institute for Theoretical Physics, University of Regensburg, Germany

Forty years after its discovery, Berry's Random Wave Model with its several modifications and variants is still the most powerful tool to understand the morphology of eigenfunctions in first-quantized chaotic (non-disordered) systems[1]. Surprisingly, the obvious question about how to construct a similarly powerful approach in the realm of interacting many-body quantum systems, with their natural description is Fock space, recieved little attention. Recently, however, this situation has dramatically changed due to the intimate connection between Berry's ansatz and the so-called eigenstate thermalization hypothesis.

While the first steps into the systematic study of the statistical distribution of Fock-space amplitudes in many-body eigenfunctions have been taken for the unexplored case of clean systems[3], a key element of a possible Random Wave Model in fock space is the universality of the two-point correlator. In this talk, we present the semiclassical theory that predicts such universal behavior and discuss its main features.

[1] See J. D. Urbina and K. Richter, Adv. Phys. (62) 363 (2013) for a recent review.
[2] M. Rigol, V. Dunjko, and M. Olshanii, Nature (452) 854 (2008).
[3] W. Beugeling, A. Baecker, R. Moessner, and M. Haque, arXiv:1710.11433 (2017).

DY 23.2 Tue 10:15 EB 107

Color mixing and beam shaping with chaotic light guides — •Julia Unterhinninghofen — Hochschule Koblenz, Konrad-Zuse-Str. 1, 56075 Koblenz

The dynamics of billiard systems has been used a model system for various applications. I.e., the ray dynamics of optical microcavities [1] for lasers and sensors can be understood as the classical nonlinear dynamics of an open billiard, while mode development and light output correspond to the dynamics of a quantum billiard. For many applications, shapes corresponding to chaotic or mixed billiards are desirable.

The ray dynamics of chaotic Bunimovich and Sinai billiards has also been used [2] to model the efficiency of color mixing in light guides with a cross-section corresponding to a chaotic billiard. Here, this approach is expanded to account for the openness (because of Fresnel losses) of such systems; we also investigate different smooth light guide cross-sections which can be easiliy fabricated. The results are applied to LED color mixing (corresponding to mixing in the spatial direction) as well as beam shaping (corresponding to mixing in the angular direction, i.e. in the far-field).

[1] J. U. Nöckel, A. D. Stone. Nature 385, 45 (1997)
[2] T. Bonenberger, J. Baumgart, S. Wendel, C. Neumann. Proc. SPIE 8641 (2013)

DY 23.3 Tue 10:30 EB 107

Semiclassical Description of Resonance-Assisted Tunneling in Deformed Optical Microdisks — •Felix Fritzsch[1,2], Arnd Bäcker[1,2], Roland Ketzmerick[1,2], and Normann Mertig[1,2,3] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden — [3]Department of Physics, Tokyo Metropolitan University, Tokyo

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 of the ray dynamics. We present a fully semiclassical description of resonance-assisted tunneling in deformed optical microdisks based on a generalization of the theory for quantum maps. This provides an intuitive ray-based picture of resonance-assisted tunneling and spoiling of Q-factors using only classical phase-space properties.

DY 23.4 Tue 10:45 EB 107

Ray-Wave correspondence in Optical and Graphene Billiards — •Guido Natura and Martina Hentschel — Technische Universität Ilmenau, Ilmenau

The development of optical resonators became essential for the improvements of optical devices such as filters, sensors or lasers. A promising application are microcavities, which allow the trapping of light by means of internal reflection. Here we are considering graphene Billiards where the resonator geometry is created by a step and a barrier on a graphene surface and allows the trapping of carriers inside [1,2]. These are assumed to behave as relativistic fermions in a finite domain as in the Neutrino *Berry-Mondragon-Billiards* [3]. The objective of this work is the invesitigation of whispering gallery modes in graphene Billiards and the study of a possible ray-wave-correspondence in the relativistic case.

[1] Katsnelson, M.I., Novoselov, K.S. and Geim, A.K., Chiral tunneling and the Klein paradox in graphene, *Nature Physics*, **2**, 620-625 (2006)
[2] Zhao et al., Creating and probing electron whispering-gallery modes in graphene, *Science*, **348**, 672-675 (2015)
[3] Berry, M.V. and Mondragon, R.J., Neutrino Billiards: Time-Reversal Symmetry-Breaking Without Magnetic Fields *Proc. Royal. Soc. A: Mathematical, Physical and Engineering Sciences*, **412**, 53-74 (1987)

15 min. break

DY 23.5 Tue 11:15 EB 107

3D billiards: visualization of regular structures and trapping of chaotic trajectories — •Markus Firmbach[1,2], Steffen Lange[1], Roland Ketzmerick[1,2], and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

Billiard systems, in which a point particle moves freely within some domain and undergoes elastic reflections at the boundary, play an important role in many area of physics, e.g. for optical microcavities. The phase-space of 2D billiards is easily displayed on a 2D Poincaré section. In contrast, 3D billiards lead to a 4D Poincaré map which is challenging to visualize. By means of the recently introduced 3D phase-space slices an intuitive representation of the organization of the mixed phase-space with regular and chaotic dynamics is obtained. Of particular interest for applications are constraints to classical transport between different regions of phase-space which can be detected by the statistics of Poincaré recurrence times. For a specific example of a 3D billiard we observe a slow power-law decay caused by long-trapped trajectories whose origin is analyzed in phase-space and frequency-space.

DY 23.6 Tue 11:30 EB 107

Microwave graphs: Transition from Symplectic to Orthogonal Symmetry — •Martin Richter[1], Aimaiti Rehemanjiang[2], Ulrich Kuhl[1], and Hans-Jürgen Stöckmann[2] — [1]Université Côte d'Azur, CNRS, Institut de Physique de Nice (InPhyNi), 06108 Nice, France — [2]Fachbereich Physik der Philipps-Universität Marburg, D-35032 Marburg, Germany

Recently an experimental realization of a system with a symplectic symmetry $\mathcal{T}$, $\mathcal{T}^2=-1$, was demonstrated [1], showing for the first time, e.g., typical level repulsion of s^4 in accordance with the Gaussian Symplectic Ensemble (GSE). It is based on a division of the whole graph into two Gaussian unitary subsystems (GUE) being the complex conjugate of each other. The coupling between these is realized by a set of microwave bonds connecting them to each other. Choosing the coupling appropriately one can realize anti-unitary symmetries of type $\mathcal{T}^2=-1$, $\mathcal{T}^2=1$, or no symmetry at all as well as a transition between them.

We will present how this transition behaves in the experimentally relevant case of a minimal number of bonds. In order to see the convergence to the corresponding Wigner predictions we accompany the experimental works with numerical random matrix simulations [2]. It allows to investigate the transition from GSE via GUE to the Gaussian Orthogonal Ensemble (GOE) by varying a phase difference between the coupling bonds.

[1] A. Rehemanjiang et. al., *Phys. Rev. Lett.* **117**, 064101 (2016)
[2] A. Rehemanjiang et. al., *arXiv*:1708.06236 [quant-ph]

DY 23.7 Tue 11:45 EB 107

Universal symmetry classes in three-terminal microwave graphs — Angel M. Martínez-Argüello[1], •Aimaiti Rehemanjiang[2], Moises Martínez-Mares[3], J. Antonio Méndez-Bermúdez[1], Hans-Jürgen Stöckmann[2], and Ulrich Kuhl[2,4] — [1]Instituto de Física, Benemérita Universidad Autónoma de Puebla, Puebla, Mexico — [2]Fachbereich Physik der Philipps-Universität Marburg, Marburg, Germany — [3]Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa, Mexico City, Mexico — [4]Université Côte d'Azur, CNRS, Institut de Physique de Nice, Nice, France

In direct analogy between electrical conduction and transport through scattering devices [1], measurements of a classical analog of a quantum observable through three-terminal microwave graphs are performed. One of the ports is placed as input and a second one as output, while a third port is used as a probe. Exact analytical predictions show good agreement with the measurements in the presence of orthogonal and unitary symmetries, provided that the absorption and coupling strength to the graphs are taken into account. In addition, the symplectic symmetry was implemented using a recent realization of graphs with such a symmetry [2]. Notably, neither the power losses nor the coupling strengths spoil the signatures of the symplectic symmetry. This represents the first classical-transport experiment that mimics a spin 1/2 system.

[1] M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).
[2] A. Rehemanjiang et al., Phys. Rev. Lett. **117**, 064101 (2016).

DY 23.8 Tue 12:00 EB 107

Bohmian trajectories for the half-line barrier — •Remy Dubertrand[1,2], Jeongbo Shim[2], and Ward Struyve[3] — [1]Institut für Theoretische Physik Universität Regensburg 93040 Regensburg, Germany — [2]Institut de Physique Nucleaire, Atomique et de Spectroscopie, CESAM, University of Liege, Bat. B15, B - 4000 Liege, Belgium — [3]Mathematisches Institut, Ludwig-Maximilians-Universität München, Theresienstr. 39, 80333 München, Germany

Bohmian trajectories are considered for a free particle that is scattered by a half-line barrier [1]. On the barrier, both Dirichlet and Neumann boundary conditions are considered. The half-line barrier yields one of the simplest cases of diffraction. Using the exact time-dependent propagator found by Schulman, the trajectories are computed numerically for different initial Gaussian wave packets. In particular, it is found that different boundary condition may lead to qualitatively different sets of trajectories. In the Dirichlet case, the particles tend to be more strongly repelled. The case of an incoming plane wave is also considered. The corresponding Bohmian trajectories are compared with the trajectories of an oil drop hopping on the surface of a vibrating bath.

[1] R. Dubertrand, J. Shim, W. Struyve, arxiv.1707.06173 (2017)

DY 24: Complex Systems

Time: Tuesday 10:00–11:00 Location: BH-N 128

DY 24.1 Tue 10:00 BH-N 128

Using quantum physics to simulate discrete-time, highly non-Markovian complex processes — •Felix Binder[1], Jayne Thompson[2], Chengran Yang[1], Varun Narasimhachar[1], and Mile Gu[1,2,3] — [1]School of Physical and Mathematical Sciences, Nanyang Technological University, 637371 Singapore, Singapore — [2]Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, 117543 Singapore, Singapore — [3]Complexity Institute, Nanyang Technological University, 639673, Singapore

Stochastic processes are as ubiquitous throughout the quantitative sciences as they are notorious for being difficult to simulate and predict. In this talk I present a unitary quantum simulator for discrete-time stochastic processes which requires less internal memory than any classical analogue throughout the simulation. The simulator's internal memory requirements equal those of the best previous quantum models. However, in contrast to previous models it only requires a (small) finite-dimensional Hilbert space. Moreover, since the simulator operates unitarily throughout, it avoids any unnecessary information loss. Interestingly, the formalism of matrix product states may be used to systematically derive the memory states and the unitary operator which define the simulator. This renders the results useful for direct experimental implementation with current platforms for quantum computation and I will present results obtained from simulation on IBM's Quantum Experience for a representative example process.

DY 24.2 Tue 10:15 BH-N 128

Analyzing the bifurcation behavior of complex systems via stochastic continuation - application to the Ising model — •Clemens Willers[1], Uwe Thiele[1], David Lloyd[2], Andrew Archer[3], and Oliver Kamps[1] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany — [2]Department of Mathematics, University of Surrey, Guildford, GU2 7XH, UK — [3]Department of Mathematical Sciences, Loughborough University, Loughborough LE11 3TU, UK

For many complex systems an analytical description of the macroscopic dynamics is not available, for instance, for systems that are described on the microscopic level by lattice- or agent-based models. These are frequently used in all natural sciences, social science, and economics. To analyse in this case the solution and bifurcation structure of the model on the level of macroscopic observables, one has to rely on equation free methods like stochastic continuation [1,2]. The question arising in this context is which kind of bifurcation diagrams can be extracted and how they relate to such diagrams of related mean-field

models if available. Our contribution briefly introduces the method of stochastic continuation. As an example, we then investigate the bifurcation diagram of the two-dimensional Ising model without and with external field both, with stochastic continuation and in the corresponding mean field model. This includes a discussion of the scaling of the extracted solutions and its relation to the known critical exponents.

[1] S.A. Thomas et. al., Physica A, 464 (2016) 27-53 [2] D. Barkley et. al., SIAM J. Appl. Dyn. Syst. 5 (2006) 403-434

DY 24.3 Tue 10:30 BH-N 128

Universal law for waiting internal time in seismicity and its implication to complex network of earthquakes — •Norikazu Suzuki — College of Science and Technology, Nihon University, Chiba, Japan

In the studies of seismicity, one can consider two different kinds of time: one is the conventional time, and the other is the internal time. Let {t_1, t_2, ..., t_N} be the conventional occurrence times of N earthquakes contained in the dataset to be analyzed. In this case, the internal time is simply the label "n" of t_n (n=1, 2, ..., N), which is henceforth referred to as the "event time". Carbone et al. (Europhys. Lett., 71 (2005) 1036) show that "unified scaling law" for conventional waiting times of earthquakes claimed by Bak et al. (Phys. Rev. Lett., 88 (2002) 178501) is actually not universal. We show that, in contrast to the conventional waiting time, the waiting "event time" obeys a power law. This implies the existence of temporal long-range correlations in terms of the event time with no sharp decay of the crossover type. The discovered power-law waiting event-time distribution turns out to be universal in the sense that it takes the same form for seismicities in California, Japan and Iran. In particular, the parameters contained in the distribution take the common values in all these geographical regions. An implication of this result to the procedure of constructing earthquake networks is discussed (S.Abe and N.Suzuki, Europhys. Lett.,65 (2004) 581; 97 (2012) 49002; 99 (2012) 39001; 110 (2015) 59001).

DY 24.4 Tue 10:45 BH-N 128

Stochastic Analysis of Snow Layers — •Pyei Phyo Lin[1], Joachim Peinke[1], Matthias Wächter[1], Isabel Peinke[2], and Pascal Hagenmuller[2] — [1]Inst Physik & ForWind Uni Oldenburg 26111 Oldenburg — [2]Météo-France - CNRS, CNRM UMR 3589, CEN, Grenoble, France

Data of high-resolution penetration tests are analyzed with stochastic methods. The measurements were performed with the snow micro penetrometer, measuring the snow resistance at micro-scale on small snow depths. We analyse this noisy data by stochastic methods. Therefore we determine drift an diffusion coefficients showing that the mean force increases with the depth. The solidity increases overall with the depth. Layer with different solidity can be detected. The noise analysis indicates that jump rise is involved, most likely due to breaking of ice bonds.

DY 25: Statistical Physics II (General)

Time: Tuesday 10:00–13:00 Location: BH-N 243

DY 25.1 Tue 10:00 BH-N 243

Analyzing tunneling time distributions on the basis of first passage time problems — •Jeanette Köppe[1], Michael Beyer[1], Markus Patzold[1], Wilfried Grecksch[2], and Wolfgang Paul[1] — [1]Institut für Physik, MLU Halle-Wittenberg — [2]Institut für Mathematik, MLU Halle-Wittenberg

In 1966, E. Nelson established a new interpretation of quantum mechanics, whereby the particles follow some conservative diffusion process, i.e. forward-backward stochastic differential equations (FBSDEs), which are equivalent to the Schrödinger equation. In analogy to classical mechanics, we show that finding the Nash equilibrium for a stochastic optimal control problem, which is the quantum equivalent to Hamilton's principle of least action, a set of quantum dynamical equations can be derived, which are the generalization of Hamilton's equations of motion to the quantum world.

On the basis of these quantum Hamilton equations, it was possible to study tunneling processes in a one-dimensional double-well potential by analyzing first passage times of the respective diffusion processes. We show that the energy splitting between the two lowest energy states $\Delta E = E_1 - E_0$ can be predicted based upon mean first passage times. Moreover, the probability density function of these first passage times is analyzed. The general form of this empircal determined distribution can be motivated by the definition of first passage times and it turns out that, independent of the considered system, tunnel times follow the same distribution qualitatively.

DY 25.2 Tue 10:15 BH-N 243

THE CONCEPT OF TEMPERATURE IN OPEN QUANTUM SYSTEMS: A MICRO-CANONICAL APPROACH — •Camilo Alfonso Moreno Jaimes and Juan Diego Urbina — Institute für Theoretische Physik, Universität Regensburg, Germany

We aim to investigate the concept of temperature in the Open Quantum System (system+reservoir) approach staring from a microcanonical bath scenario where the temperature is not a fundamental but a derived auxiliary concept. When the usual weak coupling regime is assumed, it is well known that the temperature emerges as an effective function of the energy from the saddle-point analysis that justifies the classic ensemble equivalence in the thermodynamic limit[1]. In the strong coupling regime, however, the energy is no longer an extensive quantity and we need a redefinition of temperature. We develop a microscopic analysis based on the Feynmann-Vernon approach to investigate the emergence and meaning of temperature in this strong coupling regime.

[1]: G. Horwitz. Commun. Math. Phys. 89, 11%129 (1983).

DY 25.3 Tue 10:30 BH-N 243

Efficient method of simulating with long-range interactions: The case of coarsening in the Ising model — •Henrik Christiansen, Suman Majumder, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

Simulations of systems with long range interactions are computationally more challenging than its short range counterpart, e.g., in the long range Ising model all spins have to be considered in the calculation of the local energy change. For several models, this problem has been overcome by the introduction of cluster algorithms for equilibrium simulations. As those cluster methods do not capture the dynamics, one cannot rely on them for simulating kinetics of phase transitions. Here, we present a novel and efficient approach of tackling such problems, concerning nonequilibrium dynamics via Monte Carlo simulations by storing a local "pseudo heatbath" for the energy calculation. As an illustration, we present results for coarsening of the long range Ising model in $d = 2$ dimensions. In contradiction to all available simulation results in this context (using an cut-off to make the simulation feasible), our results establish agreement with the theoretical predictions.

DY 25.4 Tue 10:45 BH-N 243

Derivation of an optimal time-dependent bias for Wang-Landau simulations — •Andreas Heuer and Myra Biedermann — Inst. f. Phys. Chemie, WWU Münster, Germany

Among the large variety of free-energy methods, the Wang-Landau approach plays an important role due to its broad applicability, e.g., in the fields of statistical physics. Empirically, it has been observed for simulations of, e.g., the Ising model, that the added bias f(t) should be chosen as M/t for long times, where M denotes the number of bins [1].

In this contribution we analyse a simple but non-trivial model system, suggested in [2], for which the impact of a time-dependent bias can be treated analytically. Key results are: (1) a minimal error requires the choice f(t) = M/t. (2) There exists a short-time regime where the optimum bias decreases exponentially with time. (3) Surprisingly, the estimation of individual free energies is systematically biased, with the bias scaling as log(t) / t.

These results are quantitatively reproduced in simulations of the Ising model and may serve as a justification for a frequently employed application scheme for Wang-Landau simulations, the 1/t algorithm [1].

[1] R.E. Belardinelli and V.D. Pereyra, Phys. Rev. E 75, 046701 (2007). [2] R.E. Belardinelli, V.D. Pereyra, R. Dickman, B. J.

Lourenco, J. Stat. Mech., P07007 (2014).

DY 25.5 Tue 11:00 BH-N 243

Interplay of fast and slow degrees of freedom in the disk to slab transition — •Andreas Tröster[1], Clemens Moritz[2], and Christoph Dellago[2] — [1]Institute of Materials Chemistry, TU Wien, Getreidemarkt 9, 1060 Wien, Austria — [2]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria

Rare transitions between long-lived stable states are often analyzed in terms of free energy landscapes computed as functions of a few collective variables. Here, using transitions between geometric phases as example, we demonstrate that the effective dynamics of a system along these variables are an essential ingredient in the description of rare events and that the static perspective provided by the free energy alone may be misleading. In particular, we investigate the disk-to-slab transition in the two-dimensional Ising model starting with a calculation of a two-dimensional free energy landscape and the distribution of committor probabilities. While at first sight it appears that the committor is incompatible with the free energy, they can be reconciled with each other using a two-dimensional Smoluchowski equation that combines the free energy landscape with state dependent diffusion coefficients. These results illustrate that dynamical information is not only required to calculate rate constants, but may also be necessary to understand how a given process occurs.

15 min. break

DY 25.6 Tue 11:30 BH-N 243

Irreversible Markov chains in spin models: Topological excitations — •Ze Lei[1] and Werner Krauth[1,2] — [1]Ecole Normale Superieure, Paris, France — [2]The University of Tokyo, Tokyo, Japan

We analyze the convergence of the irreversible event-chain Monte Carlo algorithm for continuous spin models in the presence of topological excitations.

In the two-dimensional XY model, we show that the local nature of the Markov-chain dynamics leads to slow decay of vortex–antivortex correlations in comparision with the fast decorrelation of spin waves.

We propose an assignment algorithm for pairing vortices and antivortices, and show that the maximum vortex–antivortex distance follows a Fréchet description. The contributions of topological excitations to the equilibrium correlations vary from a dynamical critical exponent $z \sim 2$ at the critical temperature to $z \sim 0$ in the limit of zero temperature.

In the harmonic approximation of spin waves for dimensions higher than 2, we confirm the event-chain algorithm's fast relaxation (corresponding to $z = 0$). Its mixing times however remain much larger than equilibrium correlation times at low temperatures.

We also describe the respective influence of topological monopole–antimonopole excitations and of spin waves on the event-chain dynamics in the three-dimensional Heisenberg model.

We expect that the fast relaxation of phonon modes explains the success of the event-chain algorithm at high densities for particle systems.

DY 25.7 Tue 11:45 BH-N 243

Lee-Yang zeros and large-deviation statistics of a molecular zipper — •Aydin Deger, Kay Brandner, and Christian Flindt — Department of Applied Physics, Aalto University, 00076 Aalto, Finland

The complex zeros of partition functions were originally investigated by Lee and Yang to explain the behavior of condensing gases. Since then, Lee-Yang zeros have become a powerful tool to describe phase transitions in interacting systems. Today, Lee-Yang zeros are no longer just a theoretical concept; they have been determined in recent experiments. In one approach, the Lee-Yang zeros are extracted from the high cumulants of thermodynamic observables at finite size [1]. Here, we employ this method to investigate a phase transition in a molecular zipper [2]. From the energy fluctuations in small zippers, we can predict the temperature at which a phase transition occurs in the thermodynamic limit. Even when the system does not undergo a sharp transition, the Lee-Yang zeros carry important information about the large-deviation statistics and its symmetry properties. Our work suggests an interesting duality between fluctuations in small systems and their phase behavior in the thermodynamic limit. These predictions may be tested in future experiments.

[1] K. Brandner, V. F. Maisi, J. P. Pekola, J. P. Garrahan, and C. Flindt, Phys. Rev. Lett. **118**, 180601 (2017)
[2] A. Deger, K. Brandner and C. Flindt, arXiv: 1710.01531 (2017)

DY 25.8 Tue 12:00 BH-N 243

Geometric frustration in non-periodic mechanical metamaterials — •Erdal C. Oğuz[1], Anne Meeussen[2,3], Martin van Hecke[2,3], and Yair Shokef[1] — [1]School of Mechanical Engineering and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel — [2]Huygens-Kamerlingh Onnes Laboratory, Universiteit Leiden, PO Box 9504, 2300 RA Leiden, the Netherlands — [3]AMOLF, Science Park 104, 1098 XG Amsterdam, the Netherlands

We investigate geometric frustration in two-dimensional lattice-based mechanical metamaterials comprised of anisotropic triangular building blocks T, where each such T possesses a nontrivial floppy mode of deformation. When each triangle is oriented randomly neighboring triangles typically cannot deform self-consistently. On the one hand, we analyze the conditions under which a non-periodic packing of these blocks form compatible and frustration-free large-scale structures, i.e., structures that exhibit a global floppy mode that is compatible with the local deformations of each T. By mapping to an antiferromagnetic Ising model, we find an extensive number of possibilities to construct a compatible structure: ($\Omega_0 \sim \exp(T)$). On the other hand, we study incompatible metamaterials in detail and we reveal two distinct types of source of frustration (defects) which either highly localize the frustrated region to a small and finite domain (local defects) or cause delocalized and long-ranged multi-stable conflicts (topological defects) whose multi-stability scales as $\Omega \sim \exp(\sqrt{T})$.

DY 25.9 Tue 12:15 BH-N 243

Explanation of Cosmic Inflation by Phase Transitions — •Hans-Otto Carmesin[1,2,3] and Matthias Carmesin[4] — [1]Universität Bremen, Fachb. 1, Pf. 330440, 28334 Bremen — [2]Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — [3]Gymnasium Athenaeum, Harsefelder Str. 40, 21680 Stade — [4]Universität Göttingen, Fak. f. Physik, 37077 Göttingen

From the Cosmic Microwave Background CMB the flatness problem and the horizon problem arose. An extraordinarily rapid increase of distances in the early universe, the Cosmic Inflation, was proposed as a possible solution (Guth, Phys. Rev. D, 1981), whereby suggested mechanisms for such an increase have been criticized (Steinhardt: Scientific American, 2011). We propose a theory that explains the Cosmic Inflation by a sequence of symmetry breaking phase transitions at critical densities (Carmesin, H.-O.: Vom Big Bang bis heute mit Gravitation - Model for the Dynamics of Space. Berlin: Verlag Dr. Köster, 2017.). Our theory applies first principles only, namely gravitation and quantum physics, contains no fit parameter, applies fundamental constants only, namely the constant of gravitation G, the velocity of light c and the Planck constant h, is in excellent quantitative agreement with observations, namely the critical density, the duration of cosmic inflation, the temperature fluctuations as well as the factor of increase correspond to the CMB and the flatness and horizon problems are solved.

DY 25.10 Tue 12:30 BH-N 243

Clock Monte Carlo: General methods for $O(1)$ complexity — •Manon Michel[1], Xiaojun Tan[2], and Youjin Deng[2] — [1]Centre de Mathématiques Appliquées, UMR 7641, Ecole Polytechnique, France. — [2]Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

Despite a now long history, the most successful and influential Markov-chain Monte Carlo (MCMC) algorithm remains the founding Metropolis algorithm. Sampling the rejection or acceptance of a proposed move requires however estimating the induced global energy change. It can lead to heavy computational overhead when simulating systems with long-range interactions or a large number of coupling terms – e.g. gravitational force, Coulomb force between electric charges, van-der-Waals force, dipole-dipole interaction etc.

Several techniques reduce the complexity but only for specific algorithms and systems. We will present a general technique for constant-time sampling: the "clock" method. We shall explain how this method draws on the factorized Metropolis filter to sample the successive steps of the chain and exhibit its performance for different long-range $O(n)-$spin systems. Besides being simple and powerful, the clock technique is general for a large class of MCMC methods and physical systems, as it relies only on the extensivity of the energy.

DY 25.11 Tue 12:45 BH-N 243

Excited States in Nelson's Stochastic Mechanics — •Markus Patzold[1], Jeanette Köppe[1], Michael Beyer[1], Wilfried Grecksch[2], and Wolfgang Paul[1] — [1]Martin Luther Universität Halle-Wittenberg, Institut für Physik — [2]Martin Luther Universität Halle-Wittenberg, Institut für Mathematik

In 1966 Edward Nelson successfully derived the Schrödinger equation for non-relativistic spinless particles in the ground state using stochastic differential equations (FBSDE). Solutions of the Schrödinger equation can be used to generate particle paths in this context. Pavon generalized his ideas 1995 to the quantum Hamilton principle, similar to the classical one, introducing a stochastic variational principle. Furthermore, a stochastic optimal control approach is equivalent to the above mentioned one and can be solved without the Schrödinger equation as it was shown by Köppe, et al. in 2017.

However, these equations lead to the ground state of the system only. In the talk I will show how to bypass this problem, adapting the stochastic equations, by exploiting the concept of supersymmetry (SUSY) to give iterative equations for all excited states in arbitary dimensions. Numerical calculations for the double well and hydrogen problem as well as analytical calculations for the harmonic oscillator in d dimensions and the radial hydrogen part including a symmetry analysis will be discussed.

DY 26: Condensed Matter Simulations augmented by Advanced Statistical Methodologies I (joint session DY/CPP)

Time: Tuesday 11:00–12:30 Location: BH-N 334

DY 26.1 Tue 11:00 BH-N 334

Markov State Modeling of Sliding Friction — •Martina Teruzzi — SISSA (International School for Advanced Studies), Trieste

Friction, despite being a well-known and studied phenomenon, still lacks a general theory or approach, mainly due to the presence of many degrees of freedom and the difficulty in identifying few relevant collective variables. We propose a method based on Markov State Modeling, a technique aimed at reducing the dimensionality of the system, by singling out the relevant slow timescales and the observables that best describe them. After successful application to a small toy model (1D Frenkel-Kontorova) we now apply this approach to more complicated systems, identifying few significant states that best characterize them through a rather general and automatic algorithm. This approach can provide insight into the main mechanisms of new frictional systems and, in perspective, could be enhanced by biased sampling to achieve a proper description of rare events, difficult to be sampled by standard dynamics.

DY 26.2 Tue 11:15 BH-N 334

Loss of Memory in Dense Sheared Particulate Systems — •Lou Kondic[1], Lenka Kovalcinova[1], Miro Kramar[2], and Konstantin Mischaikow[3] — [1]NJIT, Newark, NJ, USA — [2]INRIA Saclay, Paris, France — [3]Rutgers, Piscataway, NJ, USA

We carry out discrete element/MD simulations of dense sheared particulate systems, with the focus on understanding and characterizing dynamical properties of force networks that develop on the mesoscale. These force networks are known to play a crucial role in connecting microscale dynamics of the particles and macroscopic properties of the whole system. The results of the simulations are analysed using topological tools, that allow to fully quantify and even compare the states of the system. These tools identify in an objective and precise manner the time interval needed for the system to loose its memory, or in other words, the time interval after which any information about system state is lost. We will show that the process of memory loss may differ even if the inertial number, measuring the ratio of inertial to imposed forces, is kept constant.

This work is supported by the NSF Grant No. DMS-151717 by the DARPA contract No. HR0011- 16-2-0033.

DY 26.3 Tue 11:30 BH-N 334

Adaptive population Monte Carlo simulations — •Martin Weigel[1], Lev Yu. Barash[2,3], Lev N. Shchur[2,3,4], and Wolfhard Janke[5] — [1]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England — [2]Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia — [3]Science Center in Chenogolovka,142432 Chernogolovka, Russia — [4]National Research University Higher School of Economics, 101000 Moscow, Russia — [5]Institut für Theoretische Physik, Universität Leipzig, Postfach 100920 04009, Leipzig, Germany

Population annealing is a sequential Monte Carlo scheme that is potentially able to make use of highly parallel computational resources. Additionally, it promises to allow for the accelerated simulation of systems with complex free-energy landscapes, much alike to the much more well known replica-exchange or parallel tempering approach. We equip this method with self-adaptive schemes for choosing the algorithmic parameters, including the temperature and sweep protocols as well as the population size. The resulting method is significantly more efficient for simulations of systems with complex free-energy landscapes than some more traditional approaches, and it is particularly well suited for massively parallel computing environments such as (clusters of) GPUs.

DY 26.4 Tue 11:45 BH-N 334

Diagnostics of neural networks for machine learning phases and phase transitions — •Philippe L. Suchsland and Stefan Wessel — RWTH Aachen University, Aachen, Germany

Machine learning schemes based on neural networks have recently been proposed as new tools for classifying phases of matter as well as detecting phase transitions. One motivation behind such proposals is the ability of appropriately designed and trained neural networks to identify patterns from a large set of data without having to explicitly describe them. We apply both supervised and unsupervised machine learning schemes to basic models of statistical physics. In particular, we consider the 2D Ising model in the presence of extended domain-wall configurations as well as the 2D XY model that exhibits a Kosterlitz-Thouless transition. In both cases, we identify the physical properties of the models that are relevant for the classification task. This reveals how reliable these schemes are with respect to minimizing the amount of preprocessing of bare sample configurations before feeding them into the learning process.

DY 26.5 Tue 12:00 BH-N 334

Hyperdynamics approach to the non-equilibrium states coupled to the thermal bath — •Yuri S. Nagornov and Ryosuke Akashi — University of Tokyo, Department of Physics, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

Efficient numerical simulation method for rare events driven by thermal fluctuation has long been a hot topic in a wide range of fields in condensed-matter physics. The target phenomena in this context, such as crystal nucleation, atomic diffusion etc., occur in time scales of microseconds or even longer and are intractable by atomistic molecular dynamics simulation. Solutions to this problem have long been attempted by introducing collective variables to seek for escape paths and/or efficiently sampling the phase space to represent the canonical ensemble. However, an ideal approach is rather desired (i) not to respect the prior knowledge of appropriate collective variables and (ii) not to require the system to reach the thermal equilibrium since many of the above mentioned phenomena can occur under non-equilibrium situations. Along the line of the Langer*s theory, we formulate a differential equation for the distribution of the variables that evolve on an elevated potential surface under thermal fluctuation, from which its real probability of realization can be retrieved. This formalism enables us non-empirical exploration of rare events and evaluation of its probability to occur simultaneously. An algorithm with a modified form of the Langevin molecular dynamics is thereby constructed, which is in spirit an extension of the hyperdynamics approach. Applications to simple model systems will be presented.

DY 26.6 Tue 12:15 BH-N 334

Hyperdynamics approach to the non-equilibrium states coupled to the thermal bath — •Yuri S. Nagornov and Ryosuke Akashi — University of Tokyo, Department of Physics, 7-3-1 Hongo,

Bunkyo-ku, Tokyo 113-0033, Japan

Efficient numerical simulation method for rare events driven by thermal fluctuation has long been a hot topic in a wide range of fields in condensed-matter physics. The target phenomena in this context, such as crystal nucleation, atomic diffusion etc., occur in time scales of microseconds or even longer and are intractable by atomistic molecular dynamics simulation. Solutions to this problem have long been attempted by introducing collective variables to seek for escape paths and/or efficiently sampling the phase space to represent the canonical ensemble. However, an ideal approach is rather desired (i) not to respect the prior knowledge of appropriate collective variables and (ii) not to require the system to reach the thermal equilibrium since many of the above mentioned phenomena can occur under non-equilibrium situations. Along the line of the Langer's theory, we formulate a differential equation for the distribution of the variables that evolve on an elevated potential surface under thermal fluctuation, from which its real probability of realization can be retrieved. This formalism enables us non-empirical exploration of rare events and evaluation of its probability to occur simultaneously. An algorithm with a modified form of the Langevin molecular dynamics is thereby constructed, which is in spirit an extension of the hyperdynamics approach. Applications to simple model systems will be presented.

DY 27: Microfluidics

Time: Tuesday 11:15–12:45 Location: BH-N 128

DY 27.1 Tue 11:15 BH-N 128

Antimargination of microparticles and platelets in branching vessels — •Christian Bächer[1], Lukas Schrack[1,2], and Stephan Gekle[1] — [1]Biofluid Simulation and Modeling, Bayreuth, Germany — [2]Bio and Nano Physics, Innsbruck, Austria

A mixed suspension of red blood cells and microparticles flows through complex geometries typical for in vivo vessel networks: a vessel confluence and a bifurcation. Our three-dimensional Lattice-Boltzmann simulations show strong effects on cell and particle distribution: behind a confluence we observe an additional, surprisingly stable cell-free layer in the center containing microparticles undergoing anti-margination. In contrast to the perturbed margination in vessel confluence, we obtain full microparticle margination in branching vessels. Margination in branching vessels and antimargination behind confluences may explain in vivo findings of strongly different platelet distribution in arterioles (mainly bifurcations) and venules (mainly confluences).

DY 27.2 Tue 11:30 BH-N 128

Molecular dynamics simulations in hybrid particle-continuum schemes: Pitfalls and caveats — •Stefanie Stalter[1], Leonid Yelash[2], Nehzat Emamy[3], Maria Lukáčová-Medvid'ová[2], and Peter Virnau[1] — [1]Institute of Physics, Johannes Gutenberg University, Staudingerweg 9, 55128 Mainz, Germany — [2]Institute of Mathematics, Johannes Gutenberg University, Staudingerweg 9, 55128 Mainz, Germany — [3]Institute for Parallel and Distributed Systems, University of Stuttgart, Universitätsstraße 38, Stuttgart, Germany

Heterogeneous multiscale methods (HMM) combine molecular accuracy of particle-based simulations with the computational efficiency of continuum descriptions to model flow in soft matter liquids. In these schemes, molecular simulations typically pose a computational bottleneck. We found that it is preferable to simulate many small systems as opposed to a few large systems, and that a choice of a simple isokinetic thermostat is typically sufficient while thermostats such as Lowe-Andersen allow for simulations at elevated viscosity. We present suitable choices for time steps and finite-size effects which arise in the limit of very small simulation boxes. [1]

[1] S.Stalter et al., doi:10.1016/j.cpc.2017.10.016, CPC (2017)

DY 27.3 Tue 11:45 BH-N 128

Particle interactions in inertial microfluidics — •Christian Schaaf, Felix Rühle, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Solid particles immersed in a microfluidic Poiseuille flow at intermediate Reynolds numbers migrate laterally to discrete equilibrium positions [1]. This Segré-Silberberg effect can be explained by the inhomogeneous shear rate of the Poiseuille flow and can be rationalized by the lift force profile. In addition to this lateral inertial focusing, particles at low densities also form regular particle trains in the direction of the flow [2].

We conduct lattice-Boltzmann simulations to obtain some understanding for the formation of such structures. As a first step we focus on the dynamics of a flowing particle pair. We determine their lift force profiles as function of the lateral particle positions and axial distance as well as the Reynolds number. At small distances the profiles are dominated by viscous forces, while at large distances inertial forces take over. Additionally, we categorize the different types of trajectories and show how particles in the bound state spiral towards their equilibrium positions performing damped oscillations. In the end these results are used to explain the behavior of particle trains and to analyze their dynamics and stability.

[1] G. Segré and A. Silberberg, *Nature* **189**, 209 (1961).
[2] W. Lee, et al., *PNAS* **107**, 22413 (2010).
[3] C. Schaaf and H. Stark, submitted.

DY 27.4 Tue 12:00 BH-N 128

Mesoscopic simulations of dense suspensions of capsules in confined shear flow — •Othmane Aouane[1], Maarten Wouters[2], Andrea Scagliarini[3], and Jens Harting[1,2] — [1]Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Nürnberg, Germany — [2]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands — [3]Istituto per le Applicazioni del Calcolo, Rome, Italy

Complex fluids are ubiquitous in soft matter systems, such as colloidal suspensions and biofluids (tissues and blood). Understanding the dynamics of such systems is important for example for industrial production or disease detection. However, such systems are hard to solve analytically since they follow non-linear dynamics and might involve many-body interactions and multiscale problems. These circumstances call for numerical methods and computer simulations which can also provide access to observables not traceable in experiments such as the local fluid properties. In this work, we focus on computational simulations of dense suspensions of soft polymeric coated core-shells, i.e. capsules up to to 75% volume fraction under a confined shear flow using the lattice Boltzmann method with an emphasis on their local rheology. This study includes the effect of the mechanical properties of the individual capsules (stiffness/softness) on the flow behavior.

DY 27.5 Tue 12:15 BH-N 128

Inertial elevation of deformable particles in a shaken fluid — •Matthias Laumann[1], Andre Förtsch[1], Eva Kanso[2], and Walter Zimmermann[1] — [1]Theoretische Physik I, Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Aerospace and Mechanical Eng., University of Southern California, Los Angeles, California 90089, USA

Biological and bioinspired swimmers can move by shape actuation. Great progress has been made in understanding the direct control of shape variables for locomotory purposes. However, actuation via a time-dependent fluid motion is less well explored. Here, we examine the nonlinear coupling between shape variables and locomotion in a model system in oscillating flow including body inertia. As model we use a bead-spring tetrahedron. We determine effective conditions that lead to a non vanishing velocity in the oscillating external flow. Furthermore we give a simple explanation of the effect. These results suggest that one can tune the background flow properties to control the swimmer motion, and thus, they may have profound implications on design and employment of man-made swimmers in oscillatory flows.

DY 27.6 Tue 12:30 BH-N 128

Passive swimming of soft particles in oscillatory Poiseuille flow — •Winfried Schmidt[1], Matthias Laumann[1], Eva Kanso[2], and Walter Zimmermann[1] — [1]Theoretische Physik 1, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, California, USA

What is the dynamical behavior of soft particles in oscillatory (pul-

sating) Poiseuille flow at low Reynolds number? By investigating the overdamped motion of bead-spring models for a triangle, 2D ring polymers or 3D capsules, we predict particle actuation in the case of vanishing mean flow. This effect is generic as it does not depend on the model. Asymmetric, Janus like particles propagate in a symmetric flow. Symmetric particles swim for non-symmetric flow oscillations (non equal half periods). The mean actuation (swim) velocity of a particle is caused by its varying shape in both half periods. Since the actuation steps depend also on the size and the elasticity of soft particles, this novel actuation (passive swimming) mechanism is also appropriate for particle sorting.

DY 28: Evolutionary Game Theory (joint SOE/BP/DY) (joint session SOE/DY/BP)

Time: Tuesday 12:30–13:15 Location: MA 001

DY 28.1 Tue 12:30 MA 001

Equality-efficiency tradeoff in a dynamical Voluntary Contribution Game with Assortative Matching and heterogeneous agents. — •Stefano Duca — ETH Zurich, Zurich, Switzerland

Many scholars in the socio-economical literature have noted that any system that allows and incentivizes the transfer of wealth between agents exhibits a trade-off between efficiency and equality. Using an agent based model we study the welfare properties over time of Assortative Matching in Voluntary Contribution Games (VCM).

Every round, individuals choose how much to contribute into a group account and are ranked according to it. Based on this ranking, participants are then matched in equal-size groups; members of each group share their group output equally according to a VCM payoff function. Wealth accumulates over time and agents differ in talent and starting wealth.

In this paper, we study several ranking mechanisms based on different dimensions and ask what are the properties of these mechanisms in terms of total production of wealth and its distribution.

We find that, while in general it is impossible to determine a single best ranking system, some perform objectively better than others.

Using a computational approach we determine the mechanism that maximizes the social welfare, chosen from the Pareto frontier, depending on the preferences of a social planner.

DY 28.2 Tue 12:45 MA 001

Exiting the Primordial Soup – Transition from Pre-Darwinian to Darwinian Evolution — Charlotte V. Vogelbusch[1], Steven H Strogatz[2], •Hinrich Arnoldt[1], and Marc Timme[1] — [1]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden, Dresden, Germany — [2]Department of Mathematics, Cornell University, Ithaca, NY 14853, USA

Darwin proposed the now-accepted existence of a last universal common ancestor (LUCA) from which all species emerged in an evolutionary process. Life on earth just before LUCA was fundamentally collective - a primordial soup - as ancient life forms shared their genetic material freely through massive horizontal gene transfer (HGT). How to exit this collective state and start Darwinian evolution is far from understood and heavily debated. Here we present a minimal model for this hypothesized "Darwinian transition." The model suggests that HGT-dominated dynamics may have been intermittently interrupted by selection-driven processes during which genotypes became fitter and decreased their inclination toward HGT. Stochastic switching in the population dynamics may have destabilized the HGT-dominated collective state and led to the emergence of vertical descent, the first well-defined species, and thus started Darwinian evolution [1]. Moreover, advanced models with dynamic inclination to HGT competence suggest a viable route from collective pre-Darwinian to vertical Darwinian evolution and hint to a constrained exit window in parameter space. Ref.: [1] Phys. Rev. E 92, 052909 (2015)

DY 28.3 Tue 13:00 MA 001

Analytical approximation of temporal difference multi-agent reinforcement learning — •Wolfram Barfuss[1,2], Jonathan F. Donges[1,3], and Jürgen Kurths[1,2,4] — [1]Potsdam Institute for Climate Impact Research, GER — [2]Humboldt University, Berlin, GER — [3]Stockholm Resilience Centre, Stockholm University, SWE — [4]University of Aberdeen, UK

Reinforcement learning in multi-agent systems has been studied by the fields of economic game theory, artificial intelligence and physics. Especially an economic and physics perspective has lead to analytical approaches of learning dynamics in multi-agent systems. However, these studies put their focus on simple iterated normal form games, such as the iterated Prisoners Dilemma. Environmental dynamics, i.e. changes in the state of the agent's environment affecting the payoffs received by the agents are mostly lacking. In this work we combine the analytical approach from physics with temporal difference learning from the field of artificial intelligence. This form of learning explicitly uses the discounted value of future environmental states to adapt the agent's behavior. We develop a uniform notation for multi-agent environment systems, generalizable to any environment and an arbitrary number of agents. We find four reinforcement learning variants emerging and compare their dynamics. This work is important to advance the understanding of interlinked social and environmental dilemmas, such as climate change, pollution and biosphere degradation.

DY 29: Particulate Matter: From microscopic interactions to collective motion (joint session DY/CPP)

Time: Tuesday 14:00–15:45 Location: EB 107

DY 29.1 Tue 14:00 EB 107

Onset of anomalous diffusion in colloids confined to quasi-monolayers — •Martin Oettel[1], Johannes Bleibel[1], and Alvaro Dominguez[2] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]Fisica Teorica, Universidad de Sevilla

It has been recently shown that a colloidal monolayer, e.g., formed at a fluid interface or by means of a suitable confining potential, exhibits anomalous collective diffusion: diffusion becomes accelerated as signalled by a $1/k$–divergence of the wavenumber–dependent collective diffusion coefficient. This is a consequence of the hydrodynamic interactions mediated by the three-dimensional (3D) ambient fluid when the particles are confined to reside on a two-dimensional (2D) manifold. We study theoretically and with numerical simulations the crossover from normal to anomalous diffusion as the particles are, in real systems, confined by a 3D external potential and thus have the possibility to fluctuate out of the 2D manifold, thus forming a quasimonolayer. In essence, we always find anomalous diffusion on lateral length scales larger than the confinement width.

DY 29.2 Tue 14:15 EB 107

Microrheology in hard colloids with large tracers — •Antonio M. Puertas[1], Francisco Orts[2], Gloria Ortega[2], and Ester M. Garzon[2] — [1]Dpt. of Applied Physics, Univ. of Almeria, Almeria, Spain — [2]Dept. of Informatics, Univ. of Almeria, Agrifood Campus of Int. Excell., ceiA3, Almeria, Spain

Microrheology has become recently in a powerful technique to study the dynamics of a system in microscopic scales. A colloidal tracer is introduced in the host system, and its dynamics is monitored. When an external force acts on the tracer, the system goes out of equilibrium probing the linear regime for small forces, and entering the non-linear regime for large ones. A colloidal bath of hard spheres is probably the simplest example. Several theory models have been developed, tested by simulations, but typically these restrict to tracers of the same size as the bath particles.

Here, we present simulation results of the dynamics of a tracer pulled with a constant force in a colloidal bath. The tracer size, a_t, is larger than the bath particles, size a, up to $a_t = 5a$. Important finite size effects appear, particularly for large tracers, which have been studied and compared with predictions from hydrodynamics for the bath. Due to the massive computational demand, the simulations were computed on a multiGPU cluster and a genetic algorithm was designed to optimize the performance. The dynamics of the tracer, providing the friction coefficient with the bath and the effects of the bath (density fluctuations, and strain field) are studied for small forces. The theoretical limit of an infinite tracer, $a/a_t \to 0$, and small forces, is checked.

DY 29.3 Tue 14:30 EB 107

Efficient simulation of anisotropic particles using collective Monte Carlo moves — •Marco Klement and Michael Engel — Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Hard anisotropic particles are a classical model for the influence of shape on the thermodynamic behaviour of particulate matter. Examples are the phase diagram of liquid crystal formers and the prediction of crystal structures for polyhedral nanocrystals [1]. Here, we investigate the speed-up of hard polyhedra Monte Carlo simulations by using collective chain moves [2]. Our implementation relies on analytically detecting sweep collisions with an improved version of the Minkowski portal refinement algorithm. We validate our method by calculating equations of state and studying self-assembly phenomena.

[1] M.A. Boles, M. Engel, D.V. Talapin, Chem. Rev. 116, 11220-11289 (2016).

[2] E.P. Bernard, W. Krauth, D.B. Wilson, Phys. Rev. E 80, 056704 (2009).

DY 29.4 Tue 14:45 EB 107

Stochastic Nature of Granular Tribocharging — •Jan Haeberle[1], André Schella[2], Matthias Schröter[2], Matthias Sperl[1], and Philip Born[1] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Köln, Deutschland — [2]MPI Dynamics and Self-Organization, Göttingen, Germany

Triboelectric charging of granular media has important consequences for the bulk behaviour. Effects such as powder flowability or cluster formation due to charging are everyday experiences [1]. Triboelectric charging has also been linked to segregation [2] and suggested as a tool for structure formation in granular media [2,3]. Recently, the stochastic nature of the triboelectric charging process has become apparent [4]. To further investigate the stochastics of tribocharging, we have studied the distribution resulting after a tribocharging event in a custom-made Faraday cup setup. We measure non-Gaussian asymmetric charge distributions. We find, that we can describe the measured distributions by a model combining a distinct stochastic charging and stochastic discharging process.

[1] Duran, J., Sands, Powders, and Grains, Springer, New York (2000) [2] Schella, A., Herminghaus, S. & Schröter, M., Soft Matter 13, 394-401 (2017). [3] Cademartiri, R. et al., Soft Matter 8, 9771 (2012). [4] Apodaca, M. M., Wesson, P. J., Bishop, K. J. M., Ratner, M. A. & Grzybowski, B. A., Angewandte Chemie 122, 958-961 (2010).

DY 29.5 Tue 15:00 EB 107

Universal hidden order in amorphous cellular geometries — •Michael A. Klatt[1], Jakov Lovrić[2,3], Duyu Chen[4], Sebastian C. Kapfer[5], Fabian M. Schaller[5,1], Philipp W. A. Schönhöfer[3,5], Bruce S. Gardiner[3], Ana-Sunčana Smith[2,5], Salvatore Torquato[4,6], and Gerd E. Schröder-Turk[3,5] — [1]KIT, Institute of Stochastics, 76049 Karlsruhe, Germany — [2]Division of Physical Chemistry, Ruder Bošković Institute, Zagreb, Croatia — [3]Murdoch University, School of Engineering and Information Technology, 90 South St, Murdoch WA 6150, Australia — [4]Department of Chemistry, Princeton University, New Jersey 08544, USA — [5]Institute for Theoretical Physics, FAU, 91058 Erlangen, Germany — [6]Department of Physics, PRISM, PACM, Princeton University, New Jersey 08544, USA

Starting from an amorphous partitioning of space into cells, we iteratively optimize the "centrality" of the cells, minimizing the so-called Quantizer energy. The energy landscape is replete with local minima to which the system converges despite the existence of lower-energy crystalline configurations. Irrespective of the level and type of disorder in the initial configurations, the tessellations converge to the same amorphous state, as measured by the same structure factor and energy distributions. The final disordered configurations exhibit an anomalous suppression of long-wavelength density fluctuations, known as hyperuniformity. For systems related to the Quantizer problem, such as self-assembled copolymeric phases, our findings suggest the possibility of stable disordered hyperuniform phases.

DY 29.6 Tue 15:15 EB 107

Relaxation of hydrogen bond network in water subject to E-field — •Andreas Baer[1], Zoran Milicevic[1,2], David Matthew Smith[2,3], and Ana-Suncana Smith[1,2] — [1]PULS Group at the Institute for Theoretical Physics and EAM, FAU Erlangen-Nürnberg, Germany — [2]Division of Physical Chemistry, Institute Ruđer Bošcović, Zagreb, Croatia — [3]Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Most of the amazing properties of liquid water stem from the fluctuations in the uninterrupted network of hydrogen-bonded molecules.[1] One such phenomena is the splitting of transport coefficients in an electric field, which despite the enormous technological implication, is an effect not yet understood from the microscopic point of view. We address this problem by simulating pure water in a uniaxial E-field under ambient conditions using the GROMACS framework.[2] After quantifying the translational and orientational dynamics of water molecules, characteristic, anisotropic timescales for the reordering of hydrogen bonds are retrieved. A novel relaxation process occurring on the picosecond timescale is detected, and unambiguously associated with cooperative rotations of multiple hydrogen-bonded molecules that induce a slow relaxation of components of the macroscopic shear viscosity that are parallel to the field direction.[3] [1] Luzar, A.; Chandler, D. Nature 1996 379, 55-57. [2] Milicevic Z., Marrink S. J., Smith A.-S., Smith D. M. J. Mol Mod 2014 20, 2359 [3] Milicevic Z., Baer A., Smith D. M., Smith A.-S., PRX submitted

DY 29.7 Tue 15:30 EB 107

In-cage dynamics of molecular hydrogen in clathrates hydrates as function of the confinement size — •Margarita Russina — Helmholtz Zentrum Berlin für Materialied und Energie, Hahn-Meitner Platz 1, 14109 Berlin

To understanding the criteria governing the molecular mobility in confinement we have studied in-cage dynamics of confined molecular hydrogen as a function of confinement size. We used nanopores ice based clathrate with nanocages of two different dimensions of 0.75 and 0.946 nm, which are particularly suitable model systems since the interactions between the clathrate framework and H2 are of the same hydrophobic nature in both cages. We have found that by varying the size of the pore by only 20 % in the effective radius we can modify the diffusive mobility of confined hydrogen in both directions, i.e. both reducing and enhancing mobility compared to the bulk. In the smaller cages of clathrate hydrates with a mean size of 0.795 nm we observe strong hydrogen localization in the cage center even at temperatures up to 200K. Moderate increase of the confinement to 0.946 nm leads to the onset of jump diffusion between tetrahedrally shaped sorption sites in large cages with separation length of about 2.79 Å already at T=10 K, where bulk hydrogen is frozen at ambient pressure. The observed difference in mobility between small and large cages can be understood as a dimensional phenomenon caused by the modulation of cage potentials as a function of the cage size.

DY 30: Modeling and Simulation of Soft Matter I (joint session CPP/DY)

Time: Tuesday 14:00–16:00 Location: PC 203

Invited Talk DY 30.1 Tue 14:00 PC 203

The role of correlations in the collective behaviour of microswimmer suspensions — •Alexander Morozov — University of Edinburgh, Edinburgh, UK

Recent years witnessed a significant interest in physical, biological and engineering properties of self-propelled particles, such as bacteria or synthetic microswimmers. The main distinction of this 'active matter' from its passive counterpart is the ability to extract energy from the environment (consume food) and convert it into directed motion. One of the most striking consequences of this distinction is the appearance of collective motion in self-propelled particles suspended in a fluid observed in recent experiments and simulations: at low densities particles move around in an uncorrelated fashion, while at higher densities they organise into jets and vortices comprising many individual swimmers. Although this problem recieved significant attention in recent years, the precise origin of the transition is poorly understood.

In this talk I will present a numerical method based on a Lattice-Boltzmann algorithm to simulate hydrodynamic interactions between a large number of model swimmers (order 10^5), represented by extended force dipoles. Using this method we simulate dilute suspensions of self-propelled particles and show that, even below the transition, swimmers move in a correlated fashion that cannot be described by a mean-field approach. We develop a novel kinetic theory that captures these correlations and is non-perturbative in the swimmer density, and reveals the asymmetry between pusher and puller swimmers below the transition to turbulence.

DY 30.2 Tue 14:30 PC 203

Polymer Topology by Chain Walking Polymerization Catalysis — •Ron Dockhorn[1,2], Albena Lederer[1], 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

Monte Carlo simulations of the chain walking polymerization catalysis (CW) are performed using the bond fluctuation model to investigate the influence of the walking mechanism on the polymer topology at a given molecular weight. In agreement to previous findings, for high reaction probability/slow walking the structure growths with linear chain extensions. On the other hand, for low reaction probability/fast walking the structures show dendritic growth of the polymer. The transition region is characterized by large amount of branched side chains reflecting a cross-over regime with linear global features and dendritic local sub-structures. This is in contrast to the Zimm-Stockmayer hyperbranched (ZS-HB) scaling. Static properties are investigated by means of radius of gyration and scattering function of perfect dendrimers, ZS-HB, and CW-structures. A generalized mean-field model is applied, and is found in fair agreement with the simulation data under good solvent conditions. These findings are aimed to understand the physical properties related with the topology of the CW-structures to improve the synthesis of a new class of hyperbranched molecules.

DY 30.3 Tue 14:45 PC 203

Understanding the Dynamical Behavior of Twin Polymerization — Constantin Huster, Halit Taskin, and •Janett Prehl — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

Twin polymerization enables the formation of two different macromolecular structures of organic-inorganic hybrid materials in one single process step. To investigate the dynamical behavior and the morphology of the reaction process and the final compounds we recently developed a Monte-Carlo based reactive bond fluctuation model (rBFM) [1] that is capable to cope with the complexity of the underlying reaction mechanism. Special feature of this rBFM is the possibility to define multiple reaction centers per monomer and multiple bond vectors between two monomers that exhibit different properties.

In this presentation we introduce the rBFM and analyze first results of the diffusive behavior of the reacting twin monomers over time. By doing so we gain insights into the structure formation process of twin polymerization.

[1] K.H.Hoffmann, J.Prehl, *Reac Kinet Mech Cat* DOI: 10.1007/s11144-017-1303-y

DY 30.4 Tue 15:00 PC 203

Bridging Time Scales with Variationally Enhanced Sampling — •Omar Valsson — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany

The usefulness of atomistic simulations is generally hampered by the presence of several metastable states separated by high barriers leading to kinetic bottlenecks. Transitions between metastable states thus occur on much longer time scales than one can simulate. Numerous enhanced sampling methods have been introduced to alleviate this time scale problem, including methods based on identifying a few crucial order parameters and enhancing their sampling through the introduction of an external biasing potential.

Here will we discuss Variationally Enhanced Sampling (Valsson and Parrinello, PRL 113 090601, 2014), a generally applicable enhanced sampling method where an external bias potential is constructed by minimizing a convex functional. We present numerous examples from physics and chemistry which show the flexibility and practicality of the method. We will furthermore show how the variational property of the method can be used to extend the method in various innovative ways, e.g.: to obtain kinetic information from atomistic simulation; to accelerate nucleation events by employing models from classial nucleation theory; and to incorporate experimental information into molecular simulations.

We will also introduce the VES code (http://www.ves-code.org), an open-source library for the PLUMED 2 plugin that implements methods based on Variationally Enhanced Sampling.

DY 30.5 Tue 15:15 PC 203

Kinetics of defects in self-assembled block-copolymers using continuum models — •Juan Carlos Orozco Rey and Marcus Mueller — University of Goettingen, Institute of Theoretical Physics, Goettingen, Germany

The computational study of directed self-assembled (DSA) of copolymeric materials is a challenging task due to the disparity of length scales involved in the structure formation process. Fast simulation techniques, which enable us to conciliate the periodicity of the self-assembled structures with the large scale of devices targeted in the manufacturing of these materials, are of significant interest. Continuum models provide the highest level of coarse-graining where the polymer system is no longer described by the molecular degrees of freedom but only in terms of a local collective variable - the difference in composition. We study the ability of two continuum models - Ohta-Kawasaki and Swift-Hohenberg - to describe key aspects of defects and their dynamics: the limits of stability, the shape of the internal AB interfaces and the kinetics of motion.

We use particle-based simulations and self-consistent field theory to compare and identify the most promising model for the study of DSA. We show that in spite of the caveats of a highly coarse-grained description, a continuum model provides valuable insights into the kinetics of self-assembly as well as into the surface-directed structure formation of device-oriented structures like T-junctions. The combination with more detailed models enables us to gain better understanding of the process while reducing the computational cost.

DY 30.6 Tue 15:30 PC 203

Higher coordination of cross-links improve toughness of fiber bundles — •Huzaifa Shabbir and Markus Hartmann — Sensengasse 8 , 1090 Vienna Austria

(Physical) cross-linking is an effective strategy to tailor the mechanical properties of polymeric systems. Often, these cross-links are weaker than the covalent backbone that holds the structure together. If reversible, cross-links provide the material with some self-healing behavior.

We use Monte Carlo simulations to investigate the mechanical behavior of (reversibly) cross-linked polymeric systems. The framework of a multi-body potential is utilized to control the coordination of cross-links (coordination is defined as the number of monomers participating in one cross-link). Displacement controlled computational loading experiments are conducted to evaluate the mechanical properties of fibrous systems.

Previous work shows that the coordination of cross-links significantly influences the mechanical performance of a linear chain [1]. In this talk, the influence of the coordination of cross-links on the mechanics of aligned fiber bundles will be discussed. In particular, it will be shown that the coordination of cross-links has a large impact on the toughness of fiber bundles as higher coordination inhibits the premature rupture of the covalent backbone observed for classical cross-links of two fold coordination [2]. Special emphasis will be put on the influence of the topology of cross-links that show a much richer variety for a higher coordination compared to the classical coordination of two.

DY 30.7 Tue 15:45 PC 203

Permeability maximization in polymer gels: Modeling and simulation — •Won Kyu Kim[1], Matej Kanduč[1], Rafael Roa[1], and Joachim Dzubiella[1,2] — [1]Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

Permeability measures the ability of soft matter, such as polymer-based networks (hydrogels), to transport solvents and solutes, defining important control parameters in soft functional material applications, e.g., for filtration, drug release, and transport of reactants in responsive nano-reactors [1-4]. We study permeability by means of coarse-grained simulations and theory of a model polymer network. We find that the permeability can be maximized by optimal polymer volume fractions and inter-particle interactions between the polymer and the penetrating solutes. This nontrivial phenomenon is triggered by a competition between solute partitioning [1-3] and diffusion [2]. Throughout a wide range of parameter space of the solvent quality, solute coupling, and gel volume fraction, a rich topology of the partitioning is found. The solutes' diffusivity is highly correlated to gel structures, resulting in a drastically nonmonotonous permeability. Possible applications to hydrogel based devices such as responsive nanoreactors for catalysis [2,4] are discussed.

[1] W. K. Kim et al, Macromolecules 50, 6227 (2017). [2] R. Roa et al, ACS Catalysis 7, 5604 (2017). [3] M. Kanduč et al, Phys. Chem. Chem. Phys. 19, 5906 (2017). [4] S. Wu et al, Angewandte Chemie 51, 2229 (2012).

DY 31: Condensed Matter Simulations augmented by Advanced Statistical Methodologies II (joint session DY/CPP)

Time: Tuesday 14:00–15:15 Location: BH-N 128

DY 31.1 Tue 14:00 BH-N 128

Nonlinear Network description for many-body quantum systems in continuous space — •Markus Holzmann[1], Michele Ruggeri[2], and Saverio Moroni[3] — [1]LPMMC, UMR 5493 of CNRS, Université Grenoble Alpes, F-38100 Grenoble France — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [3]DEMOCRITOS National Simulation Center, Istituto Officina dei Materiali del CNR and SISSA, Via Bonomea 265, I-34136 Trieste, Italy

We show that the recently introduced iterative backflow renormalization [1] can be interpreted as a general neural network in continuum space with non-linear functions in the hidden units [2]. We use this wave function within Variational Monte Carlo for fermionic and bosonic liquid helium in two and three dimensions, where we typically find a tenfold increase in accuracy over currently used wave functions. For two dimensional 4 He, we also show that the iterative backflow wave function can describe both the liquid and the solid phase with the same functional form - a feature shared with the Shadow Wave Function, but now joined by much higher accuracy.

[1] M. Taddei, M. Ruggeri, S. Moroni, and M. Holzmann, Phys. Rev. B 91, 115106 (2015).

[2] M. Ruggeri, S. Moroni, and M. Holzmann, cond-mat/1711.01993 (2017).

DY 31.2 Tue 14:15 BH-N 128

Massively parallel multicanonical simulations — Jonathan Gross[1], •Johannes Zierenberg[2], Martin Weigel[3], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, D 04009 Leipzig, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany, — [3]Applied Mathematics Research Centre, Coventry University, Coventry CV1 5FB, England

Generalized-ensemble Monte Carlo simulations such as the multicanonical method and similar techniques are among the most efficient approaches for simulations of systems undergoing discontinuous phase transitions or with rugged free-energy landscapes. As Markov chain methods, they are inherently serial computationally. It was demonstrated recently, however, that a combination of independent simulations that communicate weight updates at variable intervals allows for the efficient utilization of parallel computational resources for multicanonical simulations. Implementing this approach for the many-thread architecture provided by current generations of graphics processing units (GPUs), we show how it can be efficiently employed with of the order of 10^4 parallel walkers and beyond, thus constituting a versatile tool for Monte Carlo simulations in the era of massively parallel computing. We provide the fully documented source code for the approach applied to the paradigmatic example of the two-dimensional Ising model as starting point and reference for practitioners in the field.

DY 31.3 Tue 14:30 BH-N 128

Multiferroic properties of HoMn2O5 compounds: A Monte Carlo Study — •A.S ERCHIDI ELYACOUBI, R Masrour, and A Jabar — Cady Ayyed University, National School of Applied Sciences, PB 63 46000, Safi, Morocco.

The class of HoMn2O5 compounds offers multiferroic properties where the refined magnetic zig-zag order breaks the inversion symmetry. The polarization and magnetization are found. The ferroelectric transition temperature are determined. The polarization is induced solely by different exchange couplings of the two different Mn4+ and Mn3+ magnetic ions. The magnetic and ferroelectric cycle have been deduced. The variation of the polarization by an external magnetic field depends strongly on the direction of that field. HoMn2O5 compounds;

DY 31.4 Tue 14:45 BH-N 128

Identifying the relevant degrees of freedom in mesoscale models of liquid water with Bayesian formalism — •Julija Zavadlav and Petros Koumoutsakos — Computational Science and Engineering Laboratory, ETH Zurich, Zurich, CH-8092, Switzerland

Coarse-graining (CG) has become an established methodology in molecular modeling to access time and length scales that are computationally beyond the reach of the conventional atomistic simulations. However, it often involves making several a priori assumptions, which are rarely systematically addressed. Typically, these assumptions pertain to the level of coarse-graining and the model complexity. We address this issue for mesoscale models of liquid water by investigating on an equal footing a number of CG models that differ in the level of coarse-graining and in the model complexity. To this end, we deploy the classical as well as a novel Hierarchical Bayesian methods [1,2] to quantify and calibrate the uncertainty of the models and to perform the model selection using the experimental data. Furthermore, we assess the efficiency-accuracy trade-off of developed models and provide guidelines for future water model design at the mesoscopic scale.

[1] S.Wu, P. Angelikopoulos, G. Tauriello, C. Papadimitriou, and P. Koumoutsakos, J. Chem. Phys. 145, 244112, 2016.

[2] L. Kulakova, G. Arampatzis, P. Angelikopoulos, P. Hadjidoukas, C. Papadimitriou, and P. Koumoutsakos, Sci. Rep., 7, 16576, 2017

DY 31.5 Tue 15:00 BH-N 128

Data driven inference for the repulsive exponent of the Lennard-Jones potential in molecular dynamics simulations — •Georgios Arampatzis and Petros Koumoutsakos — Computational Science and Engineering Laboratory, Clausiusstrasse 33, ETH Zürich, CH-8092, Switzerland

The Lennard-Jones (LJ) potential is a cornerstone of Molecular Dynamics (MD) simulations and among the most widely used computational kernels in science. The LJ potential models atomistic attraction and repulsion with century old prescribed parameters ($q = 6$, $p = 12$, respectively), originally related by a factor of two for simplicity of cal-

culations. We propose the inference of the repulsion exponent through Hierarchical Bayesian uncertainty quantification We use experimental data of the radial distribution function and dimer interaction energies from quantum mechanics simulations. We find that the repulsion exponent $p \approx 6.5$ provides an excellent fit for the experimental data of liquid argon, for a range of thermodynamic conditions, as well as for saturated argon vapour. Calibration using the quantum simulation data did not provide a good fit in these cases. However, values $p \approx 12.7$ obtained by dimer quantum simulations are preferred for the argon gas while lower values are promoted by experimental data. These results show that the proposed LJ 6-p potential applies to a wider range of thermodynamic conditions, than the classical LJ 6-12 potential. We suggest that calibration of the repulsive exponent in the LJ potential widens the range of applicability and accuracy of MD simulations.

DY 32: Microswimmers I (joint session DY/BP/CPP)

Time: Tuesday 14:00–15:45 Location: BH-N 243

DY 32.1 Tue 14:00 BH-N 243

Active colloidal propulsion over a crystalline surface — Udit Choudhury[1], •Arthur Straube[2], Peer Fischer[1], John Gibbs[3], and Felix Höfling[2] — [1]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — [2]Freie Universität Berlin, Institute of Mathematics, Berlin, Germany — [3]Department of Physics and Astronomy, Northern Arizona University, Flagstaff, USA

We study both experimentally and theoretically the dynamics of chemically self-propelled Janus colloids moving atop a two-dimensional (2d) crystalline surface [1]. The surface is a hexagonal close-packed monolayer of colloidal particles of the same size as the mobile one. The dynamics of the self-propelled colloid reflects the competition between hindered diffusion due to the periodic surface and enhanced diffusion due to active motion, which can be tuned by changing the concentration of a chemical fuel. Our experimental data for the mean-square displacements (MSDs) are consistent with a Langevin model for the effectively 2d translational motion of an active Brownian particle in a periodic potential, combining the confining effects of gravity and the crystalline surface with the free rotational diffusion of the colloid. Approximate analytical predictions are made for the MSD describing the crossover from free Brownian motion at short times to active diffusion at long times. The results are in semi-quantitative agreement with numerical results of a refined Langevin model that treats translational and rotational degrees of freedom on the same footing.

[1] U. Choudhury, A. V. Straube, P. Fischer, J. G. Gibbs, F. Höfling, New J. Phys. (2017), doi: 10.1088/1367-2630/aa9b4b

DY 32.2 Tue 14:15 BH-N 243

Dynamics of a single circular microswimmer in a quenched crowded media — •Oleksandr Chepizhko and Thomas Franosch — Institute for Theoretical Physics, University of Innsbruck, Innsbruck, Austria

The motion of active particles, for example, bacteria or unicellular organisms, in nature occurs in crowded environments such that the walls, boundaries, and obstacles strongly influence the dynamics of the microswimmers. Here we present a generic model for a deterministic circular microswimmer in a disordered two-dimensional quenched random array of obstacles. The microswimmer moves in circular orbits between the collisions with the obstacles, and after colliding with an obstacle the microswimmer follows the obstacle's surface for some time before detaching again.

The diffusivity of the system is studied via event-driven computer simulations for a wide range of obstacle densities and orbit radii. We find to phase boundaries of a conducting phase with an insulating and a localized phase. The phase behavior is investigated both close to these two transition lines, as well as deep in the conducting phase. The phase transitions correspond to critical phenomena with both an underlying static percolation transition, while the dynamic exponents reveal different universal classes. Furthermore, we find that the diffusivity grows with the density of obstacles up to a narrow region in the vicinity of the localization transition where it rapidly drops to zero.

DY 32.3 Tue 14:30 BH-N 243

Controlled Control of Cargo Delivery Performed by Self-Propelled Janus Droplets — •Menglin Lee[1], Martin Brinkmann[1], Ignacio Pagonabarraga[2], Ralf Seemann[1], and Jean-Baptiste Fleury[1] — [1]Saarland University, Saarbruecken, Germany — [2]University of Barcelona, Bracelona, spain

We propose a class of programmable carrier droplets that can be made of a water/ethanol mixture dispensed in a continuous oil/surfactant solution. While swimming, the droplets pass through up to three stages whose appearance and duration are determined by the chemical composition of the droplet and the surrounding phase. A spontaneous de-mixing of the initially homogeneous droplet phase controlled by an uptake of surfactant and simultaneous loss of ethanol is generally observed. The phase segregation can lead to the formation of characteristic Janus droplets which consist of a water-rich and an ethanol-rich droplet. During de-mixing cargo molecules, like DNA, can be separated in the trailing ethanol–rich droplet and are "carried like in a backpack". Delivery is obtained whenever the trailing droplet touches a wettable target. Selective attraction or repulsion from targets is determined by the long–range hydrodynamic interactions of the swimmers with the geometric shape of the targets. In combination with a controlled delay of phase separation by the initial chemical composition of the droplets, we can exploit this selectivity to deliver DNA molecules dissolved in the ethanol-rich droplet at specific target sites and during a specific timeframe.

(under review - 2017)

DY 32.4 Tue 14:45 BH-N 243

Clearing out a Maze: Chemotaxis and Percolation — Tanja Schilling[1] and •Thomas Voigtmann[2,3] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [3]Department of Physics, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

We study chemotactic motion in a random environment of obstacles by means of a lattice model that bears resemblance to the arcade game PAC-MAN®: A random walker moves on the percolating cluster of a square lattice, with steps that are biased towards the food that is initially placed on the accessible lattice sites and that is then consumed by the walker. Anomalous diffusion emerges, and is best described by a power-law with a non-trivial dynamical exponent that depends continuously on the propensity of the walker to move towards food. Although its food propensity biases the walker to explore previously unvisited sites more easily than the unbiased random walk, and thus intuitively serves to stretch out the walker's trajectories in comparison to the non-chemotactic case, the asymptotic growth of the mean-squared displacement is weaker. We suggest that getting lost in the culs-de-sac is a mechanism to explain why the chemotactic exploration of a maze thus becomes less effective than the pure diffusive one.

[1] T. Schilling and Th. Voigtmann, J. Chem. Phys. (in press, 2017); arXiv:1607.01123.

DY 32.5 Tue 15:00 BH-N 243

Theoretical study of triangular magnetocapillary microswimmers — •Alexander Sukhov[1], Sebastian Ziegler[2], Oleg Trosman[2], Ana-Suncana Smith[2], and Jens Harting[1,3] — [1]Helmholtz Institute Erlangen-Nuernberg for Renewable Energy (IEK-11), Forschungszentrum Juelich GmbH, 90429 Nuernberg, Germany — [2]Institute for Theoretical Physics, Friedrich-Alexander University Erlangen-Nuernberg, 91054 Erlangen, Germany — [3]Department of Applied Physics, Eindhoven University of Technology, NL-5600MB Eindhoven, The Netherlands

As demonstrated experimentally (for a recent review see Ref. [1]), magnetocapillary swimmers - a system of three or more magnetic beads trapped at a fluid-gas interface - prefer to form equilateral triangles due to an interplay of attractive capillary and repulsive magnetic dipole-dipole interactions. By applying additionally a time-dependent magnetic field the position of the swimmer and its velocity direction can be wirelessly manipulated. Combining the lattice Boltzmann method with the analytical force-based bead-spring model [2, 3] extended for a triangular configuration, we explain a sharp dependence of the average speed of the swimmer on the frequency of the time-dependent

magnetic field and compare our results with the experiment. In addition, we demonstrate numerically and analytically the control of the direction of the swimmer motion using magnetic fields. [1] G. Grosjean, M. Hubert and N. Vandewalle, Adv. Colloid Interface Sci., in press (2017); [2] B.U. Felderhof, Phys. Fluids **18**, 063101 (2006); [3] J. Pande *et al.*, New J. Phys. **19**, 053024 (2017).

DY 32.6 Tue 15:15 BH-N 243

The frequency-dependent behavior of microswimmers in oscillating shear flow — Kevin Schröer[1], •Patrick Kurzeja[2], and Lothar Brendel[1] — [1]Faculty of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Institue of Mechanics, Technical University Dortmund, 44227 Dortmund, Germany

One possibility to alter the macroscopic properties of a self-propelled nanoparticle suspension is the introduction of inhomogeneities in the propulsion mechanism, which leads to drastic changes in the collective behavior [1].

A new approach is presented for sheared suspensions: the control via oscillating walls. The oscillation frequency determines the thickness of a viscous boundary layer that surrounds the inertia-dominated center region. This is characterized by the Womersley number Wo, being the ratio between viscous and inertial forces [2]. As a result, regions of particle rotation and translation can be varied by this frequency.

Using this setup, we investigate the impact of Wo on the rheology of a dilute microswimmer suspension by means of Multi-Particle Collision Dynamics (MPC) simulations. This method is suited to capture hydrodynamics and thermal fluctuations and has been used in related topics like dilute suspensions in a gravity perturbed annular shear [3] or bidisperse segregation in a Hagen-Poiseuille flow [4].

[1] M. P. Magiera and L. Brendel, Phys. Rev. E 92, 1 (2015)
[2] P. Kurzeja et al., JASA 140, 4378 (2016)
[3] K. Schröer et al., EPJ Web of Conferences, 140 (2017)
[4] P. Kanehl and H. Stark, J. Chem. Phys. 142, 214901 (2015)

DY 32.7 Tue 15:30 BH-N 243

Buckling instability and swimming of elastic spherical shells — •Adel Djellouli[1], Philippe Marmottant[1], Henda Djeridi[2], Catherine Quilliet[1], and Gwennou Coupier[1] — [1]Univ. Grenoble Alpes, CNRS, LIPhy, 38000 Grenoble, France — [2]Univ. Grenoble Alpes, Grenoble INP, CNRS, LEGI, 38000 Grenoble, France

Under pressure, a hollow elastic sphere becomes unstable and collapses. It reinflates back when the pressure is decreased. The shape hysteresis associated to this deformation cycle makes this simple object a good candidate for becoming a microswimmer, that is, a swimmer able to move at low Reynolds number.

We explore this possibility through a macroscopic experiment in fluids of varying viscosities so as to explore different flow regimes [1]. We show that not only the shape sequence hysteresis leads to swimming but the asymetry in the deformation velocity makes the fast buckling phase an efficient mechanism for propulsion that implies inertial effects and subtle coupling between shape post-buckling oscillations and fluid flow patterns. Our modeling shows that such an inertial regime could even be reached at microscopic scale.

We anticipate that a conveyor made of a few of microbubbles with different shell thicknesses, would constitute a microrobot whose 3D displacement can be remotely controlled by an echographic device - a relatively cheap and widely available tool in the hospitals.

[1] A. Djellouli, P. Marmottant, H. Djeridi, C. Quilliet and G. Coupier, Phys. Rev. Lett. 119, 224501 (2017). See also P. Ball, "Focus: Elastic Spherical Shell Can Swim", Physics 10, 128 (2017).

DY 33: Delay and Feedback Dynamics

Time: Tuesday 14:00–16:00 Location: BH-N 334

DY 33.1 Tue 14:00 BH-N 334

Exploring chaos synchronization in quantum-dot micropillar lasers coupled with delay — •Xavier Porte[1], Sören Kreinberg[1], Steffen Holzinger[1], David Schicke[2], Benjamin Lingnau[2], Martin Kamp[3], Christian Schneider[3], Sven Höfling[3,4], Kathy Lüdge[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [3]Technische Physik, Julius-Maximilians-Universität Würzburg, Würzburg, Germany — [4]School of Physics and Astronomy, University of St Andrews, Scotland

Spontaneous synchronization is a universal behavior of coupled systems that only recently is being explored in the quantum domain. A particularly intriguing case is the phenomenon of chaos synchronization between nonlinear oscillators when they are coupled with delay. Semiconductor lasers are excellent examples of such systems, offering the additional key advantage of potential miniaturization to the limits of cavity quantum electrodynamics. In the present work, we explore the phenomenon of chaos synchronization applied to quantum-dot based micropillar lasers. We optically couple two nanolasers in a relay configuration, where both lasers receive self- and mutual-coupling. We investigate the coupling parameters dependencies and their influence on the correlation of the dynamics. Different synchronization regimes are demonstrated like leader-laggard and zero-lag synchronization. Our results pave the way to use nanolasers as testbed systems to study chaos synchronization in the quantum regime.

DY 33.2 Tue 14:15 BH-N 334

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

Time delay systems can be found in various fields such as engineering, biology and physics. In the scientific literature many results exist for systems with constant delay. However, in reality the delays are typically not constant but rather time-varying. Recently we found that there are two fundamental classes of time-varying delays [1, 2]. Systems with conservative delay are equivalent to systems with constant delay. On the other hand, there are systems with dissipative delay, which cannot be transformed to systems with constant delay and are associated with fundamentally different dynamic properties.

In this talk we show that nonlinear systems with large dissipative delay can exhibit a new kind of chaotic behavior characterized by laminar phases, which are periodically interrupted by irregular bursts. In particular, the output intensity during the laminar phases remains almost constant, but its level varies chaotically from phase to phase. The periodic dynamics of the lengths and the chaotic dynamics of the intensity levels can be understood and also tuned via two one-dimensional maps, which can be deduced from the nonlinearity of the delay equation and from the delay variation, respectively.

[1] A. Otto, D. Müller and G. Radons, Phys. Rev. Lett. 118, 044104 (2017).
[2] D. Müller, A. Otto and G. Radons, Phys. Rev. E 95, 062214 (2017).

DY 33.3 Tue 14:30 BH-N 334

Small changes, big effect: The dimension of chaotic attractors of dynamical systems with time-varying delay — •David Müller, Andreas Otto, and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

For many systems arising in biology, climate dynamics and engineering the influence of time-delays can not be neglected. Although taking into account environmental fluctuations by introducing time-varying delays can lead to more realistic models, the delay is often considered constant and only a few publications deal with the effect of a time-varying delay on the dynamics of the involved systems.

Recently, we identified two classes of time-varying delays, which are characterized by fundamental differences in the tangent space dynamics of the related systems [1,2]. In this talk, we demonstrate that introducing a time-varying delay also leads to drastic differences in the properties of chaotic attractors of systems with large delay. In detail, the dimension of chaotic attractors of systems with *conservative delay* is typically much larger than the dimension of attractors of systems with *dissipative delay*. Due to the fractal dependence of the delay class on the delay parameters, arbitrary small changes of the delay parameters can cause huge variations of the attractor dimension.

[1] A. Otto, D. Müller and G. Radons, Phys. Rev. Lett. 118, 044104 (2017).
[2] D. Müller, A. Otto and G. Radons, Phys. Rev. E 95, 062214

(2017).

DY 33.4 Tue 14:45 BH-N 334

Dynamics and bifurcation analysis of a passively mode-locked v-shaped semiconductor laser — •Anna-Belle Garten, Lina Jaurigue, and Kathy Lüdge — Institut f. Theo. Physik, Sekr. EW 7-1,Technische Universtität Berlin, Berlin, Germany

Passively mode-locked vertical external-cavity surface-emitting lasers (VECSEL) can produce femtoseconds pulses with high peak powers [1]. These lasers are of interest for driving nonlinear optical processes, e.g. frequency doubling for material processing and multiphoton microscopy. VECSEL mode-locked lasers typically have a v-shaped cavity, i.e. the pulse passes through gain chip twice per roundtrip.

In this contribution we investigate the influence of the geometry on the dynamics. We model the system with a set of coupled delay differential equations which take into account the v-shaped geometry. We solve these equations numerical and analyse the bifurcations of this system. Solutions are found which are not found in an equivalent linear cavity, e.g. double pulse solutions with identical puls heights but asymmetric interspike interval time. These solutions differ from double pulse solutions found in [2]. In [2] the solutions are long lived transients, arising due to the long cavity round trip time compared with the time scales of the carrier dynamics. Whereas in the v-shaped cavity they are stable solutions arising due to the geometry.

[1]C. Alfieri, D. Waldburger, S. Link, E. Gini, M. Golling, G. Eisenstein, and U. Keller, Opt. Express 25, 6402-6420 (2017)

[2] M. Marconi, J. Javaloyes, S. Balle, and M. Giudici, OSA Technical Digest (online) (Optical Society of America, 2014), paper NW3A.8.

DY 33.5 Tue 15:00 BH-N 334

Dynamics of Temporal Localized States in Passively Mode-Locked Semiconductor Lasers — •Svetlana Gurevich[1], Christian Schelte[1,2], and Julien Javaloyes[2] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany — [2]Departament de Física, Universitat de les Illes Balears, C/ Valldemossa km 7.5, 07122 Mallorca, Spain

We are interested in the emergence and the stability of temporal localized structures in the output of a semiconductor laser passively mode-locked by a saturable absorber in the long cavity regime. Our analysis is based upon a generic model of mode-locking that consists in a time-delayed dynamical system,but also upon a much more numerically efficient, yet approximate, partial differential equation. We compare the results of the bifurcation analysis of both models in order to assess up to which point the two approaches are equivalent. In particular, by a detailed bifurcation analysis we show that additional solution branches that consist in multi-pulse solutions exist. Further, we demonstrate that the various solution curves for the single and multi-peak pulses can splice and intersect each other via transcritical bifurcations, leading to a complex web of solution. In addition, we disclose the existence of secondary dynamical instabilities where the pulses develop regular and subsequent irregular temporal oscillations.

DY 33.6 Tue 15:15 BH-N 334

Localized Structures in an inhomogeneous Lugiato-Lefever equation with time-delayed feedback — •Felix Tabbert[1], Mustapha Tlidi[2], Krassimir Panajotov[3,4], and Svetlana Gurevich[1] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster — [2]Faculté des Sciences, Université Libre de Bruxelles (ULB), Code Postal 231, Campus Plaine, Bruxelles B-1050, Belgium — [3]Vrije Universiteit Brussel, Department of Applied Physics & Photonics, Pleinlaan 2, B-1050 Brussels, Belgium. — [4]Institute of Solid State Physics, 72 Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

We discuss the destabilization mechanisms of localized structures in an inhomogeneous nonlinear cavity subjected to injection and to time-delayed feedback. This simple setup is described by the delayed Lugiato-Lefever equation. We analyze the pinning behavior of spatial inhomogeneities on localized structures by introducing a potential induced by an inhomogeneous injection beam. Further, we identify conditions under which these structures are destabilized and describe different bifurcation scenarios. We show that in the presence of the inhomogeneity, delayed feedback induces an Andronov-Hopf-bifurcation that leads to oscillations of the localized structure around the inhomogeneity. Finally we show that for large values of the feedback strength, the localized structure escapes from the potential well and starts to drift and discuss different scenarios, where inhomogeneities are introduced, e.g. in the detuning parameter.

DY 33.7 Tue 15:30 BH-N 334

Feedback enhanced quantum beating due to resonant dipole-dipole coupling — •Manuel Kraft[1], Tymoteusz Tula[2], Kisa Barkemeyer[1], Anja Metelmann[3], Andreas Knorr[1], and Alexander Carmele[1] — [1]TU Berlin, Institute of Theoretical Physics — [2]Wroclaw University of Science and Technology, Faculty of Fundamental Problems of Technology — [3]Princeton University, Department of Electrical Engineering

We investigate the propagation of few-photon Fock-states in a one-dimensional waveguide scattered by two dipole-dipole coupled atoms. Using a scattering method based on the Lippmann-Schwinger equation [1], we study photon-photon correlations of the photons in the reflected and transmitted field. Depending on the dipole-dipole interaction strength, we observe highly damped oscillations in the second-order correlation function. To increase the visibility, we introduce quantum coherent time-delayed feedback [2] by terminating one end of the waveguide by a resonator, acting as a mirror. Our results clearly show that the dipole-dipole induced quantum beats can be intensified and stabilized where the long-time beating frequency is sensitive to the dipole-dipole interaction strength. Since the interaction strength depends strongly on the separation of the emitters, our method may provide a way to probe interatomic coupling and distances on a deep subwavelength scale.

[1] Zheng *et al.*, Phys. Rev. Lett. **110**, 113601 (2013)
[2] Carmele, *et al.* Phys. Rev. Lett. **110**, 013601 (2013)

DY 33.8 Tue 15:45 BH-N 334

Dynamics of Quantum-Dot Based Micropillar Lasers with Optoelectronic Feedback — •Andrej Krimlowski — Institut für Theoretische Physik, Technische Universität Berlin

Semiconductor lasers with self-coupled delayed feedback show an extensive variety of physical phenomenons including nonlinear dynamics such as stabilized laser self-pulsing and chaos. We numerically investigate an on-chip optoelectronic feedback setup in a micropillar laser-detector assembly [1]. In this setup, the optical output signal of a micropillar laser is fed back into the laser pump current with an electronic delay. The system is characterized by strong spontaneous emission as well as a temperature dependent gain. The dependence of the system's dynamics on the temperature induces a time scale separation leading to complex dynamics. We perform a linear stability analysis and a numerical bifurcation analysis in dependence on system parameters as the feedback strength, the pump current and the maximum feedback current. We find a multitude of qualitatively different dynamics including complex states with periodic and non-periodic solutions and strong multistability of the system.

DY 34: Nonlinear Stochastic Systems

Time: Tuesday 14:00–15:15 Location: BH-N 333

DY 34.1 Tue 14:00 BH-N 333

Nonequilibrium dynamics of piecewise-smooth stochastic systems — •Paul Geffert and Wolfram Just — School of Mathematical Sciences, Queen Mary University of London, United Kingdom

Piecewise-smooth systems have attracted a lot of interest in the last decade; deterministic models were studied quite intensely, but the stochastic counterpart is still in its infancy.

We study the dynamics of a simple Langevin equation with dry friction subjected to coloured noise. By applying suitable approximation schemes, we obtain analytical expressions for the stationary density and the probability of sticking. Our results show very good agreement with numerical simulations. Furthermore we explore dynamical properties of the system e.g. the spectral density.

Our analysis indicates that the observed stick-slip transitions can be linked with a "critical" value of the noise correlation time.

DY 34.2 Tue 14:15 BH-N 333

A simple parameter can switch between different weak-noise-induced phenomena in a simple neuron model. — •Marius Emar Yamakou[1] and Jürgen Jost[1,2] — [1]Max Planck Institute for Mathematics in the Sciences, Inselstrasse 22, 04103 Leipzig, Germany — [2]Santa Fe Institute for the Sciences of Complexity, NM 87501, Santa Fe, USA

In recent years, several, apparently quite different, weak noise-induced resonance phenomenon have been discovered in nonlinear systems. Here, we show that at least two of them, self-induced stochastic resonance (SISR) and inverse stochastic resonance (ISR), are mathematically related by a simple parameter switch in one of the simplest models, the FitzHugh-Nagumo (FHN) neuron model. We consider a FHN model with a unique fixed point perturbed by synaptic noise. Depending on the stability of this fixed point and whether it is located to either the left or right of the fold point of the critical manifold, two distinct weak-noise-induced phenomena, either SISR or ISR, may emerge. SISR is more robust to parametric perturbations than ISR, and the coherent oscillations generated by SISR is more robust than that generated deterministically. ISR also depends on the location of initial conditions and on the time-scale separation parameter of the model equation. Our results could also explain why real biological neurons having similar physiological features and synaptic inputs may encode very different information.

DY 34.3 Tue 14:30 BH-N 333

PDE for the "first-passage-time phase" of a stochastic oscillator — •Benjamin Lindner[1], Alexander Cao[2], and Peter J. Thomas[2] — [1]Humboldt Universität zu Berlin — [2]Case Western Reserve University (Cleveland, Ohio, USA)

Phase reduction of limit cycle dynamics provides a low-dimensional representation of high-dimensional oscillator dynamics. For a deterministic dynamical system with a stable period-T limit cycle, the change of variables $\mathbf{x} \to \theta(\mathbf{x}) \in [0, 2\pi]$ such that $d\theta/dt \equiv 2\pi/T$ is well established. In contrast, for stochastic limit cycle systems, a phase reduction can be defined in several nonequivalent ways (Freund et al. *Chaos* **13**, 225 (2003), Schwabedal and Pikovsky *Phys. Rev. Lett.* **110**, 205102 (2013), Lindner and Thomas *Phys. Rev. Lett.* **113**, 254101 (2014)]. Schwabedal and Pikovsky introduced a phase for stochastic oscillators based on a foliation of the basin of attraction, with the property that the mean transit time around the cycle from each leaf to itself is uniform and developed a numerical procedure to estimate the corresponding isochrons. For robustly oscillating planar systems driven by white Gaussian noise, we establish a partial differential equation with a mixture of reflecting and jump boundary conditions that governs this phase function. We solve this equation numerically for several examples of noisy oscillators. In addition, we obtain an explicit expression for the isochron function, $\theta(\mathbf{x})$, for the rotationally symmetric case, and compare this analytical result with oscillators that have been studied numerically in the literature.

DY 34.4 Tue 14:45 BH-N 333

Quantum Hamilton equations for multidimensional problems — •Michael Beyer[1], Jeanette Köppe[1], Markus Patzold[1], Wilfried Grecksch[2], and Wolfgang Paul[1] — [1]Institute for physics, Martin-Luther-Universität Halle-Wittenberg — [2]Institute for mathematics, Martin-Luther-Universität Halle-Wittenberg

Quantum systems can be described in terms of kinematic and dynamic equations within the stochastic picture of quantum mechanics where the particles follow some conservative diffusion process. We show that the reformulation of the quantum Hamilton principle as a stochastic optimal control problem allows us to derive these quantum Hamilton equations of motion for multidimensional systems which can be seen as a generalization of Newton's equations of motion to the quantum world. In analogy to classical mechanics one encounters some similarities for quantum systems, e.g. the decoupling of the center-of-mass motion in multi-particle systems or the Kepler problem as the special case of the two-body problem where we present numerical results for the hydrogen atom.

DY 34.5 Tue 15:00 BH-N 333

Noise and Multistability in the Square Root Map — •Eoghan J. Staunton and Petri T. Piiroinen — National University of Ireland, Galway

Many real-world mechanical systems, including systems arising in engineering such as moored ships impacting a dock or rattling gears, are modelled using impact oscillators. Near low-velocity impacts the dynamics of impact oscillators can be described by a one-dimensional map known as the square root map.

In this talk we will describe the complex structure of the basins of attraction of stable periodic orbits of the square root map and how this produces sensitivity to the addition of small-amplitude white noise. In particular we focus on the effects of noise of varying amplitudes on the square root map for parameter values that lead to multistability.

We show that there is a nonmonotonic relationship between noise amplitude and the proportion of time spent in each periodic behaviour. These relationships can be explained by comparing approximations of steady-state distributions of trajectory deviations due to noise and the deterministic structures of the map. We also show that multistability can be induced by the addition of noise of an appropriate amplitude and present the mechanisms of noise-induced transitions in this case.

DY 35: Nonequilibrium Quantum Many-Body Systems I (joint session TT/DY)

Time: Wednesday 9:30–13:00 Location: H 3010

Invited Talk DY 35.1 Wed 9:30 H 3010

Electronic Squeezing of Pumped Phonons: Negative U and Transient Superconductivity — •Dante M. Kennes[1], Eli Y. Wilner[1], David R. Reichman[2], and Andrew J. Millis[1] — [1]Department of Physics, Columbia University, New York, New York 10027, USA — [2]Department of Chemistry, Columbia University, New York, New York 10027, USA

Advances in light sources and time resolved spectroscopy have made it possible to excite specific atomic vibrations in solids and to observe the resulting changes in electronic properties but the mechanism by which phonon excitation causes qualitative changes in electronic properties, is still under debate. Here, we show that the dominant symmetry-allowed coupling between electron density and dipole active modes implies an electron density-dependent squeezing of the phonon state which provides an attractive contribution to the electron-electron interaction, independent of the sign of the bare electron-phonon coupling and with a magnitude proportional to the degree of laser-induced phonon excitation. Reasonable excitation amplitudes lead to non-negligible attractive interactions that may cause significant transient changes in electronic properties including superconductivity. The mechanism is generically applicable to a wide range of systems, offering a promising route to manipulating and controlling electronic phase behavior in novel materials. Building on these results we analyze the nonequilbrium response of the electronic system and discuss implications for experimentally accessible observables, such as optical conductivity.

DY 35.2 Wed 10:00 H 3010

Photoinduced non-thermal insulator-to-metal transition in NbO_2 epitaxial thin films — •Rakesh Rana[1], John Klopf[1], Joerg Grenzer[1], Harald Schneider[1], Manfred Helm[1,2], and Alexej Pashkin[1] — [1]Helmholtz-Zentrum-Dresden-Rossendorf, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany

The ultrafast insulator-to-metal transition in the correlated oxides such as vanadium dioxide (VO_2) has been extensively explored for its rich physics and potential applications. In this regard, its isovalent counterpart niobium dioxide (NbO_2) with considerably higher transition temperature (T_C = 1080 K) can be envisaged as a potential alternative. We have performed time-resolved optical pump-terahertz (THz) probe measurements on NbO_2 epitaxial thin-film at room temperature. The onset of the THz conductivity is followed by an exponential decay on a timescale of 400 fs. The photoinduced change in THz transmission at later delay times exhibits an excitation threshold of 17.5 mJ/cm^2. Notably, in contrast to VO_2, the pump energy required for the switching into a metastable metallic state is smaller than the energy necessary for heating NbO_2 up to T_C providing strong evidence for the non-thermal character of the photo induced insulator-to-metal transition in this system. The transient optical conductivity in the metastable state can be modelled using the Drude model confirming its metallic character.

DY 35.3 Wed 10:15 H 3010

Emergent CDW order in a 1D correlated electron system with underlying magnetic microstructure — Thomas Köhler, Sebastian Paeckel, and •Salvatore Manmana — Institut f. Theoretische Physik, U. Göttingen

We address the question of charge density wave order (CDW) emerging in a nonequilibrium situation in the course of a photo excitation. Using time-dependent matrix product states (tMPS), we model a pump excitation using Peierls substitution in a Hubbard chain at quarter filling, which is in the presence of an alternating magnetic background field. This magnetic microstructure is obtained for a 1D toy-manganate system, in which the t_{2g} electrons form a frozen lattice of Zener polarons, but do not participate in the charge transport. We investigate the interplay of the magnetic microstructure and the Hubbard U term for the dynamics of the system and discuss possible realizations with ultracold atoms on optical lattices.

We acknowledge financial support by DFG through research unit FOR1807 (project P7) and SFB/CRC1073 (project B03).

DY 35.4 Wed 10:30 H 3010

Non-monotonic response and light-cone freezing in gapless-to-(partially) gapped quantum quenches of fermionic systems — •Sergio Porta[1,2], Filippo Maria Gambetta[1,2], Niccolò Traverso Ziani[3], Dante Marvin Kennes[4], Maura Sassetti[1,2], and Fabio Cavaliere[1,2] — [1]Dipartimento di Fisica, Università di Genova, Genova, 16146 Italy — [2]SPIN-CNR, Genova, 16146 Italy — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [4]Department of Physics, Columbia University, New York, NY 10027, USA

The properties of prototypical examples of one-dimensional fermionic systems undergoing a sudden quantum quench from a gapless state to a (partially) gapped state are analyzed. By means of a Generalized Gibbs Ensemble analysis or by numerical solutions in the interacting cases, we observe an anomalous, non-monotonic response of steady state correlation functions as a function of the strength of the mechanism opening the gap. In order to interpret this result, we calculate the full dynamical evolution of these correlation functions, which shows a freezing of the propagation of the quench information (light cone) for large quenches. We argue that this freezing is responsible for the non-monotonous behaviour of observables. In continuum non-interacting models, this freezing can be traced back to a Klein-Gordon equation in the presence of a source term. We conclude by arguing in favour of the robustness of the phenomenon in the cases of non-sudden quenches and higher dimensionality.

[1] arXiv:1708.09320

DY 35.5 Wed 10:45 H 3010

The non-equilibrium Peierls transition in thermodynamic unbalanced system — •Pedro Ribeiro[1] and Stefan Kirchner[2] — [1]Affiliation: CeFEMA, Instituto Superior Técnico, Universidade de Lisboa Av. Rovisco Pais, 1049-001 Lisboa, Portugal — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, Zhejiang 310058, China

Spin- and charge density waves are a common phenomenon in condensed matter physics. Charge density waves were predicted by R. Peierls who showed that due to the electron-phonon coupling a one-dimensional lattice may become unstable and undergoes a transition into an ordered. Away from thermal equilibrium, much less is known about this transition. In this talk, we address the fate of this instability under non-equilibrium conditions created by imposing a finite voltage across the system. In particular, we explore the possibility of changing the ordering wave vector away from its equilibrium position by a finite voltage drop across the system.

DY 35.6 Wed 11:00 H 3010

Photoinduced absorptions inside the Mott gap in the two-dimensional extended Hubbard model — Kazuya Shinjo and •Takami Tohyama — Department of Applied Physics, Tokyo University of Science, Tokyo 125-8585, Japan

We theoretically investigate pump-probe optical responses in the two-dimensional extended Hubbard model describing cuprates by using a time-dependent Lanczos method. At half filling, pumping generates photoinduced absorptions inside the Mott gap. A part of low-energy absorptions is attributed to the independent propagation of photoinduced holons and doublons. The spectral weight just below the Mott gap increases with decreasing the on-site Coulomb interaction U. We find that the next-nearest-neighbor Coulomb interaction V1 enhances this U dependence, indicating the presence of biexcitonic contributions formed by two holon-doublon pairs. Photopumping in hole-doped systems also induces spectral weights below remnant Mott-gap excitations, being consistent with recent experiments. The induced weights are less sensitive to V1 and may be related to the formation of a biexcitonic state in the presence of hole carriers.

15 min. break.

DY 35.7 Wed 11:30 H 3010

Multiple particle-hole pair creation in the Fermi-Hubbard model — •Friedemann Queisser, Nicolai ten Brinke, Uwe Bovensiepen, and Ralf Schützhold — Fakultät für Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg, Germany

We study the Fermi-Hubbard model in the strongly correlated Mott phase under the influence of a harmonically oscillating hopping rate

$J(t) = J_0 + 4Jcos(\omega t)$. If ω is near an integer multiple of the gap we find higher-order resonances where multiple particle-hole pairs are created. The creation of these pairs depends crucially on the specific form of the underlying lattice geometry. We discuss the microscopic mechanism for multiple pair creation in small lattices.

[1] N. ten Brinke, M. Ligges, U. Bovensiepen and R. Schützhold, *Phys. Rev. B* **95**, 195123 (2017)

DY 35.8 Wed 11:45 H 3010

Nonequilibrium gas-liquid transition in the driven-dissipative photonic lattice — Matteo Biondi[1], Gianni Blatter[1], Hakan Tureci[2], and •Sebastian Schmidt[1] — [1]ETH Zurich, Institute for Theoretical Physics, Switzerland — [2]Princeton University, Department of Electrical Engineering, USA

We study the nonequilibrium steady state of the driven-dissipative Bose-Hubbard model with Kerr nonlinearity. Employing a mean-field decoupling for the intercavity hopping J, we find that the steep crossover between low and high photon-density states inherited from the single cavity transforms into a gas-liquid bistability at large cavity-coupling J. We formulate a van der Waals-like gas-liquid phenomenology for this nonequilibrium setting and determine the relevant phase diagrams, including a new type of diagram where a lobe-shaped boundary separates smooth crossovers from sharp, hysteretic transitions. Calculating quantum trajectories for a one-dimensional system, we provide insights into the microscopic origin of this many-body bistability.

DY 35.9 Wed 12:00 H 3010

Frustration-induced quasi-long-range order in a photonic system — •Matteo Biondi, Gianni Blatter, and Sebastian Schmidt — Institut für Theoretische Physik, Wolfgang-Pauli-Str. 27 8093 Zürich Switzerland

We investigate the interplay of geometric frustration and interactions in a nonequilibrium photonic lattice system exhibiting a photonic flat band as described by the driven-dissipative Bose-Hubbard model. We propose how to engineer quasi-long-range order in a quasi one-dimensional frustrated system by pumping the photonic lattice incoherently. Using a filter qubit to modulate the bandwidth of the pump, we demonstrate how to obtain a quasi-pure density-wave state of photons characterized by a polynomial decay of density-density correlations. We provide analytic results together with finite-size simulations of the Lindblad master equation using exact diagonalization and propose a state-of-the-art photonic realization of our system within cavity QED.

[1] M. Biondi, G. Blatter and S. Schmidt, in preparation.
[2] M. Biondi, E. v. Nieuwenburg, G. Blatter, S. Huber, and S. Schmidt, PRL 115, 143601 (2015).
[3] F. Baboux, L. Ge, T. Jacqmin, M. Biondi, E. Galopin, A. Lemaitre, L. Le Gratiet, I. Sagnes, S. Schmidt, H. E. Türeci, A. Amo and J. Bloch, PRL 116, 066402 (2016).

DY 35.10 Wed 12:15 H 3010

Thermalization of isolated Bose-Einstein condensates by dynamical heat bath generation — •Anna Posazhennikova[1], Mauricio Trujillo-Martinez[2], and Johann Kroha[2] — [1]Royal Holloway University of London, Egham, Surrey, UK — [2]Physikalisches Institut, Universität Bonn, Germany

If and how an isolated quantum system thermalizes despite its unitary time evolution is a long-standing, open problem of many-body physics. The eigenstate thermalization hypothesis (ETH) postulates that thermalization happens at the level of individual eigenstates of a system's Hamiltonian. However, the ETH requires stringent conditions to be validated, and it does not address how the thermal state is reached dynamically from an initial non-equilibrium state. We consider a Bose-Einstein condensate (BEC) trapped in a double-well potential with an initial population imbalance. We find that the system thermalizes although the initial conditions violate the ETH requirements. We identify three dynamical regimes. After an initial regime of undamped Josephson oscillations, the subsystem of incoherent excitations or quasiparticles (QP) becomes strongly coupled to the BEC subsystem by means of a dynamically generated, parametric resonance. When the energy stored in the QP system reaches its maximum, the number of QPs becomes effectively constant, and the system enters a quasi-hydrodynamic regime where the two subsystems are weakly coupled. In this final regime the BEC acts as a grand-canonical heat reservoir for the QP system (and vice versa), resulting in thermalization. We term this mechanism dynamical bath generation (DBG).

DY 35.11 Wed 12:30 H 3010

State engineering and out of equilibrium dynamics of spin models with cold bosonic atoms — •Araceli Venegas-Gomez and Andrew John Daley — University of Strathclyde, Glasgow, UK

The macroscopic control over cold atoms in optical lattices offers an excellent platform to study the out-of-equilibrium behaviour of strongly correlated systems, such as spin models, which are usually motivated by solid state physics. This offers us opportunities to study fundamental properties away from equilibrium and to probe states of the spin models, as well as providing tools to prepare states of lower temperature and entropy. We theoretically investigate a generalised Bose-Hubbard model for two-component bosonic atoms in an optical lattice, exploring the dynamics in corresponding spin-1/2 and spin-1 models. Investigating the magnetically ordered quantum states that can be engineered, we develop adiabatic state preparation techniques to achieve states with very low entropy starting from a known occupation number of particles per site. We explore this process, and ways to use non-equilibrium dynamics to probe the resulting states, using numerical methods based on tensor networks, focussing on parameters accessible in current experiments.

DY 35.12 Wed 12:45 H 3010

Reconstructing quantum states of cold atomic quantum simulators from non-equilibrium dynamics — •Marek Gluza[1], Thomas Schweigler[2], Bernhard Rauer[2], Christian Krumnow[1], Joerg Schmiedmayer[2], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [2]Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, Stadionallee 2, 1020 Vienna, Austria

Systems of ultra-cold atoms on atom chips provide an architecture to probe aspects of out-of-equilibrium quantum many-body physics including equilibration, thermalization and pre-thermalization. We present a novel tomographic reconstruction method for these quantum simulators allowing to access the expectation value of quadrature operators which are inaccessible from direct measurements but capture crucial characteristics of the elementary excitations of cold atomic systems. Specifically, we use interferometric data of non-equilibrium phase fluctuations to reconstruct the covariance matrix – including density fluctuations – of eigenmodes of the corresponding mean-field models. Experimentally, we observe quench dynamics in the non-interacting regime of particles in harmonic or box potentials. Formally, we use that one can efficiently keep track of the evolution and employ signal processing and semi-definite programming to perform a reliable reconstruction of covariance matrices. This method opens a new window into the study of dynamical quantum simulators – an insight that we exploit and discuss at the hand of several examples, including Gaussifying quantum many-body dynamics.

DY 36: Focus: Chaos and Correlation in Quantum Matter (joint session DY/TT)

The irreversibility of dynamics of complex systems ("emergent arrow of time") has been a point of controversy lasting over a century. At its heart lies the seeming contradiction between the intrinsic reversibility of the microscopic laws of nature and the manifestly time-irreversible behavior of macroscopic phenomena. Chaos plays a crucial role in resolving this paradox. The past decade has seen a great revival of interest in this question concerning the foundations of quantum statistical mechanics and how chaos arises in quantum manybody systems. It has been driven by theoretical findings involving the long sought demonstration that many-body localization (MBL) exists as well as the derivation of exact bounds on chaos. On the experimental side, significant advances have been made in the study of cold atomic gases which provide examples of closed macroscopic quantum systems for which the foundational questions of quantum statistical mechanics are especially relevant. The focus session will summarize recent advances in this very active field of studies.

Coordinators: Frank Pollmann, David Luitz

Time: Wednesday 9:30–12:15 Location: EB 107

Invited Talk DY 36.1 Wed 9:30 EB 107

Computing quantum thermalization dynamics: from quantum chaos to emergent hydrodynamics — •Ehud Altman — Department of Physics, University of California, Berkeley, CA 94720

Computing the dynamics of strongly interacting quantum systems presents a fundamental challenge due to the growth of entanglement entropy in time. In the first part of the talk I will describe a new approach that overcomes this obstruction and captures chaotic dynamics and emergent hydrodynamic transport of quantum systems. Our scheme utilizes the time dependent variational principle with matrix product states to truncate "non-useful" entanglement, while retaining crucial information on local observables. In the second part of the talk I will offer a new viewpoint on the relation between quantum and classical chaos in many body systems, using a classical version of the Sachdev-Ye-Kitaev model as an example. Chaos in this model can be understood as arising from diverging geodesics on a SO(N) manifold equipped with a random metric with locally negative curvature. The quantum bound on chaos arises from a *chaotic mobility edge* in the classical Lyapunov spectrum, separating the lower part of the spectrum for which a classical chaos picture applies from the higher part of the spectrum for which quantum interference effects are strong enough to kill classical chaos. This edge corresponds to a curvature scale of the order of the de Broglie wavelength.

DY 36.2 Wed 10:00 EB 107

Hydrodynamics of operator spreading from random circuits — •Tibor Rakovszky[1], Curt von Keyserlingk[2], Shivaji Sondhi[3], and Frank Pollmann[1] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]University of Birmingham, School of Physics & Astronomy, B15 2TT, UK — [3]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

In this talk we use random local unitary circuits to gain insight into the scrambling of quantum information in many-body systems. For a circuit with no conserved quantities we show that the average spreading of operators obeys an exact "hydrodynamic" description, in terms of a biased diffusion equation, and discuss the consequences for out-of-time ordered correlators (OTOCs) and entanglement growth. We conjecture that a similar effective description should hold in more generic ergodic systems, a claim supported by numerical results. Furthermore, we consider random circuits with a U(1) symmetry and discuss the interplay between the hydrodynamics of the conserved charge and that of operator spreading, leading to the appearance of long-time power law tails in out-of-time-ordered correlators. We also discuss the behavior of OTOCs at different chemical potentials, an analogous quantity to the finite temperature OTOCs discussed in the literature, and find that their initial spreading is slowed down when the chemical potential is large.

DY 36.3 Wed 10:15 EB 107

Out-Of-Time-Ordered Correlators in Chaotic and Critical Many-Body Systems: Path Interference and Scrambling Times — •Josef Rammensee, Benjamin Geiger, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

Out-of-time-ordered correlators $\langle[\hat{V},\hat{W}(t)]^\dagger[\hat{V},\hat{W}(t)]\rangle$ have been identified to be highly suitable tools to identify the onset of chaos in many-body quantum systems[1]. Contrary to already known indicators, the unusual time ordering of the operators is able to directly capture the local hyperbolic nature of the classical counterpart. One expects an exponential increase at short times with a rate related to classical Lyapunov exponents. Numerical studies in chaotic systems[2] indicate a saturation after the time scale for the classical-to-quantum-crossover, known as Ehrenfest or scrambling time. Our numerical studies show, that many-body criticality mimics this behaviour of chaotic systems, however with an exponent given by the local instability rate. We provide insight into the physical origin of the exponential growth and the saturation by using semiclassical methods based on the Van-Vleck-propagator for single- and many-body systems[3]. We show that the notion of interfering classical trajectories is well suited to provide a quantitative picture and we explicitly discuss the emergence of the Lyapunov exponent, resp. instability rates and the relevant time scales.
[1] J. Maldacena *et al.*, JHEP 2016:106 (2016)
[2] E. B. Rozenbaum *et al.*, PRL **118**, 086801 (2017)
[3] T. Engl, J. Dujardin, A. Argüelles *et al.*, PRL **112**, 140403 (2014)

DY 36.4 Wed 10:30 EB 107

Out of time order correlators from the time dependent variational principle — •Kevin Hemery, Frank Pollmann, and David Luitz — Department of Physics, T42, Technische Universität Muenchen, James-Franck-Strasse 1, D-85748 Garching, Germany

Out of time order correlators (OTOCs), which measure the spreading of information in quantum systems, have drawn a lot of attention recently. However, the numerical calculation of OTOCs is extremely challenging, which renders the verification of theoretical predictions difficult. We tackle this problem within the Schroedinger picture in combination with a matrix-product state formulation of the time dependent variational principle (TDVP). First, we benchmark this technique by comparing the results with exact Krylov space time evolution results for small chains. Second, we calculate the OTOCs for system sizes which are unreachable by exact methods and analyze the hydrodynamic spreading of the light cone front.

DY 36.5 Wed 10:45 EB 107

Out-of-time-ordered correlation functions in the O(N) model — •Alexander Schuckert[1] and Michael Knap[1,2] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Institute for Advanced Study, Technical University of Munich, 85748 Garching, Germany

In classical systems, chaos can be characterized by the sensitivity of the particles' trajectories with respect to small deviations in the initial state. An exponential growth in time then marks chaotic behavior. Recently, it has been proposed that certain out-of-time-ordered correlation functions (OTOCs) may be a suitable extension to characterize chaos in quantum many-body systems. OTOCs also probe the scrambling of quantum information across the system and thereby provide a direct connection between an information theoretic measure and chaotic dynamics. We calculate the time evolution of OTOCs in an O(N) symmetric scalar field theory at high temperatures using non-perturbative expansion techniques. Apart from the Lyapunov exponent quantifying a potential exponential growth of chaos, we are also interested in the emergent time scales of information propagation,

including light-cone and butterfly velocities.

15 min. break

Invited Talk DY 36.6 Wed 11:15 EB 107

Quantum Thermalization Dynamics: From Information Scrambling to Emergent Hydrodynamics — •Michael Knap — Department of Physics and Institute for Advanced Study, Technical University of Munich, 85748 Garching, Germany

Generic, clean quantum many-body systems approach a thermal equilibrium after a long time evolution. In order to reach a global equilibrium, conserved quantities have to be transported across the whole system which is a rather slow process governed by diffusion. By contrast, the scrambling of quantum information is ballistic and hence can be characterized by a "butterfly" velocity. One way of describing the propagation of quantum information is to study out-of-time ordered (OTO) correlation functions, which are unconventional correlation functions with time arguments that are not time ordered. Using matrix-product-state based numerical simulations, we compute such correlators at high temperatures in a one-dimensional Bose-Hubbard model and in generic spin-models, where well defined quasi-particles cease to exist [1]. Finally, we will discuss ways of experimentally characterizing these unconventional OTO correlation functions in synthetic quantum matter.

[1] A. Bohrdt, C. B. Mendl, M. Endres, M. Knap, New J. Phys. 19, 063001 (2017).

DY 36.7 Wed 11:45 EB 107

Entanglement Entropy in SYK — •Renato Miguel Alves Dantas[1], Daniele Trapin[1], Paul McClarty[1], Piotr Surówka[1], and Masudul Haque[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Str. 38, 01187 Dresden — [2]Department of Theoretical Physics, Maynooth University, Co. Kildare, Ireland

Eigenstates of interacting systems far from the ground state are now recognized as important for understanding non-equilibrium phenomena. We present a study of the entanglement in eigenstates of zero-dimensional fermionic models with random interactions. We consider both chaotic and integrable versions of these Sachdev-Ye-Kitaev models, respectively having quartic and quadratic couplings.

DY 36.8 Wed 12:00 EB 107

What is the right theory of transverse Anderson localization of light? — •Walter Schirmacher[1,3,4], Behnam Abaie[2], Arash Mafi[2], Giancarlo Ruocco[3,4], and Marco Leonetti[3,4] — [1]Universität Mainz — [2]Univ. New Mexico, USA — [3]Istituto Italiano di Technologia, Roma, Italy — [4]Universit'a La Sapienza, Roma, Italy

Anderson localization of light is traditionally described in analogy to electrons in a random potential. Within this description, the random potential depends on the wavelength of the incident light. For transverse Anderson localization this leads to the prediction that the distribution of localization lengths – and hence its average – strongly depends on the wavelength. In an alternative description, in terms of a spatially fluctuating electric modulus, this is not the case. Here, we report on an experimentum crucis in order to investigate the validity of the two conflicting theories using optical samples exhibiting transverse Anderson localization. We do not find any dependence of the observed average localization radii on the light wavelength. We conclude that the modulus-type description is the correct one and not the potential-type one. We corroborate this by showing that in the derivation of the traditional, potential-type theory a term in the wave equation has been tacitly neglected. In our new modulus-type theory the wave equation is exact. We check the consistency of the new theory with our data using the nonlinear sigma model. We comment on the consequences for the general case of three-dimensional disorder.

DY 37: Networks: From Topology to Dynamics (joint session SOE/DY/BP) (joint session SOE/CPP/BP/DY)

Time: Wednesday 9:30–12:15 Location: MA 001

DY 37.1 Wed 9:30 MA 001

Dynamics of interacting tipping elements on complex networks — •Jonathan F. Donges[1,2], Ann-Kristin Klose[1], and Ricarda Winkelmann[1] — [1]Earth System Analysis, Potsdam Institute for Climate Impact Research, Potsdam, Germany — [2]Stockholm Resilience Centre, Stockholm University, Stockholm, Sweden

In recent years, an increasing number of potential tipping elements have been identified in ecological, climatic and social systems. Tipping elements are defined by their ability to undergo large qualitative change that is caused by a small perturbation in a parameter or state variable. We investigate the emergent nonlinear dynamics of pairs, chains and networks of generalized tipping elements. Understanding the dynamics of systems of interacting tipping elements on complex networks is relevant for assessing the resilience and transformative capacity of complex systems such as the Earth's climate system and the World's energy system in the context of decarbonization transformation for meeting the Paris climate agreement.

DY 37.2 Wed 9:45 MA 001

The interdependent network of gene regulation and metabolism is robust where it needs to be — •Marc Hütt[1], David Klosik[2], Anne Grimbs[1], and Stefan Bornholdt[2] — [1]Jacobs University, Bremen, Germany — [2]Institute for Theoretical Physics, University of Bremen, Bremen, Germany

Despite being highly interdependent, the major biochemical networks of the living cell – the networks of interacting genes and of metabolic reactions, respectively – have been approached mostly as separate systems so far. Recently, a framework for interdependent networks has emerged in the context of statistical physics. In a first quantitative application of this framework to systems biology, here we study the interdependent network of gene regulation and metabolism for the model organism *Escherichia coli* in terms of a biologically motivated percolation model [1]. Particularly, we approach the system's conflicting tasks of reacting rapidly to (internal and external) perturbations, while being robust to minor environmental fluctuations. Considering its response to perturbations that are localized with respect to functional criteria, we find the interdependent system to be sensitive to gene regulatory and protein-level perturbations, yet robust against metabolic changes. We expect this approach to be applicable to a range of other interdependent networks.

[1] Klosik, D. F., Grimbs, A., Bornholdt, S., and Hütt, M.-T. (2017). Nature Communications, 8(1):534.

DY 37.3 Wed 10:00 MA 001

Robust connectivity in networks with groups of vulnerable nodes — •Sebastian M. Krause[1,2], Michael M. Danziger[3], and Vinko Zlatić[2] — [1]Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — [2]Theoretical Physics Division, Rudjer Bošković Institute, Bijenicka c. 54, 10000 Zagreb, Croatia — [3]Department of Physics, Bar-Ilan University, Ramat Gan 5290002, Israel

In many networked systems there are large groups of similar nodes which are vulnerable to the same failure or adversary. For example, servers in a communication network running the same software will fail together, if this software has a bug. Therefore, we are often faced with networks where all nodes of a group can fail together. Further, many different vulnerabilities can cover the whole network. This structural weakness has so far been overlooked in studies of network robustness. Here we discuss, how multiple redundant paths enable a high level of robustness, even if no node is trusted [1,2]. With each vulnerability described as a color, we discuss "color-avoiding percolation". We present a fast numerical algorithm for real world networks and analytical results for random network ensembles.

[1] Sebastian M. Krause, Michael M. Danziger, and Vinko Zlatić, Hidden Connectivity in Networks with Vulnerable Classes of Nodes, Phys. Rev. X 6, 041022 (2016).

[2] S. M. Krause, M. M. Danziger, and V. Zlatić, Color-avoiding percolation, Phys. Rev. E 96 022313 (2017).

DY 37.4 Wed 10:15 MA 001

When is a network a network? Multi-order graphical model selection in time series data on networks — •Ingo Scholtes —

Chair of Systems Design, ETH Zürich, Zürich, Switzerland

We introduce a novel framework for the modeling of time series data on networks. Such data are important, e.g., when studying click streams of users in the Web, travel patterns of passengers in transportation systems, information cascades in social networks, biological pathways, or time-stamped social interactions. While it is common to apply graph analytics and network analysis to such data, recent works have shown that temporal correlations can invalidate the results of such methods. This raises a fundamental question: When is a network abstraction of time series data justified?

Addressing this open question, we propose a framework that combines Markov chains of multiple, higher orders into a multi-layer network model that captures temporal correlations at multiple length scales simultaneously. We develop a model selection technique to infer the optimal number of layers of such a model and show that our method outperforms baseline Markov order detection techniques.

An application to eight real-world data sets capturing causal paths in time series data on networks shows that the inferred models provide an optimal summarization of the causal topologies of real-world complex systems. Our work highlights fallacies of network-based modelling techniques and provides a principled answer to the open question when they are justified. Generalizing networks to optimal multi-order models, it opens perspectives for the study of complex systems.

DY 37.5 Wed 10:30 MA 001

Exact expected cluster sizes for bond percolation in finite networks — Joan Pont Serra and •Konstantin Klemm — IFISC (CSIC-UIB), Mallorca, Spain

Bond percolation describes the statistical ensemble generated by randomly deleting edges from a given network. Traditionally studied on grids (lattices), bond percolation forms a crucial part of modern network theory with implications for epidemic spreading and network robustness under failures. For quenched systems of size well above 20 nodes, the computation of percolation quantities relies on heuristics (e.g. by the graph spectrum) or Monte Carlo sampling. Here we introduce an exact computational method that is time-efficient when the network has certain separation properties. Specifically, we work with a branch decomposition of low width. Then the network is recursively separable by removing a small number of nodes in each step. For several test networks, we present exact results for the first time. We find that the computational cost of our exact method is lower than that of Monte Carlo runs required to reach an acceptable precision.

DY 37.6 Wed 10:45 MA 001

Controlling percolation with limited resources — •Malte Schröder[1], Nuno Araújo[2], Didier Sornette[3], and Jan Nagler[3] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Universidade de Lisboa, Lisboa, Portugal — [3]ETH Zürich, Zurich, Switzerland

Connectivity - or the lack thereof - is crucial for the proper functioning of many essential socio-economic processes, from financial and economic networks over epidemic spreading in social networks to technical infrastructure. Often, connections are deliberately established or removed by various parties to induce, maintain, or destroy global connectivity. Thus, there has been a great interest in understanding how to control percolation, the transition to large-scale connectivity. Previous work studied control strategies implicitly assuming unlimited resources, leading to a large number of models of "explosive" and discontinuous percolation. Realistically, however, such control is often subject to a limited budget. We derive an efficient control strategy to delay percolation under the constraint of limited resources and study its implications. We show that the transition can be significantly delayed even with scarce resources but remains smooth and in the same universality class as random percolation. In particular, the transition never becomes "explosive". We derive an approximation for the optimal control parameters and show how resource optimal delay of percolation leads to a sudden, discontinuous transition. Thus, the percolation transition becomes effectively uncontrollable as an unintended consequence of optimal control.

DY 37.7 Wed 11:00 MA 001

Discrete reaction-diffusion models of innovations using multi-particles in networks. — •Yuki Kawasaki and Hirotada Ohashi — The University of Tokyo, Tokyo, Japan

Reaction-diffusion is a fundamental process underlying many social and economic phenomena. This process has been widely studied in continuous physical space. Different from physical and chemical phenomena, social and economic processes occur in networks connecting individuals, firms and organizations. In this study, we model reaction-diffusion processes of innovations in structured networks employing multi-particles that represent innovations and some kind of enzymes. The reaction process is that several particles react on nodes according to reaction rules and the diffusion process is that particles travel randomly to neighboring nodes. This model is able to reproduce macroscopic behaviors of systems taking account of microscopic relationships between individual particles. Simulation results are obtained for various network structures including small-world and scale-free networks. Next we extend our model to deal with simultaneous reaction and diffusion of different kinds of particles. This model can describe competition and cooperation between innovations in networks including predator-prey processes.

DY 37.8 Wed 11:15 MA 001

Probabilistic Quantifiers for Deterministic Spreading — •Justine Wolter[1,2], Benedict Lünsmann[3], Xiaozhu Zhang[1,2], Malte Schröder[1,2], and Marc Timme[1,2,3] — [1]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden, Dresden, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — [3]Max Planck Institute for the Physics of Complex Systems, 01069 Dresden

How do signals spread across dynamical systems? Spreading may be stochastic, e.g., during epidemic outbreaks or deterministic, e.g., in electrical or other supply networks. Due to mathematical challenges, it remains unknown how to robustly quantify even simple characteristics such as peak times or amplitudes of a spreading signal propagating across a network. Here we change the perspective and propose to analyze deterministic spreading dynamics employing concepts of probability theory. We characterize generic spreading dynamics by expectation values to work out a theory explicitly quantifying when and how strongly a perturbation initiated at one unit of a network impacts any other [1]. The theory provides this information as a function of the relative position of initially perturbed and responding unit as well as on the entire network topology. Furthermore, asymptotically exact approximation schemes enable to well predict previously inaccessible peak times and amplitudes. These insights may open up a new realm of quantifying characteristics of deterministic processes through probability theory. Ref.: [1] J. Wolter et al., http://arXiv.org/abs/1710.09687

DY 37.9 Wed 11:30 MA 001

Perturbation spreading on diffusively-coupled networks and power grids — •Xiaozhu Zhang[1,2], Dirk Witthaut[3], and Marc Timme[1,2] — [1]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden, Dresden, Germany — [2]Network Dynamics, Max Planck Institute for Dynamics and Self-organization, 37077 Göttingen — [3]Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Spreading phenomena on networks essentially underlie the collective dynamics of systems across physics, biology and engineering. Yet, how local changes dynamically spread in such networked systems is still far from fully understood. Here we analyze the spreading dynamics for diffusively-coupled networks close to given operating points. We provide analytical solutions of transient nodal responses via linear response theory and approximate the perturbation arrival times via Taylor expansion. In homogeneous networks, we find the spreading speed based on the estimated arrival times decreases and converges to a constant at large distance. Intriguingly, the asymptotic spreading speed is essentially determined by the network topology, i.e. the limiting behavior of the number of shortest paths at large distance. These results shed light on the qualitatively universal asymptotic spreading behavior in networks and its quantitative dependence on the underlying network topology.

DY 37.10 Wed 11:45 MA 001

Temporal networks with geometric constraints and protein folding — •Nora Molkenthin[1], Marc Timme[2,1], and Steffen Mühle[3] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — [2]Chair for Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute for Theoretical Physics, TU Dresden, 01062 Dresden — [3]Physics Department III, University of Göttingen, D-37077 Göttingen, Ger-

many

The structure of many complex networks is highly constrained by geometric factors, affecting a broad range of systems from polymer aggregates to traffic and supply networks. On the microscopic scale, folding proteins constitute paradigmatic systems for spatial network formation. They are well characterized as Protein Residue Networks (PRN) yet their statistical properties seem to be diverse and general rules are largely unknown. Here, advancing a recent graph-theoretical mapping [1], we develop a temporal network model for the aggregation of connected, spatially extended units, thereby reproducing key features of PRN*s. In stark contrast to network models without geometric constraints, we observe algebraic scaling of the network diameter with system size and predict the characteristic link length distribution, both features fitting with those experimentally observed in PRN*s.

[1] Molkenthin & Timme, Scaling Laws in Spatial Network Formation, Phys. Rev. Lett. 117:168301 (2016)

DY 37.11 Wed 12:00 MA 001

Non-inertial reference frames for inferring networks from dynamics — •Jose Casadiego[1,2] and Marc Timme[1,2] — [1]Chair for Network Dynamics, Institute of Theoretical Physics and cfaed - Center for Advancing Electronics Dresden, Technical University of Dresden, Dresden, Germany — [2]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization (MPIDS), Goettingen, Germany

The dynamics of complex networks are determined to a great extent by the connectivity of their units. Given that measuring the connectivity by direct methods is often infeasible, researchers typically apply inverse approaches to infer links between units from the collective dynamics. Current state-of-the-art methods rely on either (i) quantifying functional links through statistical dependencies, or (ii) approximating the possibly nonlinear interactions between units via modeling of differential equations. Yet, functional links frequently do not match physical links, and finding an appropriate model may be computationally demanding and also require a prior knowledge about the interactions. Here we develop a model-independent theory to reconstruct the connectivity of networks from transients states to stable dynamics. Specifically, we demonstrate that representing these transients with respect to non-inertial reference frames provides simple linear mappings between network connectivity and dynamics. Furthermore, we show the robustness of our framework by reconstructing the full connectivity of different network dynamical systems exhibiting phase-locking, periodic orbits and collective synchronization.

DY 38: Modeling and Simulation of Soft Matter II (joint session CPP/DY)

Time: Wednesday 9:30–12:00 Location: C 230

Invited Talk DY 38.1 Wed 9:30 C 230

The favorite polymer libations — •Carlos M. Marques[1], Debashish Mukherji[2], and Kurt Kremer[2] — [1]Institut Charles Sadron, UdS-CNRS, Strasbourg, France — [2]Max-Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz Germany

Macromolecular solubility in solvent mixtures often strikes as a paradoxical phenomenon. In a system where all particle interactions are repulsive, chains can nevertheless collapse. And when attractive interactions settle in, they might collapse or swell the chain. We will review in this contribution how the puzzling behavior of polymers in aqueous alcohol solutions triggered a better understanding of the interplay between solvent composition and polymer conformation. And how the resulting view on polymer collapse and swelling takes us well beyond mean-field descriptions ... and alcohol.

[1] Mukherji, D., Marques, C. M., Kremer, K. (2014). Polymer collapse in miscible good solvents is a generic phenomenon driven by preferential adsorption. Nature communications, 5882, 5.

[2] Mukherji, D., Marques, C. M., Stuehn, T., Kremer, K. (2015). Co-non-solvency: Mean-field polymer theory does not describe polymer collapse transition in a mixture of two competing good solvents. The Journal of chemical physics, 142(11), 114903.

[3] Mukherji, D., Wagner, M., Watson, M. D., Winzen, S., de Oliveira, T. E., Marques, C. M., & Kremer, K. (2016). Relating side chain organization of PNIPAm with its conformation in aqueous methanol. Soft Matter, 12(38), 7995.

[4] Mukherji, D., Marques, C. M., Stuehn, T., Kremer, K. (2017). Depleted depletion drives polymer swelling in poor solvent mixtures. Nature communications, 1374, 8.

[5] Mukherji, D., Marques, C. M., Kremer, K. (2017). Collapse in two good solvents, swelling in two poor solvents: defying the laws of polymer solubility? Journal of condensed matter, 024002, 30.

DY 38.2 Wed 10:00 C 230

Studying Polymer-induced Depletion Effects via Grid-based Simulations — •Qiyun Tang and Marcus Müller — Universität Göttingen, Institute für Theoretische Physik, Friedrich-Hund- Platz 1, 37077 Göttingen, Germany

Recently we found that our modified grid-based coarse-grained simulations could be employed to study the polymer induced depletion effects between nanoparticles in the nanoparticle/protein limit. By analysing the radial distribution function of nanoparticles from simulations, we systematically study the influence of polymer density and also the nanoparticle density on these depletion effects. Results show that in the semidilute region of polymer solution, the contact depletion potential is gradually reduced by increasing nanoparticle's concentration. Similar behavior is also observed in the polymer melt. The simulation results are also compared to the theories, and are consistent with the theoretical prediction in the dilute polymer solutions.

DY 38.3 Wed 10:15 C 230

Process-directed assembly of copolymer materials — •Marcus Müller — Georg-August-Universität Göttingen, Institut für Theoretische Physik, Göttingen, Germany

Process-directed self-assembly of block copolymers refers to rapid thermodynamic processes that reproducibly direct the kinetics of structure formation from a starting, unstable state into a selected, metastable mesostructure. We investigate the kinetics of self-assembly of linear block copolymers after different rapid changes of thermodynamic control parameters (e.g., photochemical transformations, stretching or mechanical deformation, or pressure changes). These thermodynamic processes convert an initial, equilibrium mesophase of the copolymer material into a well-defined but unstable, starting state. The spontaneous structure formation that ensues from this unstable state becomes trapped in a metastable mesostructure, and we systematically explore, which metastable mesostructures can be fabricated by varying the physical properties of the copolymers in the starting and final state and a step-shear deformation. In addition to the equilibrium mesophases of linear AB diblock copolymers, this diagram of process-accessible states includes multiple, novel, metastable periodic mesostructures; inter alia, Schoen's F-RD periodic minimal surface. Strategies and challenges for studying process-directed self- assembly by particle-based simulations and self-consistent field theory are discussed and the role of non-equilibrium chain conformations and the diffusive dynamics is highlighted.

DY 38.4 Wed 10:30 C 230

Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning — •Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Classical intermolecular potentials typically require an extensive parametrization procedure for any new compound considered. To do away with prior parametrization, we propose a combination of physics-based potentials with machine learning (ML), which is transferable across small neutral organic and biologically-relevant molecules. ML models provide on-the-fly predictions for environment-dependent local atomic properties across conformations and chemical compositions of H, C, N, and O atoms. These parameters enable accurate calculations of intermolecular contributions. Unlike other potentials, this model is transferable in its ability to handle new molecules and conformations without explicit prior parametrization: All local atomic properties are predicted from ML, leaving only eight global parameters—optimized once and for all across compounds. We validate IPML on various gas-phase dimers at and away from equilibrium separation, where we obtain mean absolute errors between 0.4 and 0.7 kcal/mol for several chemically and conformationally diverse datasets representative of non-covalent interactions in biologically-relevant molecules. We fur-

ther focus on hydrogen-bond complexes—essential but challenging due to their directional nature—where datasets of DNA base pairs and amino acids yield an extremely encouraging 1.4 kcal/mol error.

15 min. break

DY 38.5 Wed 11:00 C 230

Investigating structural and thermodynamic representability for coarse-grained models of ionic liquids — •Svenja Wörner[1], Joseph Rudzinski[1], Tamisra Pal[2], Michael Vogel[2], Kurt Kremer[1], and Tristan Bereau[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany. — [2]Technische Universität Darmstadt, Darmstadt, Germany.

Coarse-grained models are usually parameterized to reproduce either structure or thermodynamic properties. The coarse-grained model for the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate developed by Bhargava et al was parameterized to reproduce density and surface tension and therefore lacks detailed structural accuracy. In this work, we investigate to what extent the structural accuracy of this model can be improved while retaining the original thermodynamic target properties. We employ the generalized Yvon-Born-Green framework, which utilizes an integral equation theory that systematically connects the coarse-grained model parameters to the pair correlation functions. This methodology is not only useful for parameterizing new force fields , but can also be used to systematically perturb parts of potentials or to incorporate information from other state points to refine an existing force field. We demonstrate that perturbing only the hard core of the potential of the non-bonded interactions for ionic liquid model significantly improves the structure while retaining thermodynamic information included in the original model. Adding information from multiple temperatures may further improve representablility.

DY 38.6 Wed 11:15 C 230

Mapping onto ideal chains profoundly overestimates self-entanglements in polymer melts — •Hendrik Meyer[1], Eric Horwath[2], and Peter Virnau[2] — [1]Institut Charles Sadron, CNRS and Université de Strasbourg — [2]Institut f. Physik, Universität Mainz

In polymer physics it is typically assumed that excluded volume interactions are effectively screened in polymer melts. Hence, chains could be described by an effective random walk. In this letter, we show that this mapping is problematic by analyzing the occurrence of knots, their spectrum and sizes in polymer melts, corresponding random walks and chains in dilute solution. The effective random walk severely overrates the occurrence of knots and their complexity, particularly when compared to melts of flexible chains, indicating that non-trivial effects due to remnants of self-avoidance still play a significant role for the chain lengths considered in this numerical study. For melts of semiflexible chains, the effect is less pronounced. In addition, we find that chains in a melt are very similar in structure and topology to dilute single chains close to the collapse transition, which indicates that the latter are also not well-represented by random walks. We finally show that typical equilibration procedures are well-suited to relax the topology in melts. [1] arXiv:1710.11077

DY 38.7 Wed 11:30 C 230

Collective dynamics in liquid water: Molecular dynamics simulations — •Ari Paavo Seitsonen[1] and Taras Bryk[2] — [1]Département de Chimie, Ecole Normale Supérieure, Paris — [2]Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv

Water, as the most important substance for life, has always attracted the researchers to explore and explain its numerous anomalous properties. Collective dynamics in simple and molecular liquids is so far well understood only on macroscopic length and time scales. Experiments on Brillouin scattering of light on liquids can be described by the hydrodynamic theory, which explains the main relaxation and propagation processes contributing to the scattered intensity of light. Atomistic molecular dynamics simulations is an efficient tool in exploration of the dynamic properties, providing precious information on time-dependent correlations in liquids on nano- and atomic-scale resolution.

Here we report molecular dynamics simulations using density functional theory (DFT), in particular the BLYP approximation to the exchange-correlation term with the augmented D3 empirical term to account for the London dispersion interactions missing in the BLYP. We present results on the collective dynamics [1], and the recently evaluated [2] melting temperature of water using this approach.
[1] Taras Bryk & Ari P Seitsonen Condensed Matter Physics 19 (2016) 23604; DOI: 10.5488/CMP.19.23604
[2] Ari P Seitsonen & Taras Bryk Physical Review B 94 (2016) 184111; DOI: 10.1103/PhysRevB.94.184111

DY 38.8 Wed 11:45 C 230

Molecular Origin of Urea-driven Hydrophobic Collapse of Polyacrylamides — •Divya Nayar, Angelina Folberth, and Nico van der Vegt — Technische Universität Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany

Osmolytes modulate protein folding and affect the water solubility of macromolecules [1]. The osmolyte-induced hydrophobic polymer collapse due to osmolyte depletion from the solvation shell is well-known, however, evidences have indicated direct preferential osmolyte binding that may lead to polymer collapse [2]. To understand the underlying molecular mechanisms better, we examine the role of urea in strengthening and attenuating the hydrophobic collapse of thermo-responsive polyacrylamides i.e. Poly-N-isopropylacrylamide (PNIPAM, secondary amide) and Poly-N,N,-diethylacrylamide (PDEA, tertiary amide) respectively [3]. Using extensive molecular dynamics simulations and large-scale polymer conformational sampling, we show that urea collapses PNIPAM by "preferentially binding" to it. We propose an osmolyte stabilizing mechanism driving PNIPAM collapse, based on the balance in opposing loss of entropic degrees of freedom of urea and water [4]. The study provides new physical insights into the interplay between polymer side-chain chemistry, solvent entropic degrees of freedom and polymer-solvent interactions to understand the osmolyte effects on hydrophobic collapse. [1] D. R. Canchi et al. Annu. Rev. Phys. Chem., 2013, 64, 273. [2] N. F. A. van der Vegt et al. J. Phys. Chem. B 2017, 121, 9986. [3] J. Wang et al. Macromolecules, 2016, 49, 234. [4] D. Nayar et al. Phys. Chem. Chem. Phys. 2017, 19, 18156.

DY 39: Wetting, Microfluidics and Confined Liquids I (joint session CPP/DY)

Time: Wednesday 9:30–13:00 Location: C 264

Invited Talk DY 39.1 Wed 9:30 C 264

Slippage over superhydrophobic surfaces: fundamentals and local phenomena — •Clarissa Schönecker[1,2], David Schäffel[2], Kaloian Koynov[2], Doris Vollmer[2], and Hans-Jürgen Butt[2] — [1]Lehrstuhl für Mikrofluidmechanik, TU Kaiserslautern — [2]Max-Planck-Institut für Polymerforschung, Mainz

Superhydrophobic surfaces can provide a significant slip to a fluid flowing over the surface, making them attractive for the development of functional coatings. Although the global behaviour of flow past such surfaces has been widely investigated, understanding the local fundamentals that lead to slippage is still lacking. We studied in detail the local slip length and local flow field for water in the Cassie state on a structured superhydrophobic surface. Using fluorescence correlation spectroscopy, we revealed that the local slip length of a superhydrophobic surface is finite, non-constant and anisotropic. Furthermore, it can be strongly influenced by the presence of surface active substances. All these properties are in accordance with and can be explained by a theoretical model of the local hydrodynamics close to the surface. The study shows the effect of surface properties, like the surface geometry or interfacial forces.

DY 39.2 Wed 10:00 C 264

How drops start sliding over solid surfaces — Doris Vollmer[1], Nan Gao[1,2], Florian Geyer[1], Dominik Pilat[1], Sanghyuk Wooh[1], Hans-Jürgen Butt[1], and •Rüdiger Berger[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Fudan University, 220 Handan Road, Shanghai 200433, People's Republic of China

We report that the lateral adhesion force between a liquid drop and a solid can be divided into a static and a kinetic regime. This striking analogy with solid-solid friction is a generic phenomenon that holds for liquids [1]. We have investigated the lateral adhesion forces of liquids of different polarities and surface tensions on smooth, rough and structured surfaces. The lateral adhesion forces were measured with a home build instrument [2] and calculated by the occurring changes of the rear and the front of the drop, its changes in drop widths and the liquid-air surface tension. Our studies indicate that the lateral adhesion force is dominated by contact line friction and interfacial friction only plays a minor role. Finally, the lateral adhesion force measurements can provide quantitative information on the homogeneity or cleanliness of surfaces.

References:

[1] N. Gao, F. Geyer, D.W. Pilat, S. Wooh, D. Vollmer, H.-J. Butt, R. Berger, Nature Physics (2017), doi: 10.1038/NPHYS4305

[2] D. W. Pilat, P. Papadopoulos, D. Schäffel, D. Vollmer, R. Berger, H.-J. Butt, Langmuir 28, 16812-16820(2012), doi 10.1021/la3041067

DY 39.3 Wed 10:15 C 264

Beyond the Navier-de Gennes Paradigm: Slip Inhibition on Ideal Substrates — Mark Ilton[1,2], Thomas Salez[3,4], Paul Fowler[1,5], Marco Rivetti[5], Mohammed Aly[6], Michael Benzaquen[4,7], Joshua McGraw[1,6], Elie Raphael[4], Kari Dalnoki-Veress[1], and •Oliver Bäumchen[5] — [1]McMaster University, Hamilton, Canada — [2]University of Massachusetts, Amherst, MA, USA — [3]Univ. Bordeaux, Talence, France — [4]ESPCI Paris, Paris, France — [5]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [6]Ecole Normale Supérieure, Paris, France — [7]Ecole Polytechnique, Palaiseau Cedex, France

Hydrodynamic slip of a liquid at a solid surface governs liquid transport at small scales. For polymeric liquids, de Gennes predicted that the Navier boundary condition together with the theory of polymer dynamics imply extraordinarily large slip for entangled polymer melts on ideal surfaces; this Navier-de Gennes paradigm was confirmed using dewetting experiments on ultra-smooth, low-energy substrates. Here, we use capillary leveling of polymeric films on these same substrates to measure the slip length from a robust one-parameter fit to a lubrication model. We show that at the low shear rates involved in leveling experiments, the employed substrates can no longer be considered ideal. The data is instead consistent with physical adsorption of polymer chains at the solid/liquid interface. We extend the Navier-de Gennes description using one additional parameter, namely the density of physically adsorbed chains per unit surface. The resulting model is found to be in excellent agreement with the experimental observations.

DY 39.4 Wed 10:30 C 264

Consistency condition for macro- and mesoscopic descriptions of contact line with surfactant — •Uwe Thiele[1], Sarah Trinschek[1], Jacco H. Snoeijer[2], and Karin John[3] — [1]Institut für Theoretische Physik, Universität Münster, Wilhelm-Klemm-Str. 9, Münster — [2]Physics of Fluids Group, Faculty of Science and Technology, University of Twente, Enschede — [3]Laboratoire Interdisciplinaire de Physique, Université Grenoble-Alpes, CNRS

Consider a three-phase contact line where a liquid-gas interface meets a solid. For a simple liquid at equilibrium it is described on the macroscale by the Young-Dupré law relating the three interfacial energies to the equilibrium contact angle θ_e. On the mesoscale, it is modelled by a film-height-dependent wetting energy $f(h)$. Macro- and mesoscale description are consistent if $\gamma \cos\theta_e = \gamma + f(h_a)$ where γ and h_a are the liquid-gas interface energy and the thickness of the equilibrium adsorption layer, respectively.

Our contribution discusses the incorporation of insoluble surfactant. We derive the macro- and mesoscopic equilibrium models for spatially inhomogeneous states (consistent with the dynamic approach of [1,2]). Discussing the case of a static contact line with surfactant, we show that again there exists a consistency condition between macro- and mesoscopic descriptions. It imposes a particular dependence of the wetting energy on surfactant concentration. This is illustrated at a simple example. [1] U. Thiele, A. J. Archer and M. Plapp, *Phys. Fluids* **24**, 102107 (2012). [2] U. Thiele, A. J. Archer and L. M. Pismen, *Phys. Rev. Fluids* **1**, 083903 (2016).

15 min. break

DY 39.5 Wed 11:00 C 264

What determines the lateral adhesion force? — •Doris Vollmer, Nan Gao, Sanghyuk Wooh, Rüdiger Berger, and Hans-Jürgen Butt — MPI für Polymerforschung, Mainz

The mobility of drops on surfaces depends on the interactions between the drop, the surface and its surrounding medium. The strength of the interactions is reflected in the lateral adhesion force, FLA. We have investigated the lateral adhesion forces of droplets of water on a superhydrophobic periodic structure made of TiO2 pillars or varying distance, using a laser deflection system. The force per pillar across the effective contact width did not change with the spacing ratio. Notably, the lateral adhesion force can be calculated, knowing either (i) the apparent contact width and the apparent contact angles or the (ii) real contact width and the contact angle on the corresponding flat surface.

DY 39.6 Wed 11:15 C 264

Efficient Condensation and Droplet Removal on Electrowetting-Functionalized Surfaces — Davood Baratian, Ranabir Dey, Harmen Hoek, Dirk van den Ende, and •Frieder Mugele — University of Twente; Physics of Complex Fluids, Enschede, The Netherlands

Efficient condensation of vapor and collection of fog from the atmosphere are important to life in arid environments. Nature has come up with various strategies to optimize the processes by a combination of both topographic and chemical functionalization of solid surfaces that are imprinted passively into the structure of the surface. One crucial aspect in this process is the removal of liquid from the solid surface once it has condensed. In here, we present a novel active approach to improve the efficiency of vapor condensation onto hydrophobic surfaces that are functionalized by electrowetting. We fabricated electrowetting-functionalized surfaces with submerged interdigitated electrodes. Upon exposure to supersaturated vapor droplets condense onto these surfaces in an initially random pattern. As the droplets grow, electrowetting mobilizes the growing drops and induces early coalescence, giving rise to alignment of drops and to early shedding. Mobilization and early shedding are controlled by the effective reduction of contact angle hysteresis in AC electrowetting. Drops are found to grow algebraically, initially with a self-similar growth law as in conventional drop condensation. At a later stage, self-similarity is broken and the statistical drop size distribution is altered. We discuss potential applications in terms of heat transfer.

DY 39.7 Wed 11:30 C 264

Forced dynamic dewetting of structured surfaces: Influence of surfactants — •Günter K. Auernhammer[1,4], Franziska Henrich[1], Dorota Linke[1], Hans Martin Sauer[2], Edgar Dörsam[2], Steffen Hardt[3], and Hans-Jürgen Butt[1] — [1]MPI Polymer Research, Mainz, Germany — [2]TU Darmstadt, IDD, Germany — [3]TU Darmstadt, Nano- und Mikrofluidik, Germany — [4]IPF, Dresden

We investigate dynamic dewetting on structured surfaces. The focus lies on the interplay between surface structure and surfactants concentration in forced dewetting. The structured surfaces are printing plates for gravure printing with different sizes of the gravure cells. These plates were mounted on a rotating horizontal cylinder that is half-immersed in an aqueous solution of the anionic surfactant sodium 1-decanesulfonate. On the printing plates, structured and unstructured areas were side by side to enable a direct comparison. When rotating the cylinder a liquid meniscus is partially drawn out of the liquid. The moving contact line was pinned on the borders of the gravure cells, leading to a strongly varying receding contact angle. For this reason we compare the height differences of the meniscus on the structured and unstructured area. With increasing size of the gravure cells this height difference increases. By adding surfactant, the height difference for the same surface decreases. We conclude that the surfactant reduces the influence of a structured surface on dynamic dewetting. Characterizing the emptying mechanism of the gravure cells revealed that some liquid is left in the gravure cell.

DY 39.8 Wed 11:45 C 264

Spatially Resolved NMR with Micrometer Resolution in Static Field Gradients — •Benjamin Kresse, Mark Höfler, Alexei F. Privalov, and Michael Vogel — TU Darmstadt, Hochschulstr. 6, 64289 Darmstadt, Germany

A new probe head is presented which is specially designed for magnetic resonance imaging (MRI) with ultrahigh resolution in one dimension using a static field gradient magnet. In contrast to clinical MRI scan-

ners with a spatial resolution of typically 0.1 to 1 mm a resolution of about 2 μm is reached due to the high field gradient of 73 T/m. Systems with a rotational symmetry can be investigated by scanning the sample slice-wise. The key feature of the probe is a precise computer controlled adjustment of the sample position and orientation e.g. to adjust the sample axis parallel to the gradient of the magnetic field.

Wetting processes can be investigated. For example, droplets on surfaces can be studied in terms of density by inspecting the signal amplitude and in terms of molecular dynamics by measuring the relaxation time of the nuclear spins. Furthermore, concentration gradients of mixtures can be examined by measurements on different isotopes. It is also possible to investigate biological objects with flat geometries like skin. In principle non-stationary processes like in microfluidics can be explored with an increased time resolution by a boosted signal-to-noise ratio using stripline designs.

DY 39.9 Wed 12:00 C 264

Feedback-Control of Photoresponsive Fluid Interfaces — •Josua Grawitter and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Deutschland

New microfluidic devices promise powerful applications in diagnosing and combatting illness around the world. Conventional, pressure-driven devices rely on static channel geometries designed for specific flow patterns. Light-driven devices instead use photosensitive surfactants to produce surface tension gradients that drive Marangoni currents. By changing their light patterns in response to fluid flow, light-driven devices add feedback control methods to the microfluidic toolbox.

To explore their potential, we develop a diffusion-advection-reaction equation for photosensitive surfactants and calculate Marangoni currents at fluid-fluid interfaces. We then study how the interface responds when illuminated by spots of light. Switching on a single light spot, the density of the switched surfactant spreads in time and assumes an exponentially decaying profile in steady state. Simultaneously, the induced radial Marangoni flow reverses its flow direction from inward to outward. We use this feature to set up specific feedback rules, which couple advection velocities sensed at the light spots to their intensities. As a result two neighboring spots switch on and off alternately. When we arrange more light spots on regular polygons, regular and irregular oscillations in light intensity emerge for certain numbers of spots. This demonstrates how light-driven feedback control may be used to create responsive and versatile microfluidic devices.

DY 39.10 Wed 12:15 C 264

Collective Orientational Order and Phase Behavior of a Discotic Liquid Crystal under Confinement — •Arda Yildirim[1], Kathrin Sentker[2], Patrick Huber[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Institut für Materialphysik und -technologie, Technische Universität Hamburg, Eißendorfer Str. 42, 21073 Hamburg, Germany

Discotic liquid crystals (DLCs) are a promising class of soft matter for electronic applications. This is due to their ability to self-organize into columns in a hexagonal columnar mesophase, driven by the overlapping of the π orbitals of their aromatic cores. This leads to a high charge-carrier mobility along the column axis. Previous studies on DLCs showed that their properties, such as phase transition temperatures and enthalpies, are susceptible to nanoconfinement [1,2]. In this study, 2,3,6,7,10,11 hexakis[hexyloxy] triphenylene (HAT6) was confined into parallel aligned cylindrical nanopores of anodic aluminum oxide (AAO) membranes by melt infiltration. Furthermore, the pore surfaces of a series of membranes were chemically modified, resulting in a more hydrophobic pore surface than the unmodified ones. Collective orientational order and phase behavior of HAT6 confined into modified and unmodified nanopores of AAO were investigated by broadband dielectric spectroscopy and differential scanning calorimetry respectively.
[1] C. Krause and A. Schönhals, J. Phys. Chem. C, 2013, 117, 19712.
[2] C. Krause et al., Colloid Polym. Sci., 2014, 292, 1949

DY 39.11 Wed 12:30 C 264

Reversible smectic layer buckling of a ferroelectric liquid crystal confined in anodic aluminium oxide nanochannels — •Mark Busch[1], Andriy V. Kityk[2,1], Tommy Hofmann[3], Dirk Wallacher[3], and Patrick Huber[1] — [1]TU Hamburg-Harburg, Hamburg, Germany — [2]Czestochowa University of Technology, Czestochowa, Poland — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

The temperature-dependent structural and electro-optical properties of the ferroelectric liquid crystal 2MBOCBC inside the confining cylindrical nanochannels of anodic aluminium oxide are investigated.[1] The channel walls of the 42 nm diameter pores are coated with a polymer to enforce a planar anchoring of this chiral mesogens. By means of neutron diffraction a fully reversible temperature-dependent smectic C* layer buckling towards a symmetric chevron-like structure is found. The formation of this structure coincides with a dramatic decrease in the linear electro-optical response, being explained by the aforementioned structural rearrangement.
[1] Busch et al., Nanoscale (2017), DOI: 10.1039/C7NR07273B

DY 39.12 Wed 12:45 C 264

Transport processes in water vapour sorption experiments on grained hygroscopic materials — •Alexander Murr — Institute for Structural Engineering and Material Science, University of Innsbruck

Water vapour sorption (WVS) experiments are frequently used to characterise the behaviour of hygroscopic materials for a variation in humidity. Sample material is exposed to a step change in relative humidity (RH) and the mass change is measured gravimetrically.

In order to identify the involved transport processes, WVS experiments on grained wood and cellulose have been performed. A comparison on the sorption kinetics of four different grain layer filling levels indicates the necessarity of including the water vapour transport between the sample surface and the forced air stream. Analysing the initial kinetics shows this transport being relevant for the whole range of RH. Additionally, the limitation of a non-instantaneous step change in RH will be discussed. An analysis based on a simple diffusion equation with an instantaneous sink provides further insights on the measured sorption kinetics. Consequently, the relaxation and reorganisation processes could be more easily separated and characterised in future experiments.

DY 40: Talk J. Bechhoefer

Time: Wednesday 9:30–10:00 Location: BH-N 243

Invited Talk DY 40.1 Wed 9:30 BH-N 243

Measurement of the functional form of Shannon entropy by partial erasure of a bit — •John Bechhoefer[1], Momčilo Gavrilov[1,2], and Raphaël Chétrite[1,3,4] — [1]Dept. of Physics, Simon Fraser University, Burnaby, British Columbia, Canada — [2]Present address: Dept. of Biophysics and Biophysical Chemistry, Johns Hopkins University, Baltimore, MD, USA — [3]Pacific Institute for the Mathematical Sciences, UMI 3069, Vancouver, British Columbia, Canada — [4]Permanent address: Université Côte d'Azur, CNRS, LJAD, Parc Valrose, NICE, France

We use a feedback trap to erase a fraction of a bit of information from a memory whose states are encoded in the two states of a double-well potential. The system consists of a colloidal particle in water in a "virtual" potential. We show experimentally that the minimum amount of work required is proportional to the Shannon entropy function for a two-state system, for arbitrary state probabilities. This is the first experimental confirmation that the Shannon function is the appropriate definition for nonequilibrium system entropy as it relates to thermodynamics.

DY 41: Talk U. Thiele

Time: Wednesday 9:30–10:00 Location: BH-N 334

Invited Talk DY 41.1 Wed 9:30 BH-N 334

From bifurcations of single sliding drops to their ensemble statistics — •Uwe Thiele — Institute for Theoretical Physics and Center of Nonlinear Science (CeNoS), WWU Münster, 48149 Münster.

We study the nonlinear dynamics of individual sliding drops and of large ensembles. After introducing the modelling of capillarity and wettability in mesoscopic hydrodynamics we first employ path-continuation [1] to analyse periodic trains of stationary sliding drops and show that qualitative transitions occur at saddle-node bifurcations. A global bifurcation results in pearling-coalescence cycles that show the period-doubling route to chaos [2]. Second, we simulate the evolution of large drop ensembles and show that the interplay of coalescence and pearling results in a stationary drop size distribution that may be understood from the single-drop bifurcation diagram. Then a coarse-grained statistical model for the dynamics of the drop size distribution is developed that well captures the features of the evolution [3]. Finally, we consider the effects of substrate heterogeneities and continuous condensation of liquid onto the substrate. We show that then the interplay of condensation, (de)pinning, coarsening and pearling also results in a stationary distribution that can be related to single-drop bifurcation diagrams. [1] Using PDE2PATH, see H. Uecker, D. Wetzel and J.D.M Rademacher, Num. Math.-Theory Meth. Appl. 7, 58 (2014); [2] S. Engelnkemper, M. Wilczek, S.V. Gurevich and U. Thiele, Phys. Rev. Fluids 1, 073901 (2016); [3] M. Wilczek, W. Tewes, S. Engelnkemper, S.V. Gurevich and U. Thiele, Phys. Rev. Lett. 119, 204501 (2017).

DY 42: Turbulence

Time: Wednesday 10:00–12:45 Location: BH-N 128

DY 42.1 Wed 10:00 BH-N 128

On the small-scale structures of the turbulent velocity gradient and the resulting pressure field — •Dimitar G Vlaykov and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The non-local nature of the pressure in incompressible flows is at the heart of the complexity of the turbulence problem. Through a Poisson equation it is intimately related to the non-linear structures of the velocity gradient field in fully developed turbulence. To address both issues, we present a statistical characterization of the spatial structure of the second invariant of the velocity gradient tensor in homogeneous and isotropic turbulence. We distinguish regions of different intensity and type – vorticity or strain dominated, and provide estimates on their scales and relative separation. The results inform a comparative statistical study of the dependence of the pressure nonlocality on the local conditions for a range of Taylor-based Reynolds numbers between 123 and 433. It is found that in strongly vorticity-dominated regions a shielding mechanism is responsible for localizing the dominant pressure contributions to a dissipation-scale neighborhood. Moreover, this neighborhood is smaller than the underlying vortex structure. In strain-dominated regions, on the other hand, the same mechanism leads to the pressure statistics being determined on inertial scales. Finally, the well-known long-range pressure correlations stem from the strong non-locality of the contributions to the pressure in regions of low velocity-gradient intensity.

DY 42.2 Wed 10:15 BH-N 128

Scalable exact coherent structures for the turbulent cascade — •Stefan Zammert and Bruno Eckhardt — Philipps-Universität Marburg, Marburg, Germany

Exact solutions of the Navier-Stokes equations play a key role in the formation of subcritical turbulence. The appearance of three-dimensional turbulence was shown to be connected to secondary bifurcations of such structures in various flows. However, an explanation of the evolution of the observed spatial complexity, e.g. the multiple scales of turbulence, is still missing.

We will show different families of exact coherent states of plane Couette flow which can be scaled in their spatial extends to obtain a hierarchy of exact coherent states (*Eckhardt & Zammert: Nonlinearity, to appear*). While one of these families is localized in the center of the channel and independent of the walls, another one is attached to the walls and reminiscent of so-called attached eddies. The structures propose a potential entry to explain the turbulent cascade using exact coherent structures and thus by methods from dynamical systems theory.

DY 42.3 Wed 10:30 BH-N 128

Filtered kinetic energy budget in two-dimensional Rayleigh-Bénard convection — •Gerrit Green[1,2], Dimitar Vlaykov[1], Juan-Pedro Mellado[3], and Michael Wilczek[1] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August-University Göttingen — [3]Max-Planck-Institute for Meteorology, Hamburg, Germany

The dynamics of turbulent Rayleigh-Bénard convection (RBC) exhibits a complex interaction between coherent large-scale flow patterns, so-called superstructures, and small-scale fluctuations. It is largely unexplained how such superstructures trigger small-scale turbulence and, conversely, how turbulence sustains or inhibits superstructures. In this contribution, we employ two-dimensional direct numerical simulations to investigate the interaction between scales. A filtering approach is used to separate the large and small scales. This allows us to systematically study the distinct contributions to the large-scale kinetic energy budget. Different Rayleigh and Prandtl numbers are explored with this method. We show that most of the energy tranfer between scales occurs near the wall and that in the bulk it is approximately independent of height. The ultimate goal is to find an effective description of turbulent superstructures in RBC, and the presented results will help to understand how to establish such a description.

DY 42.4 Wed 10:45 BH-N 128

Edge states in the climate system: exploring global instabilities and critical transitions — •Valerio Lucarini[1,2,3] and Tamas Bodai[1,2] — [1]Department of Mathematics and Statistics, University of Reading — [2]Centre for the Mathematics of Planet Earth, University of Reading — [3]CEN, University of Hamburg

Multistability is a ubiquitous feature and provides key challenges for our ability to predict a system's response to perturbations. The Earth climate is multistable: present astronomical conditions support two stable regimes, the warm and the snowball climate. We study the global instability giving rise to the snowball/warm multistability in the climate system by identifying the climatic edge state, a saddle embedded in the boundary between the two basins of attraction of the stable climates. The edge state attracts initial conditions belonging to such a boundary and is the gate facilitating noise-induced transitions between competing attractors. We use a simplified yet Earth-like climate model constructed by coupling a primitive equations model of the atmosphere with a simple diffusive ocean. We refer to the climatic edge states as Melancholia states. We study their dynamics, their symmetry properties, and we follow a complex set of bifurcations. We find situations where the Melancholia state has chaotic dynamics. In these cases, the basin boundary between the two basins of attraction is a strange geometric set with a nearly zero codimension, and relate this feature to the time scale separation between instabilities occurring on weather and climatic time scales. We also discover a new stable climatic state characterized by non-trivial symmetry properties.

DY 42.5 Wed 11:00 BH-N 128

Statistical and Dynamical Properties of Covariant Lyapunov Vectors in a Coupled Atmosphere-Ocean Model - Multiscale Effects and Geometric Degeneracy — •Valerio Lucarini[1,2,3] and Stephane Vannitsem[4] — [1]Department of Mathematics and Statistics, University of Reading — [2]Centre for the Mathematics of Planet Earth, University of Reading — [3]CEN. University of Hamburg — [4]Royal Meteorological Institute, Bruxelles

We study a simplified coupled atmosphere-ocean model using the formalism of covariant Lyapunov vectors (CLVs). The model is obtained via a severe truncation of quasi-geostrophic equations for the two fluids, has 36 degrees of freedom, features a chaotic dynamics. One finds 2 positive Lyapunov exponents (LEs), 16 negative LEs, and 18 near-zero LEs. The presence of many near-zero LEs results from the vast time-scale separation between the time scales of the two fluids. The tangent space spanned by the CLVs corresponding to the positive and negative LEs has a non-pathological behaviour, while strong degeneracies are found for the near neutral modes. Our results underline the difficulties in using hyperbolicity as a conceptual framework for multiscale chaotic dynamical systems, whereas the framework of partial hyperbolicity seems better suited, possibly indicating an alternative definition for the chaotic hypothesis. Our results suggest the need for accurate analysis of error dynamics on different time scales and domains and for a careful set-up of assimilation schemes when looking at coupled atmosphere-ocean models.

15 min. break

DY 42.6 Wed 11:30 BH-N 128

Directed locomotion fuelled by turbulent fluid motion — Nicolas Francois, Hua Xia, Horst Punzmann, and •Michael Shats — Centre for Plasmas and Fluids, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601, Australia

Chaotic horizontal motion of fluid at the liquid-gas interface is a ubiquitous phenomenon since such a motion can be driven by surface waves. When waves are steep, such motion is not just chaotic. It becomes turbulent in the sense of Kraichnan's two-dimensional turbulence, a state strongly out of equilibrium. We show that a properly shaped floating object on the liquid surface can tap energy of turbulent fluctuations to fuel its self-propulsion along a trajectory which can be viewed as a rectified random walk. If a floating device is fixed at one position on the surface, making a horizontal rotor, it can convert turbulent fluctuations into unidirectional rotation. The effect relies on the momentum transfer from the underlying fabric of the flow to the floating object. The shape of the object controls its ability to become a 'Lagrangian ratchet' that can tap the energy of correlated bundles of fluid trajectories.

DY 42.7 Wed 11:45 BH-N 128

Tuning diffusion of finite size particles in turbulent flows — •Hua Xia, Nicolas Francois, Horst Punzmann, and Michael Shats — Research School of Physics and Engineering, The Australian National University, Canberra, Australia

The motion of a large floater on a liquid surface perturbed by Faraday waves was shown to be erratic and share features similar to the Brownian motion of particles in contact with a thermal bath. In particular a fluctuation-dissipation relationship was uncovered. This similarity with systems at thermodynamic equilibrium seems at odds with the fact that Faraday waves generate turbulent flows, a state strongly out of equilibrium.

Here we show that the law of dispersion in chaotic flows can be widely tuned due to the coupling of diffusing particles with the fabric and memory of the flow. We demonstrate a sharp change in the law of diffusion as a function of scales seen as a transition from *thermal* diffusion at large scales to strongly non-equilibrium regime at small scales. The chaotic flow is dominated by underlying coherent bundles executing random walk. Large particles interact with many bundles, disperse similar to a Brownian particle in a thermal bath. For particles smaller than the characteristic length scale, the coherent bundles push the particles resulting in a much faster dispersion.

DY 42.8 Wed 12:00 BH-N 128

Fluid surface particle control and transition to order in wave-based liquid metamaterials — Nicolas Francois[1], Hua Xia[1], •Horst Punzmann[1], Paul Fontana[2], and Michael Shats[1] — [1]Research School of Physics and Engineering, Australian National University, Canberra, Australia — [2]Physics department, Seattle University, Seattle, USA

This work demonstrates a method of remotely shaping the trajectories of floating particles on a liquid-gas interface through the external control of surface waves. The underlying principle is a combination of rotating waves, created by a superposition of two orthogonal standing waves, and the Lagrangian drift of particles along closed paths in such waves. This mechanism offers a high degree of control over the particle motion and provides the ability to confine particles to a spatially periodic lattice of nested orbits. The key parameter in the transition from ordered to disordered flow (or vice versa) is the temporal phase shift between the two orthogonal standing waves. We present experimental results on the creation and control of such dynamical liquid interface materials, complemented with a theoretical model of particle trajectories based on the wave-driven Lagrangian drift at the surface of an ideal fluid. In analogy of solid metamaterials which guide waves through matter, liquid metamaterials allow the guidance of matter through control of the imposed surface wave topology. By dynamically shaping a fluid interface using rotating waves, it is possible to effectively produce a 2D material with prescribed transport properties [N. Francois, et. al. Nat. Commun. 7, 14325 (2017)].

DY 42.9 Wed 12:15 BH-N 128

The Statistical Properties of Ultra-Strong Turbulence — •Christian Küchler[1], Gregory P. Bewley[2], and Eberhard Bodenschatz[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Cornell University, Ithaca, USA

How do the two-point statistical quantities of the velocity field depend on the turbulence level? Is turbulence universal? Answering these questions requires access to a sufficiently wide inertial range over which the turbulence can be considered universal. The Variable Density Turbulence Tunnel at the Max Planck Turbulence Facility can reach extremely high turbulence levels under experimentally resolvable conditions. The VDTT is a closed- loop wind tunnel of 80 m^3 volume filled with pressurized sulfur-hexaflouride at 0.5 bar to 15 bar. This allows to change the turbulence levels over two orders of magnitude, while keeping the geometry of the flow the same. The turbulence is generated by an unique active grid consisting of 111 individually controllable flaps. By using nanoscale thermal anemometry probes developed at Princeton University we record ultra long time series of the turbulent velocity field at a single point 9 m downstream of the active grid. Using these techniques we compiled datasets at turbulence levels that hereto-forth could not experimentally resolved. In the talk we report the evolution of two-point statistics as a function of turbulence level and present insights on the inertial range scaling and intermittency effects of turbulent flows.

DY 42.10 Wed 12:30 BH-N 128

The decay of grid-generated wind tunnel turbulence — •Lisa Rademacher, Lars Kröger, Joachim Peinke, Gerd Gülker, and Michael Hölling — ForWind - Institute of Physics, University of Oldenburg, 26111 Oldenburg, Germany

Producing turbulent inflow conditions inside a wind tunnel by passive and active grids is an important measuring tool to simulate real wind conditions. Especially active grids have shown to be indispensable for controlling the inflow turbulence more precisely and reproducing unsteady processes. This is for instance important for examining wind turbines and how they perform in highly intermittent wind fields. Depending on the investigated problem different wind fields are required e.g. shear flows or unsteady flow events to simulate the turbulent atmospheric boundary layer or gusty wind loads. Since turbulence is characterised by its highly chaotic nature the reproducibility and controllability of the inflow conditions are of high importance. Also the invasive character of the grid itself should be as small or short-living as possible to prevent interfering of grid wake and measurement model. Ideally the grid wake should decay fast compared with the decay of the turbulent structures, which should last as long as possible - so the generated turbulence would exist without traces of the generating grid over the most parts of the measuring section. In this contribution the decay of the generated turbulence and the grid wake considering different flap movement patterns of a Makita-designed active grid are examined by the use of PIV.

DY 43: Stochastic thermodynamics and information processing

Time: Wednesday 10:00–13:45 Location: BH-N 243

DY 43.1 Wed 10:00 BH-N 243

Stochastic thermodynamics in the strong coupling regime: An unambiguous approach based on coarse graining — •Philipp Strasberg and Massimiliano Esposito — Complex Systems and Statistical Mechanics, Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We consider a classical and possibly driven composite system XY weakly coupled to a Markovian thermal reservoir R so that an unambiguous stochastic thermodynamics ensues for XY. This setup can be equivalently seen as a system X strongly coupled to a non-Markovian reservoir YR. We demonstrate that only in the limit where the dynamics of Y is much faster than X, our unambiguous expressions for thermodynamic quantities, such as heat, entropy, or internal energy, are equivalent to the strong coupling expressions recently obtained in the literature using the Hamiltonian of mean force. By doing so, we also significantly extend these results by formulating them at the level of instantaneous rates and by allowing for time-dependent couplings between X and its environment. Away from the limit where Y evolves much faster than X, previous approaches fail to reproduce the correct results from the original unambiguous formulation, as we illustrate numerically for an underdamped Brownian particle coupled strongly to a non-Markovian reservoir.

DY 43.2 Wed 10:15 BH-N 243

Conservation Laws in Nonequilibrium Thermodynamics — •Riccardo Rao and Massimiliano Esposito — Complex Systems and Statistical Mechanics, Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, G.D. Luxembourg

Starting from the most general formulation of stochastic thermodynamics—i.e. a thermodynamically consistent nonautonomous stochastic dynamics describing systems in contact with several reservoirs—, we define a procedure to identify the conservative and the minimal set of nonconservative contributions in the entropy production. The former is expressed as the difference between changes caused by time-dependent drivings and a generalized potential difference. The latter is a sum over the minimal set of flux–force contributions controlling the dissipative flows across the system. When the system is initially prepared at equilibrium (e.g. by turning off drivings and forces), a finite-time detailed fluctuation theorem holds for the different contributions. Our approach relies on identifying the complete set of conserved quantities and can be viewed as the extension of the theory of generalized Gibbs ensembles to nonequilibrium situations.

[1] R. Rao & M. Esposito. arXiv 1709.01951.

[2] M. Polettini, G. Bules-Cuetara & M. Esposito. Phys. Rev. E 94, 052117 (2016).

DY 43.3 Wed 10:30 BH-N 243

Fluctuation theorems for detached path probabilities — •Jannik Ehrich and Andreas Engel — Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Systems with interacting degrees of freedom play a prominent role in stochastic thermodynamics. We apply the concept of causal conditioning to define a detached entropy production for a general bipartite Markov process. This quantity simplifies the dissection of the mutual influence the interacting degrees of freedom have on each other [1]. We elaborate on a series of special cases including measurement-feedback systems, sensors and hidden Markov models. For these special cases we show that fluctuation theorems involving the detached entropy production recover known results which have been obtained separately before. Additionally, we show that the fluctuation relation for the detached entropy production can be used in model selection for data stemming from a hidden Markov model.

[1] J. Ehrich and A. Engel, Phys. Rev. E **96**, 042129 (2017)

DY 43.4 Wed 10:45 BH-N 243

Fluctuations of Apparent Entropy Production in Networks with Hidden Slow Degrees of Freedom — •Matthias Uhl, Patrick Pietzonka, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart

The fluctuation theorem for entropy production is a remarkable symmetry of the distribution of produced entropy that holds universally in non-equilibrium steady states with Markovian dynamics. However, in systems with slow degrees of freedom that are hidden from the observer, it is not possible to infer the amount of produced entropy exactly. Previous work suggested that a relation similar to the fluctuation theorem may hold at least approximately for such systems if one considers an apparent entropy production. By extending the notion of apparent entropy production to discrete bipartite systems, we investigate which criteria have to be met for such a modified fluctuation theorem to hold in the large deviation limit [1]. We use asymptotic approximations of the large deviation function to show that the probabilities of extreme events of apparent entropy production always obey a modified fluctuation theorem and, moreover, that it is possible to infer otherwise hidden properties.

[1] M. Uhl, P. Pietzonka, U. Seifert, arXiv:1708.09786

15 min. break

DY 43.5 Wed 11:15 BH-N 243

Stochastic thermodynamics of a self-oscillating isothermal machine — •Christopher W. Wächtler[1], Philipp Strasberg[2], Sabine H. L. Klapp[1], Gernot Schaller[1], and Chrisotpher Jarzynski[3] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Complex Systems and Statistical Mechanics, University of Luxembourg, Luxembourg — [3]Institute for Physical Science and Technology, University of Maryland, USA

Self-oscillation describes the generation and maintenance of a periodic motion by a source of energy that is lacking a corresponding periodicity. We here examine a theoretically and experimentally studied model of a nanomechanical resonator coupled to a single-electron transistor, i.e. a single electron shuttle. While the dynamics of this system has been studied from different points of view the thermodynamical aspects have not been addressed before. Within the formalism of stochastic thermodynamics we are able to find a consistent thermodynamical description of the system at the semiclassical level including two sources of noise: thermal fluctuations of the resonator and stochastic jumps of the electrons. We derive the first and second law and, furthermore, demonstrate that the system can also serve as an isothermal machine, which performs useful work while maintaining its periodic motion.

DY 43.6 Wed 11:30 BH-N 243

Stochastic thermodynamics of periodically driven systems: Fluctuation theorem for currents and unification of two classes — •Somrita Ray and Andre Barato — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden

Periodic driving is used to operate machines that go from standard macroscopic engines to small nonequilibrium microsized systems. Two classes of such systems are small heat engines driven by periodic temperature variations, and molecular pumps driven by external stimuli. Well-known results that are valid for nonequilibrium steady states of systems driven by fixed thermodynamic forces have been generalized to heat engines operated by external periodic drive only recently [1]. These results include a general expression for entropy production in terms of currents and affinities, and symmetry relations for the Onsager coefficients from linear-response theory. For nonequilibrium steady states, the Onsager reciprocity relations can be obtained from the more general fluctuation theorem for the currents. We present a fluctuation theorem for the currents for periodically driven systems [2] that implies a fluctuation dissipation relation, symmetry relations for Onsager coefficients, and further relations for nonlinear response coefficients. Our results are valid for both heat engines and molecular pumps.

1. K. Brandner, K. Saito and U. Seifert, Phys. Rev. X 5, 031019 (2015) 2. SR and A. C. Barato, Phys. Rev. E 96, 052120 (2017)

DY 43.7 Wed 11:45 BH-N 243

Relations between long-time and finite-time fluctuation theorems in 2-level system under periodic drive — •Ivan Khaymovich[1,2] and Avinash Mandaiya[3] — [1]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [2]Institute for Physics of Microstructures, Russian Academy of Sci-

ences, 603950 Nizhny Novgorod, GSP-105, Russia — [3]Indian Institute of Science, Bangalore 560012, India

Mesoscopic systems driven out of equilibrium experience large fluctuations of a stochastic entropy production. Fluctuation relations (FR) taking into account these fluctuation and generalizing the second law of thermodynamics are of particular interest for last decades. Gallavotti-Cohen relation being a remarkable example of long-time (LT) FR focuses on the large deviation regime and it is insensitive to initial conditions, while Crooks relation works with finite-time (FT) protocols and needs a special initial conditions both for forward and reversed system evolution in time. In general all FR are based on a some kind of reversion of a time-dependent protocol applied to a system. These FR are significantly simplified for the protocols symmetric to that reversion operation. In the present work we find sufficient conditions for asymmetric protocols for which simplified versions of LT and FT FR are still valid and derive the relation between these conditions. We give several examples of these protocols in a simplest case of 2-level system showing the link between LT and FT fluctuation relations.

DY 43.8 Wed 12:00 BH-N 243

Collective power: Minimal model for thermodynamics of nonequilibrium phase transitions — •Tim Herpich, Juzar Thingna, and Massimiliano Esposito — Complex Systems and Statistical Mechanics, Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We establish a direct connection between the linear stochastic dynamics, the nonlinear mean-field dynamics, and the thermodynamic description of a minimal model of driven and interacting discrete oscillators. These exhibit at the mean-field level two bifurcations separating three phases: a single stable fixed point, a stable limit cycle indicative of synchronization, and multiple stable fixed points. The apparent contradiction with the underlying linear Markovian dynamics which ensures convergence to a unique steady state is resolved via metastability, i.e. the appearance of gaps in the upper real part of the spectrum of the Markov generator. The dissipated work of the stochastic dynamics exhibit signatures of nonequilibrium phase transitions over long metastable times which disappear in the infinite-time limit. Remarkably, it is also reduced by attractive interactions between oscillators. When operating as a work-to-work converter we study the power output and efficiency of our device in the presence of nonequilibrium phase transitions. We find that the maximum power output is achieved far-from-equilibrium in the synchronization regime and that the efficiency at maximum power is surprisingly close to the universal linear regime prediction. Our work builds bridges between thermodynamics of nonequilibrium phase transitions and bifurcation theory.

15 min. break

DY 43.9 Wed 12:30 BH-N 243

Records of entropy production in a double quantum dot — •Edgar Roldan[1], Shilpi Singh[2], Izaak Neri[1], Ivan Khaymovich[1], Dmitry Golubev[2], Ville Maisi[3], Joonas Peltonen[2], Frank Jülicher[1], and Jukka Pekola[2] — [1]Max Planck Institute for the Physics of Complex System (Dresden, Germany) — [2]Low Temperature Laboratory, Aalto University (Aalto, Finland) — [3]Lund University (Lund, Sweden)

Little is known about extreme-value statistics of thermodynamic fluxes characterising the most extreme deviations from the average behaviours. We report on the experimental measurement of stochastic entropy production and of records of negative entropy. For this purpose we employ a metallic double dot under a constant external DC bias which realizes Markovian nonequilibrium steady states. We find that the cumulative distribution of entropy production's negative record is bounded at all times by a limiting exponential distribution with a mean value equal to minus the Boltzmann constant. Using this result, we derive an upper bound for the average maximal entropy influx from the environment to a mesoscopic system in a finite time, and demonstrate this result with experimental data. Our work provides bounds for the maximal fluctuations of single-electronic currents against the direction of the electric field. Furthermore, our results may shed light on the statistics of overheating events in single-electronic devices which are key for the design of reversible computing nano-devices operating near Landauer's principle of minimal heat dissipation.

DY 43.10 Wed 12:45 BH-N 243

Testing optimality of sequential decision-making — •Izaak Neri[1,2,5], Meik Dörpinghaus[3,5], Édgar Roldán[1,5], Heinrich Meyr[4,5], and Frank Jülicher[1,5] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstraße 108, 01307 Dresden, Germany — [3]Vodafone Chair Mobile Communications Systems, Technische Universität Dresden, 01062 Dresden, Germany — [4]Institute for Integrated Signal Processing Systems, RWTH Aachen University, 52056 Aachen, Germany — [5]Center for Advancing Electronics Dresden, 01062 cfaed, Germany

Sequential decision making studies how a device makes as fast as possible decisions based on the sequential observation of a stochastic process. Here, a statistical test for the optimality of black box decision devices and a related measure for the divergence to optimality of black box decision devices are presented; a device is optimal if the average decision time – over different realisations of the observed process – is minimal given a certain maximal allowed error probability. A relation between the presented statistical test and the recently derived fluctuation theorems for first-passage times of entropy production is discussed [1]. Numerical experiments illustrate the use of the test for practical purposes.

[1]I Neri, É Roldán, F Jülicher, Statistics of Infima and Stopping Times of Entropy Production and Applications to Active Molecular Processes, Physical Review X 7, 011019 2017

DY 43.11 Wed 13:00 BH-N 243

Towards a (stochastic) thermodynamic description of non-Markovian delayed systems — •Sarah A. M. Loos and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

Stochastic thermodynamics provides a consistent description of a wide class of Langevin systems, but the Markov assumption is often crucial [1]. However, time-delayed feedback control – which commonly arises for example in biological processes and technical applications – renders stochastic dynamics non-Markovian [2]. Therefore, some basic concepts need to be revisited [3]. Time-delay further pushes the steady states out of thermodynamic equilibrium (even in the absence of probability currents), as reflected by a non-zero mean entropy production. This is explicitly shown in [4] for the case of linear forces and an exponential memory kernel in one dimension.

Here, we discuss the possibility of calculating key thermodynamic quantities in the steady state of overdamped Langevin systems involving different memory kernels and nonlinear external forces. Using a Markovian embedding, we find a divergent entropy production in the case of error-free and continuous measurement. Furthermore, we present an analytical expression for the heat exchange rates that only involves positional moments.

[1] U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012).
[2] S. A. M. Loos and S. H. L. Klapp, PRE **96**, 012106 (2017).
[3] M. L. Rosinberg, T. Munakata, G. Tarjus, PRE **91**, 042114 (2015).
[4] A. Crisanti, A. Puglisi, D. Villamaina, PRE **85**, 061127 (2012).

DY 43.12 Wed 13:15 BH-N 243

Stochastic aspects of thermodynamic irreversibility in nanoscale friction — •Paola Carolina Torche, Andrea Silva, Denis Kramer, Tomas Polcar, and Ondrej Hovorka — University of Southampton, Southampton, UK

Understanding the energy dissipation occurring during the nanoscale friction processes remains an open challenge. This is partly due to the lack of availability of a consistent and sufficiently general thermodynamic framework that would allow separating the microscopic, fluctuating, work performed by a nanoscale slider into the relevant internal energies and the irreversible heat produced during the motion.

In this talk we discuss the possibility of applying the principles of the modern stochastic thermodynamics [1] to quantify the fluctuating work and irreversible heat at the coarse-grained level of description of nanoscale friction, namely to the stochastic trajectories generated by the tip of Friction Force microscope [2]. By considering the Prandtl-Tomlinson model of a stick-slip frictional motion augmented by thermal fluctuations modelled by the transition state theory, we show that it is possible to fully quantify the stochastic entropy, work and heat distributions associated with the sliding motion. We then discuss the possibilities of validating the developed computational approach with Atomic Force Microscopy experiments.

[1] U. Seifert, Stochastic thermodynamics, fluctuation theorems, and molecular machines, Rep. Prog. Phys. 75, 126001 (2012).
[2] Gnecco et al, Velocity dependence of atomic friction, Phys. Rev.

Lett. 84, 1172 (2000).

DY 43.13 Wed 13:30 BH-N 243

Coherence of biochemical oscillations is bounded by driving force and network topology — •Andre Barato — Max Planck Institute for the Physics of Complex Systems

Biochemical oscillations are prevalent in living organisms. Systems with a small number of constituents cannot sustain coherent oscillations for an indefinite time because of fluctuations in the period of oscillation. We show that the number of coherent oscillations that quantifies the precision of the oscillator is universally bounded by the thermodynamic force that drives the system out of equilibrium and by the topology of the underlying biochemical network of states. Our results are valid for arbitrary Markov processes, which are commonly used to model biochemical reactions. We apply our results to a model for a single KaiC protein and to an activator-inhibitor model that consists of several molecules. From a mathematical perspective, based on strong numerical evidence, we conjecture a universal constraint relating the imaginary and real parts of the first nontrivial eigenvalue of a stochastic matrix.

A. C. Barato and U. Seifert; Phys. Rev. E 95, 062409 (2017)

DY 44: Pattern Formation I

Time: Wednesday 10:00–13:00 Location: BH-N 334

Invited Talk DY 44.1 Wed 10:00 BH-N 334

Self-organisation and positioning of sub-cellular protein clusters — •Sean M. Murray — Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

Many cellular processes require proteins to be precisely positioned within the cell. In some cases this can be attributed to passive mechanisms such as recruitment by other proteins in the cell or by exploiting the curvature of the membrane. However, in bacteria, active self-positioning is likely to play a role in multiple processes, including the positioning of the future division site and cytoplasmic protein clusters. How can such dynamic clusters be formed and positioned? Here, we present a model for the self-organization and positioning of dynamic protein clusters into regularly repeating patterns based on a phase-locked Turing pattern. A single peak in the concentration is always positioned at the midpoint of the model cell and two peaks are positioned at the midpoint of each half. Furthermore, domain growth results in peak-splitting and pattern doubling. We argue that the model may explain the regular positioning of the highly conserved Structural Maintenance of Chromosomes (SMC) complexes on the bacterial nucleoid and provides an attractive mechanism for the self-positioning of dynamic protein clusters in other systems.

We also briefly present recent results on the role this mechanism may play in bacterial chromosome segregation.

DY 44.2 Wed 10:30 BH-N 334

Active phase separation: A generic approach — •Fabian Bergmann, Lisa Rapp, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

Many non-equilibrium systems with conservation constraints show self-organization phenomena resembling classic phase separation: from cell polarization to cell populations communicating via chemotaxis, and from dense active Brownian particles to mussels in ecology. We identify this behavior as kinetic phase separation and suggest for its generic description near onset a Cahn-Hilliard (CH) model [J. Chem. Phys. **28**, 258 (1958)]. We introduce a general perturbative reduction scheme to establish the mathematical link between the proposed generic CH equation and system-specific models. We show this explicitely for two examples - cell polarization and chemotactic cells. The comparison of the cell polarization model to its approximation by the CH model veryfies the valitity of our generic approach. We thus suggest the CH equation as a generic model for phase separation applicable to many systems both in and outside of equilibrium.

DY 44.3 Wed 10:45 BH-N 334

Active Phase Separation vs Pattern Formation in Conserved Systems — •Lisa Rapp, Fabian Bergmann, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth

Active phase separation takes place in non-equilibrium systems such as during cell polarization or in active colloidal particle suspensions. These systems are typically described by conserved order parameters. Surprisingly, however, these conserved systems can also show spatially periodic patterns. We formulate the criteria for this transition from phase separation to periodic patterns in terms of a generic Cahn-Hilliard model and a recent model for cell polarization. In addition, the nonlinear properties of spatially periodic patterns in conserved systems are characterized.

DY 44.4 Wed 11:00 BH-N 334

Interrupted coarsening in a generalized Cahn-Hillard model with long-range interactions — •Simon Villain-Guillot and Mahdi Mcheik — Laboratoire Ondes et Matière d Aquitaine, Université de Bordeaux, 351 Cours de la Libération F-33405 Talence Cedex

The Cahn-Hilliard equation describes the dynamics of phase separation in the conservative case. This process is driven by the minimization of the free energy, especially of its interfacial part, during the Ostwald ripening, or coarsening. In 1D however, the lower energy state that should end the dynamics is very slow to reach. This is even more critical when the Cahn-Hilliard dynamics is modified to take into account long range interaction terms. A dynamical criterion proposed by Misbah and Politi [3] predict the interuption of the coarsening process and the stabilazation of a microstructured pattern.

We have explored a model where the Cahn Hilliard dynamics is coupled with a diffusion equation of a surfactant that favors interfaces. This scenario enables to speed up the dynamics and favors various pattern formation or micro-structuration.

References

[1] When does coarsening occur in the dynamics of one-dimensional fronts? P.Politi and C. Misbah, Phys. Rev. Lett. 92, 090601 (2004).

15 min. break

Invited Talk DY 44.5 Wed 11:30 BH-N 334

Spatial heterogeneities shape collective behavior of the signaling amoeboid cells — •Azam Gholami — Max-Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Dictyostelium discoideum organism, naturally occurring in forest soil, is an important model system for the study of chemotaxis, cell differentiation, and morphogenesis. We present novel experimental results on pattern formation of signaling Dictyostelium discoideum amoeba in the presence of a periodic array of millimeter-sized pillars. We observe concentric cAMP waves that initiate almost synchronously at the posts and propagate outwards. These waves have higher frequency than the other firing centers and dominate the system dynamics. The cells respond chemotactically to these circular waves and stream towards the pillars, forming periodic Voronoi domains that reflect the periodicity of the underlying lattice. These experiments are crucial to understand the signaling mechanism of Dictyostelium cells that experience external obstacles in its natural habitat. We expect our observations to be generic to other excitable media governed by reaction-diffusion dynamics, where spatial heterogeneities can significantly influence the wave generation process.

DY 44.6 Wed 12:00 BH-N 334

Mass-conserved Excitable Waves in the interior of Giant Amoeboid Cells — •Francesc Font[1], Sven Flemming[1], Carsten Beta[2], and Sergio Alonso[2] — [1]Department of Physics, Universitat Politecnica de Catalunya, Barcelona, Spain — [2]Institute of Physics and Astronomy, Universität Potsdam, Potsdam, Germany

Spiral waves and complex patterns have been observed in the interior of Dictyostelium discoideum cells. The amoebas have typically around 10 μm length, and the waves are on the similar scale than the cell size. Recent experiments have shown that a set of similar Dictyostelium discoideum cells can fuse into a single, larger cell when exposed to repeated electric pulses. The relatively large size of the resulting cell permits a clearer observation of the wave dynamics and pattern formation within the cell domain. For a systematic characterization of the

internal waves, we present a mathematical model of pattern formation in the amoeboid interior that combines noisy excitable kinetics with a mass-conservation constrain, together with a dynamic phase field for the cell shape. We will conclude by comparing numerical simulations of our model to experiments with giant amoeba Dictyostelium discoideum.

DY 44.7 Wed 12:15 BH-N 334

Spontaneous formation of target centers in D.discoideum — •Estefania Vidal-Henriquez[1], Vladimir Zykov[1], Bodenschatz Eberhard[1,2,3], and Gholami Azam[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077 Goettingen, Germany — [2]Institute for Nonlinear Dynamics, University of Goettingen, D-37073 Goettingen, Germany — [3]Laboratory of Atomic and Solid-State Physics and Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, New York 14853, USA

Dyctiostelium discoideum is a social amoeba that produces target patterns and spiral waves of cyclic AMP as a way to form multicellular aggregates when subjected to adverse environmental conditions. The stability of pacemakers at the interior of a target wave presents a modeling challenge in such organism, since in its classical description the limit cycle produces bulk (whole system) oscillations. We present a novel and robust way of producing target waves based on non-artificial conditions. Using the cell density in a discrete way, the bigger cell clusters become centers, as observed in experiments. We characterize the emission frequency of the centers and the capability of the rest of the system to react to them, depending on the cell coverage. The wave velocity is density dependent, thus producing aggregation streams. This model emphasizes the importance of external unbounded phosphodiesterase, upon which the system can change between oscillatory and excitable regimes allowing to reproduce many of the experimentally observed properties. Finally we discuss boundary conditions and the density differences necessary to artificially induce target centers.

DY 44.8 Wed 12:30 BH-N 334

Spontaneous membrane formation and self-encapsulation of active rods in an inhomogeneous motility field — •Jens Grauer[1], Hartmut Löwen[1], and Liesbeth Janssen[1,2] — [1]Institute for Theoretical Physics II: Soft Matter, Heinrich-Heine University Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany — [2]Theory of Polymers and Soft Matter, Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands

We study the collective dynamics of self-propelled rods in an inhomogeneous motility field. At the interface between two regions of constant but different motility, a smectic rod layer is spontaneously created through aligning interactions between the active rods, reminiscent of an artificial membrane. This 'active membrane' engulfes rods which are locally trapped in low-motility regions and thereby further enhances the trapping efficiency by self-organization, an effect which we call 'self-encapsulation'. Our results are gained by computer simulations of self-propelled rod models confined on a sphere with a stepwise constant motility field, but the phenomenon should be observable in any geometry with sufficiently large spatial inhomogeneity. We also discuss possibilities to verify our predictions of an active membrane in a motility field in experiments of self-propelled colloidal Janus rods and vibrated granular matter.

DY 44.9 Wed 12:45 BH-N 334

Influence of fast advective flows on pattern formation of *Dictyostelium discoideum* — •Torsten Eckstein, Estefania Vidal, Albert Bae, Vladimir Zykov, Eberhard Bodenschatz, and Azam Gholami — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

We report experimental and numerical results on pattern formation of self-organizing *Dictyostelium discoideum* cells in a microfluidic setup under a constant buffer flow. The external flow advects the signaling molecule cyclic adenosine monophosphate (cAMP) downstream, while the chemotactic cells attached to the solid substrate are not transported with the flow. At high flow velocities, elongated cAMP waves are formed that cover the whole length of the channel and propagate both parallel and perpendicular to the flow direction. While the wave period and transverse propagation velocity are constant, parallel wave velocity and the wave width increase linearly with the imposed flow. We also observe that the acquired wave shape is highly dependent on the wave generation site and the strength of the imposed flow. We compared the wave shape and velocity with numerical simulations performed using a reaction-diffusion model and found excellent agreement. These results are expected to play an important role in understanding the process of pattern formation and aggregation of *D. discoideum* that may experience fluid flows in its natural habitat.

DY 45: Statistical Physics in Biological Systems (joint session DY/BP)

Time: Wednesday 10:00–13:30 Location: BH-N 333

DY 45.1 Wed 10:00 BH-N 333

Fluctuation effects in single-molecule dynamics: From subergodic time-scales to the kinetics in the few-encounter limit — Alessio Lapolla, David Hartich, and •Aljaz Godec — Mathematical Biophysics Group, Max-Planck-Institute for Biophysical Chemistry (Göttingen)

Single-molecule (SM) dynamics evade the confines of traditional ensemble statistical mechanics. A correct theoretical description of SM dynamics requires a time-average statistical mechanics – the explicit consideration of trajectory-to-trajectory fluctuations over finite observation times. Similarly, a new paradigm emerges when considering molecular reaction kinetics in the few-encounter limit occurring, e.g. in transcription regulation or in diseases triggered by protein misfolding, where already the first reactive event is 'catastrophic'.

We will review our recent theoretical results on a rigorous formulation of occupation-time statistical mechanics, and a first passage time theory of few-encounter kinetics. We will discuss why our results are relevant for explaining quantitatively emerging biophysical phenomena at low-copy numbers.

DY 45.2 Wed 10:15 BH-N 333

Extreme value statistics of mutation accumulation in renewing cell populations — •Philip Greulich[1,2] and Benjamin D. Simons[3,4] — [1]Mathematical Sciences, University of Southampton, UK — [2]Institute for Life Sciences, University of Southampton, UK — [3]Cavendish Laboratory, University of Cambridge, UK — [4]Gurdon Institute, University of Cambridge, UK

The emergence of a predominant phenotype within a cell population is often triggered by a rare accumulation of DNA mutations in a single cell. For example, tumors may be initiated by a single cell in which multiple mutations cooperate to bypass a cell's defense mechanisms. The risk of such an event is thus determined by the extremal accumulation of mutations across tissue cells. To address this risk, we studied the statistics of the maximum mutation numbers in a Moran process, as a model for a renewing cell population. By drawing an analogy between the genealogy of a cell population and the theory of branching random walks, I will present new analytical estimates for the probability of exceeding a threshold number of mutations, and show how the statistical distribution of maximum mutation numbers scales with age and cell population size.

DY 45.3 Wed 10:30 BH-N 333

The rate of recombination and its effect on mutational robustness — •Alexander Klug and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln, Germany

Mutational robustness refers to the effect of mutations on the fitness of a population. In case of high mutational robustness most mutations do not change the fitness or have only a minor effect on it. Hence from the point of view of fitness landscapes, mutational robustness describes the occurrence of clusters of genotypes of almost equal fitness. Using a deterministic population model with selection and mutation it can be shown that the population slightly favours genotypes inside such clusters which therefore results in increased mutational robustness[1]. We show that this effect is strongly enhanced by the introduction of recombination on the basis of analytical results for a two-locus landscape and numerical results for different neutral landscape models with multiple loci.

[1] E. van Nimwegen, J. P. Crutchfield, M. Huynen, PNAS 96:9716-9720 (1999)

DY 45.4 Wed 10:45 BH-N 333

Accelerating Evolution With Dynamic Fitness Landscapes — •Alexander Leonard[1,2] and Sebastian Ahnert[1,2] — [1]Cavendish Laboratory, Univeristy of Cambridge — [2]Sainsbury Laborary, University of Cambridge

Using a tractable lattice self assembly model to produce polyomino phenotypes from numeric genotypes, along with genetic algorithms and fitness proportional selection, allows abstract evolutionary behaviour to be probed in great detail. Comparing a static fitness landscape with a landscape with periodically changing fitness sub goals yields novel behaviour that can be approached analytically. In particular, we find dynamic landscapes, despite only selecting for subsets of goals at any given time, on average solve the total fitness goal faster than static landscapes.

The genotype space, and hence the genotype to phenotype mapping, is unchanged between the static and dynamic cases. As such, the distinct evolutionary behaviour must originate from the paths through the landscape populations take to reach global fitness peaks. Considering purely information-theoretic quantities like the genotype robustness, upper and lower bounds can be found for the oscillation period yielding optimal solving discovery rates.

Additionally, landscapes with longer oscillation periods typically use more genotype coding to produce an equivalent phenotype, indicating that more rapidly oscillating landscapes yield more modular genotypes in response to the more dynamic environment. Such findings are widely applicable to genetic algorithms with complex fitness landscapes.

DY 45.5 Wed 11:00 BH-N 333

Active textiles with Janus filaments — •Len Pismen and Andrei Zakharov — Technion - Israel Institute of Technology

We describe reshaping of active textiles actuated by bending of Janus filaments comprising both active and passive components. A great variety of shapes, determined by minimising the overall energy of the fabric, can be produced by varying bending directions determined by the orientation of Janus filaments. Under certain conditions, alternative equilibrium states, one absolutely stable and the other metastable coexist, and their relative energy may flip its sign as system parameters, such as the extension upon actuation, change. A snap-through reshaping in a specially structured textile reproduces the Venus flytrap effect.

DY 45.6 Wed 11:15 BH-N 333

Local weather driven model for the potential West Nile Virus spread in Germany — •Suman Bhowmick[1,3], Hartmut H. K. Lentz[1], Philipp Lorentz[2], Philipp Lorentz Hövel[2], and Igor Sokolov[3] — [1]Institut für Epidemiologie, Friedrich Loeffler Institut, Germany — [2]Institut für Theoretische Physik, TU Berlin, Germany — [3]Institut für Physik, HU Berlin, Germany

We endeavoured to explore the possible role of the migratory birds in the potential spread of West Nile Virus (WNV) in Germany through a compartment based, mechanistic model. It is of SEIR (susceptible-exposed-infected-removed) type to decipher the intricacy of the spreading dynamics of the WNV. The parameters associated with the model are temperature driven. In addition to that we have considered the seasonal appearance and disappearance of the migratory birds. As results, we will present the numerical solutions of the local infection model as well as an analytical expression for the basic reproduction number R0 and its dependence on the temperature. The phase plots demonstrate two very different kinds of dynamics in Germany. In the north where the temperature is quite low, the phase portrait shows the stable nontrivial equilibrium where as in the south due to the warmer weather, we have found stable limit cyclic behaviour. Potential risk map of the spread of WNV shall be investigated through the coupling of local ODE model with the constructed migratory birds network. Keywords Epidemiological model, Bird migration, Network, Sensitivity analysis, Vector borne disease

15 min. break

DY 45.7 Wed 11:45 BH-N 333

Nonlinear Dynamics of Calcium Cycling in Cardiomyocytes — •Filippo G. Cosi[1], Stefan Luther[1,2,3,4,5], and Ulrich Parlitz[1,2,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August-Universität Göttingen, Institute for Nonlinear Dynamics, Göttingen, Germany — [3]University Medical Center Göttingen, Institute of Pharmacology and Toxicology, Göttingen, Germany — [4]DZHK (German Center for Cardiovascular Research), partnersite Göttingen, Germany — [5]Department of Physics and Department of Bioengineering, Northeastern University, Boston, USA

Delayed or early after depolarisations and Calcium alternans inside single cardiomyocytes are known to alterate the sane dynamics of the muscle cell leading to heart defects and even failure on a greater scale.

Defects in the subcellular components, like Rynodine Receptors (RyR) or Sodium-Calcium Exchangers (NCX) are believed to be the cause of these depolarisations and alternans. In our project, we therefore investigate how these defects are influencing the Calcium and membrane potential dynamics on a cellular scale. A mathematical model including both, the stochastic nature of the cellular components and the whole cell Calcium dynamics, is developed.

Calcium waves, showing a sequential and spontaneous activation of the cell, are presented as results of the model together with the main structure of the algorithm. Diffusive Calcium waves are assumed to be one of the symptoms of diseased ventricular cardiomyocytes causing Calcium alternans and delayed after depolarisations.

DY 45.8 Wed 12:00 BH-N 333

A minimal model to study pH-dependent phase separation — •Omar Adame-Arana[1], Christoph A. Weber[1,2], Vasily Zaburdaev[1], Jacques Prost[3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Paulson School of Engineering and Applied Sciences, Harvard University, Pierce Hall 412, 28 Oxford Street Cambridge, MA 02138, USA — [3]Institut Curie, 26 rue d'Ulm, 75248 Paris Cedex 05, France

Liquid phase separation is ubiquitous in nature. There is an increasing interest in studying the role of the formation of liquid like droplets as an organizer of the cell cytoplasm. pH influences the charge state of macromolecules such as proteins and can therefore affect phase separation. We propose a minimal model to study how pH can influence the phase separation of a solution composed of macroions of different charge states. We couple a phase separating system to chemical reactions associated with pH. Using this model we first construct the corresponding phase diagrams at the isoelectric point and study the effects of different interaction parameters on the phase diagrams. We then study the effects of changes of pH on phase diagrams. We find that phase separation is most pronounced near the isoelectric point.

DY 45.9 Wed 12:15 BH-N 333

Nonequilibrium force-velocity relation for single polymerization motor — •Thomas Niedermayer[1,2] and Reinhard Lipowsky[2] — [1]Physikalisch-Technische Bundesanstalt (PTB), Berlin — [2]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam

In biological cells, the force generating assembly of cytoskeletal filaments is a nonequilibrium process which is coupled to the hydrolysis of bound nucleotides. This complex phenomenon may be captured by a stochastic process involving the association, aging, and dissociation of subunits. Necessarily, aging increases the shrinkage velocity of filaments under load and decreases the stall force. A recently proposed recursive solution for the stochastic process enables us to calculate the force-velocity relation for single cytoskeletal filaments in agreement with extensive stochastic simulations. Both for actin filaments and microtubules, we predict the onset of fast depolymerization slightly above the stall force. This effect involves strong correlations of the subunit states, underlining the failure of mean field calculations.

DY 45.10 Wed 12:30 BH-N 333

Dynamics and Thermodynamics of Chemical Reaction Networks — •Riccardo Rao and Massimiliano Esposito — Complex Systems and Statistical Mechanics, Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, G.D. Luxembourg

Chemical Networks (CN) are large sets of coupled chemical reactions where some of the species are externally controlled. Cell metabolism and biochemical signal transduction networks are notable examples of CN. We present a rigorous nonequilibrium thermodynamic description of CN in terms of deterministic rate equations. Our description is inspired by Stochastic Thermodynamics and is based on Chemical Re-

action Network Theory. The energy and entropy balances of CN are derived and a nonequilibrium Gibbs free energy is introduced. This latter is related to the chemical work necessary to sustain nonequilibrium steady states and to the driving work necessary to control the network far from equilibrium. We finally discuss these different forms of work in the stochastic framework.

[1] R. Rao and M. Esposito, Nonequilibrium Thermodynamics of Chemical Reaction Networks: Wisdom from Stochastic Thermodynamics, Phys. Rev. X, 2016, 6, 041064.

DY 45.11 Wed 12:45 BH-N 333

Thermodynamically Consistent Coarse Graining of Biocatalysts beyond Michaelis–Menten — •Artur Wachtel, Riccardo Rao, and Massimiliano Esposito — Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg

Virtually all processes in living cells involve catalytic molecules to enhance chemical reactions: various enzymes process metabolites and signaling molecules, catalytically active membrane proteins serve as transporters or receptors for chemical signals.

In this talk we start from the detailed catalytic mechanism of a single biocatalyst and we provide a coarse-graining procedure which, by construction, is thermodynamically consistent even out of equilibrium: This procedure provides stoichiometries, reaction fluxes (kinetic rate laws), and reaction forces (Gibbs energies of reaction) for the coarse-grained level. It can treat active transporters and molecular machines, and thus extends the applicability of ideas that originated in enzyme kinetics. We thus identify the conditions under which a relation between one-way fluxes and forces holds at the coarse-grained level as it holds at the detailed level. In doing so, we clarify the speculations and broad claims made in the literature about such a general flux–force relation. As a further consequence we show that, in contrast to common belief, the second law of thermodynamics does not require the currents and the forces of biochemical reaction networks to be always aligned.

[1] A. Wachtel, R. Rao and M. Esposito, arXiv:1709.06045 (2017)

DY 45.12 Wed 13:00 BH-N 333

Entropic Allostery of Protein Binding and 'Allosteron' Networks — •Alice C. von der Heydt and Tom C.B. McLeish — Dept of Physics, Durham University, Durham, DH1 3LE, UK

Proteins form an essential part of all living organisms. Effector-binding and self-assembly are vital to their biological function. Allostery, *i.e.*, non-local signal transduction and co-operativity among distant sites of a protein, does not imply binding to cause major structural changes. Entropic allostery, instead, rests upon a subtle tuning of the amplitudes and the spectrum of thermal fluctuation modes, to enable binding co-operativity. This mechanism (Cooper and Dryden, 1984) may provide the main part of the allosteric free energy if collective, long-wavelength modes dominate the density of thermally accessible states, and thus, coarse-grained models apply. In an effort to establish a theory of entropic allostery and to elucidate the range of applications, we construct and analyse a basic toy-model unit, the 'allosteron', and its association into networks akin to protein complexes. An allosteron is equipped with both internal and coupling, harmonic degrees of freedom whose interaction strengths can be modified through binding of ligands. Physical interaction strengths derive from a class of Lennard-Jones potentials defined via the balance of attractive and repulsive (entropic) forces. The impact of entropic allostery is demonstrated and discussed for the binding of proteins and their assemblies, such as ring oligomers, that are suitably modelled by coupled allosterons.

DY 45.13 Wed 13:15 BH-N 333

Estimation of the infinitesimal generator by square-root approximation — •Luca Donati[1], Martin Heida[2], Bettina Keller[1], and Marcus Weber[3] — [1]Freie Universität Berlin, Berlin, Germany — [2]WIAS, Berlin, Germany — [3]ZIB, Berlin, Germany

The dynamics of molecular systems can be represented by a continuous operator, called Propagator, that propagates probability densities with time. Associated to the Propagator, there exists another operator, called infinitesimal Generator, that defines the Fokker-Planck equation and provides information about the dynamics of the system in terms of transition rates between states. We have studied a method to obtain the discretized version of the Generator.

The method considers a Voronoi tasselleation of the conformational space and exploits the Gauss theorem to write the instantaneous rate between adjacent cells in terms of the Boltzmann weight of the intersecting surface. This quantity can be approximated by the geometric average of the Boltzmann weights of the cells.

We also show that there exists a direct correlation between the Generator and the potential energy function of the system. The method can be used to study the effect on dynamics of the system of small thermodynamic changes or perturbations of the potential energy function. We present results for 2d diffusion process and Alanine dipeptide.

DY 46: Microswimmers (joint session BP/CPP/DY)

Time: Wednesday 15:00–17:30 Location: H 1028

Invited Talk DY 46.1 Wed 15:00 H 1028

Emergent Dynamics of Active Particles — •Roland G. Winkler — Institute for Advanced Simulation, Forschungszemtrum Jülich, 52425 Jülich, Germany

The stationary-state structural and dynamical properties of microswimmers are governed by their shape and hydrodynamic interactions, but also the effective dimensionality of the system matters, i.e., three-dimensional bulk versus thin film. As a generic approach for microswimmers, we have developed a model for a spheroidal squirmer, with hydrodynamics implemented by the multiparticle collision dynamics approach [1,2]. We study the swimming behavior, cooperative motion, and motility-induced phase separation (MIPS) of such squirmers in a narrow slit. For two squirmers, surface hydrodynamic interactions strongly influences their cooperative motion [2]. Considering the phase behavior of many squirmers, hydrodynamic interactions suppress MIPS for spherical squirmers. In contrast, hydrodynamic interactions enhance MIPS for elongated squirmers. Moreover, the shape affects the rheological properties of squirmers in shear and Poiseuille flow.

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

[2] M. Theers, E. Westphal, G. Gompper, R. G. Winkler, Soft Matter 12, 7372 (2016)

DY 46.2 Wed 15:30 H 1028

Magnetic behavior and chemotaxis of magnetic bacteria — •Agnese Codutti[1], Damien Faivre[1], and Stefan Klumpp[2] — [1]Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany — [2]Georg-August-Universität Göttingen Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Chemotaxis is the bacterial ability to bias their motility toward a preferred concentration of attractants or repellents. This chemotactic ability can be used by magnetic bacteria, coupling it to a passive alignment to external magnetic fields. Magnetic bacteria include the naturally-occurring magnetotactic bacteria, and lab-produced biohybrids, in which for example E. coli can be coupled to external magnetic beads. Therefore, a model to understand the coupling between magnetic fields, active swimming, and chemotaxis is needed to predict the behavior of these systems. We perform simulations based on an Active Brownian Particle model, modified to include active swimming, active changes of directions, chemotaxis, and passive alignment with external magnetic fields. The model allows us to reproduce the capillary experiments, and to throw some light on the possible aerotaxis models shown by magnetotactic bacteria. As main results, we show how run and tumble motion hinders the chemotactic/aerotactic abilities of the bacteria when coupled with magnetic fields, while run and reverse motility benefits from the magnetic field, leading to faster chemotaxis. We explore different magnetic behaviors of magnetotactic bacteria, where cells are either simply aligned by the external field or alternatively using it as proxy of oxygen gradient.

DY 46.3 Wed 15:45 H 1028

The bacterial soliton in a nutrient field – re-examined — •Andrzej Palugniok[2], Maximilian Seyrich[1], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Worcester College, University of Oxford, Walton Street, OX1 2HB Oxford, United Kingdom

The gut bacterium *E. coli* with its run-and-tumble walk is a well-studied model swimmer in the active-matter field. One of the various interesting collective phenomena is a bacterial soliton or a traveling concentration pulse of bacteria [1]. It develops when bacteria start to consume a nutrient in an initially uniform field, in which they also perform chemotaxis.

To describe such a situation, we start from a Smoluchowski equation of a run-and-tumble particle in a chemotactic field. A Markovian tumble rate is derived from the usual linear response theory. We perform a multipole expansion to derive equations for the bacterial density and the local polar order decribed by the bacterial polarization. On times longer than the typical relaxation time for the polarization, one recovers the Keller-Segel equation. Solving it together with the diffusion equation for the nutrient, we are able to reproduce the bacterial soliton. Thereby, we demonstrate that one does not need a second, signalling chemical field as introduced in Ref. [1] nor a singular chemotactic drift term as demanded in Ref. [2].

[1] J. Saragosti et al., PNAS **108**, 39 (2011).
[2] E.F. Keller and L.A. Segel, J. Theor. Biol., **30**, 2 (1971).

DY 46.4 Wed 16:00 H 1028

Dynamic Propulsion Force Measurements of Chlamydomonas Microalgae using Micropipette Force Sensors — •Thomas Josef Böddeker, Christian Titus Kreis, Quentin Magdelaine, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, D-37077 Göttingen, Germany

Although the swimming dynamics of microbes, such as bacteria and microalgae, have received a lot of attention in recent years, methods for direct propulsion force measurements are still limited. We present a new approach utilizing micropipettes as force sensors to study the propulsion forces and wall interactions of the unicellular, biflagellated microswimmer *Chlamydomonas*. Fourier signal analysis of the micropipette deflection reveals a clear signature of the energy output of the microswimmer and provides a handle to measure the frequency and energy associated to the flagella beating. Continuous measurements in a liquid cell allow us to characterize the propulsion of individual cells and to probe the extent of steric and hydrodynamic interactions between beating flagella and solid interfaces. For controlled environmental conditions, we quantify the difference in propulsion energy and beating frequency between swimming in bulk and in close proximity to solid interfaces.

DY 46.5 Wed 16:15 H 1028

Applying an Extended Kalman Filter to extract bacteria statistics — •Oliver Köhn — Universität des Saarlandes

Bacteria tend to swim in liquids in absence of food facilitated by creation of flagella. The trajectories are determined by slightly curved lines (running states) and randomly interrupted by short intervals with strong direction changes (tumbling state)[1]. This behavior seems to be efficient in finding food in unknown environments. We assume an intrinsic randomness in the running states as well in the appearance of the tumbling intervals.[1] Furthermore in real experiments the extracted positions are influenced by a detection noise. Estimating the stochastic trajectory properties requires the distinction between bacteria intrinsic randomness and the measurement noise. From the engineers it is known that the Kalmann filter algorithm provide this in an optimal way [2]. We adapted and implemented this filter for simulated as well as measured bacteria trajectories.

[1] Enhancing bacterial motility and search efficiency by genetic manipulation of flagellar number; Javad Najafi, M. Reza Shaebani, Thomas John, Florian Altegoer, Gert Bange & Christian Wagner; submitted to PNAS [2] Forecasting, structural time series models and the Kalman filter; Andrew C. Harvey; 1989; Cambridge University Press

DY 46.6 Wed 16:30 H 1028

Phase diagram of a low Reynolds number swimmer near a wall — •Abdallah Daddi-Moussa-Ider[1], Maciej Lisicki[2,3], Christian Hoell[1], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, Düsseldorf 40225, Germany — [2]Department of Applied Mathematics and Theoretical Physics, Wilberforce Rd, Cambridge CB3 0WA, United Kingdom — [3]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

The hydrodynamic flow field generated by self-propelled active particles and swimming microorganisms is strongly altered by the presence of nearby boundaries in a viscous flow. Using a simple model swimmer composed of three-linked spheres, we show that the swimming trajectories near a non-slip wall reveal various interesting scenarios of motion depending on the initial orientation and the distance separating the swimmer from the wall. Accordingly, the swimmer can either be trapped by the wall, totally escape from the wall, or undergo an oscillatory gliding motion at a constant mean height above the wall. Using a far-field approximation, we find that the wall-induced correction at leading order has a quadrupolar flow structure where the translational and angular velocities of the swimmer decay as inverse third and fourth power with distance, respectively. The resulting equations of motion for the trajectories and the relevant order parameters fully characterize the transition between the phases and allow for an accurate description of the swimming behavior near a wall.

DY 46.7 Wed 16:45 H 1028

Three-dimensional simulation of sperm in structured microfluidic channels — •Sebastian Rode, Jens Elgeti, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems (ICS-2) , Forschungszentrum Jülich, 52425 Jülich, Germany

Sperm cells propel themselves by a periodic wave-like beating of their flagellum [1-3]. At low Reynolds numbers and in confinement, the directed motion of sperm and other microswimmers is strongly influenced by steric and hydrodynamic surface interactions [1]. We model sperm motility in our mesoscale hydrodynamics simulations by imposing a planar traveling bending wave along the flagellum [2]. For swimming in zigzag shaped microchannels, we find that the deflection angle of a sperm cell at sharp corners depends on the orientation of its beating plane. Our results are in good agreement with recent microfluidic experiments, and help to improve the understanding of sperm cell navigation under strong confinement. We show that the emergence of a nonplanar component of the flagellar beat with increasing wavelength drastically increases surface attraction.

[1] J. Elgeti et al., Rep. Prog. Phys. 78, 056601 (2015) [2] J. Elgeti et al., Biophys. J. 99, 1018 (2010) [3] G. Saggiorato et al., Nat. Commun. 8, 1415 (2017)

DY 46.8 Wed 17:00 H 1028

Altering diffusion by interaction of microalgae with micron-sized objects — •Francine Kolley[1,2], Patricia Dähmlow[2], Hajnalka Nadasi[2], Florian von Rüling[2], and Alexey Eremin[2] — [1]Technical University Dresden — [2]Otto-von-Guericke-University Magdeburg

The enhancement of passive particles, single silica spheres and their doublets, was studied in suspensions containing microswimmers Chlamydomonas reinhardtii. These green algae move with a flagellar motor, reaching typical velocities up to 150 μm/s. Stimulated by phototaxis, their motion is similar to humans doing breaststroke. The induced flow of the puller affects the translational as well as the rotational diffusion of the passive particles. The corresponding diffusion coefficients were obtained from the measurement of the mean square displacements of the passive particles for various concentrations of the algae. The Brownian Motion of the silica beads was observed in a quasi-2D system in flat cappilaries.To avoid cell immobilization by adsorption to the glass substrate the capillary surface was silanized. Additionally, a polymer was introduced to the suspension to optimize the diffusive behavior. In the range of small algae concentrations, the diffusion coefficients exhibited a linear dependence on the cell density of Chlamydomonas reinhardtii.

DY 46.9 Wed 17:15 H 1028

Dynamics of chemotactic and chemokinetic bacterial populations — •Theresa Jakuszeit[1], James Lindsey-Jones[1], François J. Peaudecerf[2], and Ottavio A. Croze[1] — [1]Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Institute of Environmental Engineering, ETH Zürich, Stefano-Franscini-Platz 5, 8093 Zürich, Switzerland

Several motile bacteria are able to sense chemical gradients much larger than their own size, and perform a random walk biased up attractant gradients ('chemotaxis') by varying their reorientation rate. In addition to this well-known chemotactic behaviour, several soil and marine bacterial species are known to modify their swimming speed according to the local concentration of chemoattractant ('chemokinesis'). Therefore, a chemical field of attractant induces a spatially varying swimming speed, which results in a drift towards lower attractant

concentrations – contrary to the drift created by chemotaxis.

Here, to explore the biological benefits of chemokinesis and investigate its impact on the chemotactic response, we extend a Keller-Segel type model to include a dependence of the swimming speed on the attractant concentration. Even though chemokinesis on its own results in a dispersion of the population away from high attractant concentrations, it can not only enhance the chemotactic response but also modify it qualitatively. We apply the model to predict the dynamics of bacteria capable of chemokinesis and chemotaxis in experimentally inspired chemoattractant fields, such as those generated in capillary migration assays and around environmental nutrient sources.

DY 47: Nonequilibrium Quantum Many-Body Systems II (joint session TT/DY)

Time: Wednesday 15:00–18:30 Location: H 3010

Invited Talk DY 47.1 Wed 15:00 H 3010

Efficient Simulation of Quantum Thermalization and Dynamics — •Frank Pollmann — Department of Physics, Technical University of Munich, 85748 Garching, Germany

The past decade has seen a great interest in the question about whether and how quantum many-body system locally thermalize. It has been driven by theoretical findings involving the long sought demonstration that many-body localization (MBL) exists as well as the derivation of exact bounds on chaos. In my talk, I will introduce matrix-product state (MPS) based methods that allow for an efficient numerical simulation of the quantum thermalization dynamics. Firstly, I will show that, contrary to the common belief that the rapid growth of entanglement restricts simulations to short times, the long time limit of local observables can be well captured using the MPS based time-dependent variational principle. Secondly, I will discuss how mixed states can be represented using dynamically disentangled purified states. These novel methods allow to extract transport coefficients, e.g. the energy diffusion constant, efficiently.

DY 47.2 Wed 15:30 H 3010

Prethermalization without canonical transformations — Marc Alexander and •Marcus Kollar — Theoretische Physik III, Universität Augsburg

Weakly quenched quantum systems often exhibit a prethermalization regime on short to intermediate time scales, which is usually derived using canonical transformations [1,2]. We show how to skip this step and directly obtain the transient behavior, the long-time average, and the dressed constants of motion for arbitrary time-dependent protocols. We apply these results to fermionic Hubbard models for a variety of time-dependent perturbations.

[1] M. Moeckel and S. Kehrein, Phys. Rev. Lett. **100**, 175702 (2008)
[2] M. Kollar et al., Phys. Rev. B **84**, 054304 (2011)

DY 47.3 Wed 15:45 H 3010

Universal prethermal states in slowly driven many-body systems — •Tobias Gulden[1], Netanel Lindner[1], Erez Berg[2], and Mark Rudner[3] — [1]Technion - Israel Institute of Technology — [2]University of Chicago — [3]University of Copenhagen

A key challenge in the search for new non-equilibrium phases of matter is the tendency of closed many-body systems to indefinitely absorb energy from a driving field. Generically this leads to an infinite temperature state where any interesting quantum, and in particular topological, effects are washed out. Here we show that in fact heating can be used as a resource for establishing universal prethermal behavior which exhibits topological phenomena. The prethermalization regime which we consider occurs for low driving frequencies, and persists throughout a long time window. Recently such prethermal states were found in one dimensional topological pumps [Lindner, Berg, Rudner, PRX 2017]. We provide bounds on the lifetimes of states, study different manifestations of universal prethermal behavior in a variety of systems, and discuss probes for observing topological properties.

DY 47.4 Wed 16:00 H 3010

Non-Equilibrium Steady State Quantum Systems — •Michael Schuett and Markus Mueller — Condensed Matter Theory Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Recent experimental advances have sparked a growing interest in quantum systems out of equilibrium. Such systems can exhibit phenomena not found in equilibrium. A frequent price payed for this freedom is the intractability of the non-equilibrium system. Here we consider a tractable toy model, rich enough to exhibit interesting non-equilibrium properties in a driven steady state. Being a well characterized fixed point, the steady state selects a specific state from the vast set of out of equilibrium states. The scenario we consider are non-interacting Fermions driven around a mesoscopic scatterer. We construct the driven, current-carrying many-body state, based on non-interacting scattering states and determine the non-equilibrium Friedel oscillations. We show, based on non-interacting scattering states that experimentally detectable oscillatory magnetic field patterns arise from the emerging current pattern. Finally we generalize our construction of the steady states to include interactions and conclude with an outlook on interaction induced instabilities or chaoticity.

DY 47.5 Wed 16:15 H 3010

Non-equilibrium steady state of the ionic Hubbard model in strong electric fields — •Yusuf Mohammed[1] and Martin Eckstein[2] — [1]Universität Hambrug, Hamburg, Germany — [2]FAU, Erlangen, Germany

We investigate the transport properties and non-equilibrium steady state phases of the dissipative ionic Hubbard model driven by an electric field. In the ionic Hubbard model, metallic behavior is enhanced by a competition of band insulating and Mott insulating behavior. The system is analyzed by means of the inhomogeneous dynamical mean-field theory (DMFT), using the iterated perturbation theory as impurity solver. The steady states of this model are accessed directly through the Keldysh contour formalism. We found that with increasing electric field the sublattice polarization reduces, leading to a decrease in the screening of the gap and an increase in the electronic scattering rate. This results in a smaller current in the nonlinear regime of correlated ionic insulators compared the non interacting case. In addition, we observed a quasi-thermal distributions even in the negative differential resistance regime, due to electron-electron scattering.

15 min. break.

DY 47.6 Wed 16:45 H 3010

Irreversible dynamics in quantum many-body systems — •Markus Schmitt[1,2] and Stefan Kehrein[1] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany

Irreversibility, despite being a necessary condition for thermalization, still lacks a sound understanding in the context of quantum many-body systems. In our work [1] we approach this question by studying the behavior of generic many-body systems under imperfect effective time reversal, where the imperfection is introduced as a perturbation of the many-body state at the point of time reversal. Based on numerical simulations of the full quantum dynamics we demonstrate that observable echos occurring in this setting decay exponentially with a rate that is intrinsic to the system meaning that the dynamics is effectively irreversible.

[1] M. Schmitt and S. Kehrein, arXiv:1711.00015

DY 47.7 Wed 17:00 H 3010

Absence of dynamical localization in interacting driven systems — •David J. Luitz[1], Yevgeny Bar Lev[2,3], and Achilleas Lazarides[3] — [1]Physik Department T42, Technische Universität München, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

Using a numerically exact method we study the stability of dynamical localization to the addition of interactions in a periodically driven isolated quantum system which conserves only the total number of particles. We find that while even infinitesimally small interactions destroy dynamical localization, for weak interactions density transport is sig-

nificantly suppressed and is asymptotically diffusive, with a diffusion coefficient proportional to the interaction strength. For systems tuned away from the dynamical localization point, even slightly, transport is dramatically enhanced and within the largest accessible systems sizes a diffusive regime is only pronounced for sufficiently small detunings.
[1] D. J. Luitz, Y. Bar Lev, A. Lazarides, *SciPost Phys.* **3**, 029 (2017)

DY 47.8 Wed 17:15 H 3010

Impurity induced quench dynamics in shallow Fermi seas: an analytic treatment — •Conor Jackson and Bernd Braunecker — University of St Andrews, St Andrews, United Kingdom

We investigate the Loschmidt echo for a system of free fermions after the introduction of a local quench impurity, taking account of the finite band depth. For a system with a large bandwidth, the sudden introduction of an impurity leads to the well-known Fermi-Edge Singularity and a characteristic power law decay in the Loschmidt echo in the long time limit. We examine analytically the effect of the finite band bottom at intermediate time scales, using a Riemann-Hilbert approach to evaluate the functional determinants induced by the fermionic statistics. On these time scales we find disruption of the entire Fermi sea, rather than simply the surface shakeup which leads to the standard result, and we can provide an analytic explanation of previous numerical results.

DY 47.9 Wed 17:30 H 3010

Anomalous Spin Precession under a Geometrical Torque — •Christopher Stahl[1,2] and Michael Potthoff[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg

Precession and relaxation predominantly characterize the real-time dynamics of a spin driven by a magnetic field and coupled to a large Fermi sea of conduction electrons. We demonstrate an anomalous precession with frequency higher than the Larmor frequency or with inverted orientation in the limit where the electronic motion adiabatically follows the spin dynamics. For a classical spin, an analytic expression which identifies the finite spin Berry curvature of the conduction electrons as the origin of the anomalous frequency is derived. Complementary studies for the minimal model of two coupled spins and calculations for the Kondo-impurity model verify that the anomalous precession is also present for a quantum spin and suggest that the derived formula for the frequency of the classical spin can be applied to the quantum case by replacing the classical spin components by the corresponding expectation values.
[1] C. Stahl and M. Potthoff, PRL 119, 227203 (2017)

DY 47.10 Wed 17:45 H 3010

The Lipkin-Meshkov-Glick model with Markovian dissipation — •João S. Ferreira and Pedro Ribeiro — CeFEMA, Instituto Superior Técnico, Universidade de Lisboa Av. Rovisco Pais, 1049-001 Lisboa, Portugal

Motivated by recent prototypes of engineered atomic spin devices, we study a fully connected system of n spins 1/2, modeled by the Lipkin-Meshkov-Glick (LMG) model of a collective spin $s = n/2$, in the presence of Markovian dissipation processes. Employing semi-classical and variational methods and a systematic Holdstein-Primakov mapping, we determine the semi-classic equations of motion, the phase diagram and spectral properties of the Liouvillian by studying both the thermodynamic limit and $1/s$ corrections. Our approach reveals the existence of: dynamical phase transitions for finite s, tri-stable steady state regions and recurrent regions where the system fails to thermalize.

DY 47.11 Wed 18:00 H 3010

Tripartite information and scrambling in quantum lattice models — •Oskar Schnaack[1], Sebastian Paeckel[1], Thomas Köhler[1], Salvatore R. Manmana[1], Stefan Kehrein[1], and Markus Schmitt[1,2] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

The tripartite information has been introduced as a quantitative observable-independent measure of scrambling by Hosur et al. [1]. We investigate its time-evolution for quantum lattice models with tunable integrability breaking and demonstrate that in contrast to integrable models generic systems scramble information irrespective of the chosen partitioning of the lattice. To compute the information measures of interest we introduce exact representations of permutation operators to obtain entanglement entropies of embedded subsystems using matrix product states.
[1] P. Hosur, X.-L. Qi, D. A. Roberts, B. Yoshida, JHEP02 (2016) 004

DY 47.12 Wed 18:15 H 3010

Real-time dual bosons: role of magnetic time scales. — •Sergey Brener — Universität Hamburg, Germany

We describe magnetic dynamics within the framework of dual bosons on keldysh contour. In particular the role of separating of electron and magnetic time-scales is considered.

DY 48: Talk V. Latora (joint session DY/SOE)

Time: Wednesday 15:00–15:30 Location: MA 001

Invited Talk DY 48.1 Wed 15:00 MA 001

Network structure and dynamics: when and how multiplex really matters? — •Vito Latora — School of Mathematical Sciences, Queen Mary University of London, London E1 4NS, United Kingdom

After almost ten years of research on characterising the properties of real-world multiplex networks, describing mathematically their structure, and modelling different types of dynamical process occurring over them, it is now time to draw the first conclusions and to try to answer a fundamental question: Does multiplex really matter? Focusing here both on the structure and on dynamics of multiplex networks, we discuss some cases where multiplexity gives rise to the emergence of novel behaviors, otherwise unobserved in single-layer networks.

DY 49: Talk J. Lagerwall

Time: Wednesday 15:00–15:30 Location: BH-N 334

Invited Talk DY 49.1 Wed 15:00 BH-N 334

Nanorod fractionation via lyotropic liquid crystal formation, and its effect on phase diagram and gelation — Camila Honorato-Rios[1], Claudius Lehr[1], Christina Schütz[1], Roland Sanctuary[1], Mikhail Osipov[2], Jörg Baller[1], and •Jan Lagerwall[1] — [1]University of Luxembourg, Physics and Materials Science Research Unit, Luxembourg — [2]University of Strathclyde, Mathematics & Statistics, Glasgow, Scotland (UK)

Colloidal nanorod suspensions of sufficient volume fraction may undergo two characteristic macroscopic phenomena, both related to the nanorod shape. On the one hand, the rods may spontaneously develop long-range order, i.e., they form a nematic liquid crystal phase. In case of length-disperse suspensions at phase coexistence, the higher aspect ratio rods preferentially go to the nematic fraction. On the other hand, connectivity percolation between rods may take place and the macroscopic sample arrests into a gel phase. The threshold for both phenomena decreases with increasing rod aspect ratio. We use the spontaneous fractionation by rod aspect ratio upon liquid crystal formation, repeatedly, to separate cellulose nanocrystals by length. Interestingly, an increased aspect ratio strongly benefits liquid crystal formation, but it has no impact on gelation. We argue that the critical factor for the gelation is not the physical rod aspect ratio but rather the amount of counter ions in solution. Above threshold the rods aggregate in an aligned manner, forming 'suprarods' that reach the required length for percolation, triggering the macroscopic gelation.

DY 50: Quantum Dynamics, Decoherence and Quantum Information (joint session DY/TT)

Time: Wednesday 15:30–18:15 Location: EB 107

DY 50.1 Wed 15:30 EB 107

Modeling Dye-Mediated Photon-Photon Interaction in Condensates of Light — Milan Radonjić[1], •Wassilij Kopylov[2], Antun Balaž[1], and Axel Pelster[3] — [1]Institute of Physics Belgrade, University of Belgrade, Serbia — [2]Department of Physics, TU Berlin, Germany — [3]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany

Based entirely on the Lindblad master equation approach we obtain a microscopic description of photons in a dye-filled cavity, which features condensation of light [1,2]. To this end we generalize the nonequilibrium approach of Ref. [3] such that the dye-mediated contribution to the photon-photon interaction in the light condensate is accessible. We describe the dynamics of the system by analyzing the resulting equations of motion. In particular, we discuss the existence of two limiting cases for steady states: photon BEC and laser-like. In the former case, we determine the corresponding dimensionless interaction strength relying on realistic experimental data and find a good agreement with the previous theoretical estimate [4]. Furthermore, we investigate how the dimensionless interaction strength depends on the respective system parameters such as the effective temperature of the dye and the number of the dye molecules.

[1] J. Klaers et al., Nature 468, 545 (2010)
[2] R. A. Nyman and M. H. Szymanska, Phys. Rev. A 89, 033844 (2014)
[3] P. Kirton and J. Keeling, Phys. Rev. Lett. 111, 100404 (2013)
[4] E. C. I. van der Wurff et al., Phys. Rev. Lett. 113, 135301 (2014)

DY 50.2 Wed 15:45 EB 107

Optimized polarization control in a Central-Spin System — •Alessandro Ricottone[1], Yi Nan Fang[2], Stefano Chesi[2], and William Coish[1] — [1]Department of Physics, McGill University, Montréal, Québec H3A 2T8, Canada — [2]Beijing Computational Science Research Center, Beijing 100084, China

We study the dissipative dynamics of the central-spin system, where one central spin is homogeneously coupled with many ancilla spins. We find that, due to a combination of the quantum Zeno effect and many-body collective behaviour of the ancilla spins, the dissipation rate can be optimized to minimize the time scale for polarization dynamics. An archetypical example of this model is given by an electron spin coupled to nuclear spins in a quantum dot via hyperfine interactions, but the same Hamiltonian can be applied in many other physical scenarios. These results may be important for protocols to quickly polarize nuclear spins in semiconductor quantum dots or to rapidly and efficiently equilibrate a quantum annealer.

DY 50.3 Wed 16:00 EB 107

Quantum heat transport and rectification through anharmonic chains between reservoirs — •Thomas Motz, Joachim Ankerhold, and Jürgen Stockburger — Ulm University, Institute for Complex Quantum Systems

We present a novel dynamical description of quantum heat transfer through anharmonic chains between thermal reservoirs [1,2]. The approach is non-perturbative in the system-bath coupling and also allows to include disorder and the presence of external driving. Technically, we start from the formally exact stochastic Liouville-von Neumann (SLN) treatment of open quantum dynamics [3] and consider the situation of ohmic dissipation. For purely harmonic chains this leads to a very efficient scheme to study also very long chains and flux-flux correlations. In the anharmonic situation, we particularly study thermal rectification, the impact of disorder, and strong coupling to the heat baths.

[1] J. T. Stockburger and T. Motz, Fortschr. Phys. **65**, 1600067 (2017)
[2] T. Motz et al., New J. Phys. **19** 053013 (2017)
[3] J. T. Stockburger and H. Grabert, PRL **88** 170407 (2002)

DY 50.4 Wed 16:15 EB 107

Stochastic simulation of open-system quantum dynamics: overcoming the curse of non-Hermitian propagation — Konstantin Schmitz[1], Thomas Unden[2], and •Jürgen Stockburger[1] — [1]Ulm University, Institute for Complex Quantum Systems — [2]Ulm University, Intstiute for Quantum Optics

The Stochastic Liouville-von Neumann equation [1] provides an exact numerical simulation strategy for quantum systems coupled to a reservoir with Gaussian fluctuations of arbitrary spectrum (linear dissipation). Individual stochastic samples are propagated with Hamiltonians containing random non-Hermitian terms, leading to poor signal-to noise ratios in some cases. However, the efficiency of this approach has recently improved dramatically through time-domain projection techniques, implemented as reduction operations [2]. In addition, we present two recently developed sampling strategies which show significantly improved scaling with the strength of the dissipative interaction and with the reservoir memory time: a) anticorrelated sampling, exploiting a gauge-like symmetry and b) reducing the non-unitary terms in sample propagation through convex optimization techniques.

[1] J. T. Stockburger and H. Grabert, PRL **88** 170407 (2002)
[2] J. T. Stockburger, EPL **115**, 40010 (2016)

DY 50.5 Wed 16:30 EB 107

Fidelity plateaux from correlated noise in cold-atom quantum simulators — •Scott R Taylor and Chris A Hooley — University of St Andrews, St Andrews, UK

We demonstrate that, in a quantum simulation protocol based on the Hubbard model, correlated noise in the Hubbard parameters leads to arbitrarily long plateaux in the state-preparation fidelity as a function of elapsed time. We argue that this correlated-noise scenario is the generic one in the cold-atom context, since all of the Hubbard-model parameters ultimately depend on the same set of lasers. We explain the formation of such a plateau using the Bloch-sphere representation, deriving analytical expressions for its start and end times and its height.

15 min. break

DY 50.6 Wed 17:00 EB 107

Non-Markovian Quantum Dynamics - On the way to real-time simulations of heat engines — •Michael Wiedmann, Jürgen T. Stockburger, and Joachim Ankerhold — Institute for Complex Quantum Systems, Ulm University, Albert-Einstein- Allee 11, D-89069 Ulm

The experimental miniaturization of heat engines down to the single-atom level questions classical concepts such as work and heat flux. In the regime of higher temperatures, well-established theories from classical thermodynamics apply, where surrounding heat baths exchange energy and particles with a much smaller system of interest. Quantum mechanically, the situation is more intricate though. The non-locality of quantum mechanical wave functions induces system-reservoir correlations and entanglement which may have profound impact on thermodynamic properties, particularly for condensed phase systems at cryogenic temperatures. The fully dynamical approach of the stochastic Liouville-von Neumann equation (SLN) builds an exact, time-local and non-perturbative framework to tackle non-Markovian dynamics at low temperatures, for arbitrarily driven systems and strong coupling [1]. With emphasis on particularities induced by anharmonic potentials, we present an efficient real-time propagation scheme for a single quantum oscillator coupled to dissipative reservoirs. Aspects of work and heat flux are analyzed in the regime of strong system-reservoir couplings and in the context of reservoir fluctuations far from equilibrium.

[1] M. Wiedmann et al., Phys. Rev. A **94**, 052137 (2016).

DY 50.7 Wed 17:15 EB 107

Jump-based feedback control in the Lipkin-Meshkov-Glick model — •Sven Zimmermann — Technische Universität Berlin, Deutschland

We apply a measurement based feedback control scheme to the dissipative Lipkin-Meshkov-Glick model to affect the quantum phase transition [1-3]. Here we use the Wiseman-Milburn control scheme and apply it on the level of the master equation to the system dissipator [4, 5]. Our interest lies in the steady state properties of the Lipkin-Meshkov-Glick system under the feedback action. By numerically calculating the average spin expectation values, we show that the considered control scheme changes the critical point of the phase transition. Furthermore, by investigating the waiting time distribution and the concurrence, we show, that the emission properties of the system and the entanglement can be significantly modified by the considered closed-loop control scheme.

[1] H.J. Lipkin, N. Meshkov and A. Glick, Nucl. Phys., 62, 188 (1965)

[2] S. Morrison and A. S. Parkins PRL 100, 040403 (2008)

[3] W. Kopylov and T. Brandes, NJP 17, 103031 (2015)

[4] H. M. Wiseman and G. J. Milburn, Quantum Measurment Control, Cambrige University Press, Campridge (2010)

[5] G. Kießlich, C. Emary, G. Schaller and T. Brandes, NJP 14, 123036 (2012)

DY 50.8 Wed 17:30 EB 107

Architectures for quantum simulation showing a quantum speedup — •Juan Bermejo-Vega[1], Dominik Hangleiter[1], Martin Schwarz[1], Robert Raussendorf[2], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, Freie Universitat Berlin, 14195 Berlin, Germany — [2]University of British Columbia, Department of Physics and Astronomy, Vancouver, BC, V6T 1Z1, Canada

A main goal in the field of quantum simulation is to demonstrate a quantum speedup (or "quantum computational supremacy"), referring to the experimental realization of a quantum device that computationally outperforms classical computers. In this talk, we present simple and feasible schemes of two-dimensional dynamical quantum simulators with the potential to show such a quantum speedup. In each of the schemes, an initial (potentially disordered) product state is prepared, followed by a short-time evolution under a basic translationally invariant Hamiltonian with nearest-neighbor interactions, and a final measurement in a fixed basis. The correctness of the final state preparation in each scheme is fully efficiently certifiable. Our schemes are tailored to platforms of cold atoms in optical lattices, and cannot be efficiently classically simulated under plausible complexity-theoretic assumptions. This work shows that benchmark settings exhibiting a quantum speedup may require little control in contrast to universal quantum computing. Thus, our proposal puts a convincing experimental demonstration of a quantum speedup within reach in the near term.

DY 50.9 Wed 17:45 EB 107

Analytical results for the non-Markovianity of quantum spin ensembles — •Remy Dubertrand[1,2], Alexandre Cesa[2], and John Martin[2] — [1]Institut für Theoretische Physik Universität Regensburg 93040 Regensburg, Germany — [2]Institut de Physique Nucleaire, Atomique et de Spectroscopie, CESAM, University of Liege, Bat. B15, B - 4000 Liege, Belgium

We study the non-Markovian character of spin ensembles. The ensemble is assumed to be isolated and a subset of spins is taken as the system, while the remaining part of the ensemble is taken as the environment. For a large class of interaction range, we derive analytical expressions for the non-Markovianity [1] following a recently introduced measure [2]. In particular, we investigate the thermodynamic limit and derive conditions to observe a Markovian dynamics or not. For a system of a single spin, it is explicitly shown that our results agree with the other known measures of non-Markovianity. We believe that our work can be used to investigate further the dynamics of fundamental models in condensed matter physics from the new perspective of (non-)Markovianity.

[1] R. Dubertrand, A. Cesa, J. Martin, to be submitted

[2] S. Lorenzo, F. Plastina, and M. Paternostro, Phys. Rev. A 88 (2013)

DY 50.10 Wed 18:00 EB 107

Quantum Dynamics beyond Gaussians: from Coarse Graining to a Tower of Scales via Multiresolution — •Antonina N. Fedorova and Michael G. Zeitlin — Russia, 199178, St.Petersburg, V.O. Bolshoj pr., 61, IPME RAS, Mathematical Methods in Mechanics Group

We present a family of methods which can describe complex behaviour in quantum ensembles. We demonstrate the creation of nontrivial (meta) stable states (patterns), localized, chaotic, entangled or decoherent, from the basic localized modes in various collective models arising from the quantum hierarchy described by Wigner-Moyal-von Neumann-like equations. The advantages of such an approach are as follows: i). the natural description of localized states in any proper functional realization of (Hilbert) space of states, ii). the representation of hidden symmetry of a chosen representation of the functional model describes the (whole) spectrum of possible states via the multiresolution decomposition. Effects we are interested in are as follows: 1. a hierarchy of internal/hidden scales (time, space, phase space); 2. non-perturbative multiscales: from slow to fast contributions, from the coarser to the finer level of resolution/decomposition; 3. the coexistence of the levels of hierarchy of multiscale dynamics with transitions between scales; 4. the manifestation of the key features of the complex quantum world such as the existence of chaotic and/or entangled states with possible destruction in "open/dissipative" regimes due to interactions with quantum/classical environment and transition to decoherent states.

DY 51: Networks: From Topology to Dynamics (joint session DY/SOE)

Time: Wednesday 15:30–18:00 Location: MA 001

DY 51.1 Wed 15:30 MA 001

Mapping and discrimination of networks in the complexity-entropy plane — •Marc Wiedermann[1,2], Jonathan F. Donges[1,3], Jürgen Kurths[1,2], and Reik V. Donner[1] — [1]Potsdam Institute for Climate Impact Research — [2]Humboldt University of Berlin — [3]Stockholm Resilience Centre

Complex networks are usually characterized in terms of their topological, spatial, or information-theoretic properties and combinations of the associated metrics are used to discriminate networks into different classes or categories. However, even with the present variety of characteristics at hand it remains a subject of current research to appropriately quantify a network's complexity and correspondingly discriminate between different types of complex networks on such a basis. Here we explore the possibility to classify complex networks by means of a statistical complexity measure that has formerly been successfully applied to distinguish different types of chaotic and stochastic time series. It is composed of a network's averaged per-node entropic measure characterizing the network's information content and the associated Jenson-Shannon divergence as a measure of disequilibrium. We study 29 real-world networks and show that networks of the same category cluster in distinct areas of the resulting complexity-entropy plane. In particular, connectome networks exhibit among the highest complexity while transportation and infrastructure networks display significantly lower values. We further show that the proposed framework is useful to objectively construct threshold-based networks by choosing the threshold such that the statistical complexity is maximized.

DY 51.2 Wed 15:45 MA 001

Renormalisation group theory for percolation in time-varying networks — •Jens Karschau, Marco Zimmerling, and Benjamin M. Friedrich — cfaed | TU Dresden, Dresden, Germany

Wireless communication networks require reliable routing of messages, despite the fact that individual networks links are unreliable. Multi-hop routing protocols propose a promising solution to overcome the issue of message loss. For these protocols, successful relay of a message defines a percolation problem.

Here, we present a percolation theory for a minimal model, where individual links switch between an active and an inactive state according to a two-state Markov process. Using renormalization group theory, we analytically compute the complete statistics of failure events. We show how the time-dependent probability to find a path of active links between two designated nodes converges towards an effective Bernoulli process, i.e. without memory, as the hop distance between the nodes increases. Our work extends classical percolation theory to the dynamic case. It elucidates temporal correlations of message losses with implications for the design of communication protocols and control algorithms.

Reference: arXiv:1708.05704

DY 51.3 Wed 16:00 MA 001

Self-organized cluster formation in neural networks — •Rico Berner[1,2], Eckehard Schöll[1], and Serhiy Yanchuk[2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Institut für Mathematik, Technische Universität Berlin, Germany

We investigate collective behaviour in a network of adaptively coupled phase oscillators, where the coupling topology depends on the dynamics of oscillators. We show that such a system gives rise to numerous dynamics, including hierarchical multi-clusters and chimera states. Our numerical and analytical results are compared and interpreted with respect to pattern formation due to learning processes and the multi-layer structure of the human brain.

DY 51.4 Wed 16:15 MA 001

Coarsening dynamics of ferromagnetic granular networks - experiment and simulation — •Pedro A. Sanchez[1], Armin Kögel[2], Robin Maretzki[2], Tom Dumont[2], Elena S. Pyanzina[3], Sofia S. Kantorovich[1], and Reinhard Richter[2] — [1]Univ. of Vienna, Sensengasse 8, Vienna, 1090, Austria — [2]Experimentalphysik 5, Univ. of Bayreuth, 95440 Bayreuth, Germany — [3]Federal Univ., Lenin av. 51, Ekaterinburg, 620000, Russia

We investigate the phase separation of a shaken mixture of glass and magnetised steel spheres after a sudden quench of the shaker amplitude. Then transient networks of steel spheres emerge in the experiment. For the developing network we observe an initial regime, where the network incubates, followed by a regime where network structures are elongated and broken, and finally a regime where the structures have relaxed to compact clusters of rounded shapes. This phaenomenology resembles the initial, elastic and hydrodynamic regimes observed by H. Tanaka [J. Phys.: Cond. Mat., 2000] during the viscoelastic phase separation for dynamically asymmetric mixtures of polymers. In order to unveil the three regimes we measure order parameters like the mean number of neighbors and the efficiency.

To eluzidate the origin for a viscoelastic phase separation, we use a simple simulation approach to define the key interactions in the experimental system. This way, we discover that along with dipolar and steric interactions, a central attraction between the magnetised spheres is decisive for the coarsening dynamics. Our simulations show three regimes in the evolution of characteristic order parameters.

DY 51.5 Wed 16:30 MA 001

Coherence resonance in a network of FitzHugh-Nagumo systems: interplay of noise, time-delay and topology — •Maria Masoliver[1], Nishant Malik[2], Eckehard Schöll[3], and Anna Zakharova[3] — [1]Department of Physics, DONLL, Universitat Politècnica de Catalunya — [2]Department of Mathematics, Dartmouth College, Hanover, USA — [3]Institut für Theoretische Physik, Technische Universität, Berlin

The FitzHugh-Nagumo system is a paradigmatic model which describes the excitability and spiking behavior of neurons. This model, in the excitable regime under the influence of noise exhibits the counterintuitive phenomenon of coherence resonance: there exists an optimum intermediate value of the noise intensity for which noise-induced oscillations become most regular. We systematically investigate the phenomena of coherence resonance in time-delay coupled networks of FitzHugh-Nagumo elements in the excitable regime [1]. Using numerical simulations, we examine the interplay of noise, time-delayed coupling and network topology in the generation of coherence resonance. We demonstrate the possibility of controlling coherence resonance by varying the time-delay and the number of nearest neighbors. For a locally coupled ring, we show that the time-delay weakens coherence resonance. For nonlocal coupling with appropriate time-delays, both enhancement and weakening of coherence resonance are possible.

[1] M. Masoliver, N. Malik, E. Schöll, A. Zakharova, Chaos 27, 101102 (2017)

15 min. break

DY 51.6 Wed 17:00 MA 001

A Network Approach to Spin Systems Beyond Nearest-Neighbor Interactions — •Kathinka Gerlinger[1], Julian Heiss[1], Matthias Weidemüller[1,2], Andreas Spitz[3], and Michael Gertz[3] — [1]Physics Institute, Heidelberg University, Heidelberg, Germany — [2]Shanghai Branch, University of Science and Technology of China, Shanghai 201315, China — [3]Institute of Computer Science, Heidelberg University, Heidelberg, Germany

Investigating spin systems as examples of strongly-interacting systems and determining their phase diagram is a central research challenge in complex many-body physics. For the 1D Ising model with only nearest-neighbor interactions, Valdez et al. (arXiv:1508.07041) have recently shown the veracity and efficiency of complex network models with regard to finite-size scaling. We expand the task of finding the quantum phase transition of such spin systems beyond nearest neighbor interactions. To this end, we discuss suitable mappings of spin systems to complex networks and their analysis based on complex network analytic methods. Furthermore we investigate the evolution of spin states on dynamic networks and their relation to physical systems.

DY 51.7 Wed 17:15 MA 001

Self-consistent correlations of randomly coupled rotators in the asynchronous state — •Alexander van Meegen[1,2,3] and Benjamin Lindner[1,2] — [1]Humboldt Universität zu Berlin — [2]Bernstein Zentrum Berlin — [3]Forschungszentrum Jülich

We present a study of a network of unidirectionally coupled rotators with i.i.d. frequencies and i.i.d. coupling coefficients. Similar to bi-

ological networks, this system can attain an asynchronous state with pronounced temporal autocorrelations of the rotators.

Using an approach based on the system's generating functional, we derived a differential equation for the self-consistent autocorrelation function of the network noise. Its numerical solution has been confirmed by simulations of networks with Gaussian or sparsely distributed coupling coefficients. Explicit expressions for correlation function, power spectra, correlation time, noise intensity, and quality factor for the case of identical frequencies for all rotators in the limits of weak or strong coupling strength have been obtained.

This work paves the way for more detailed studies of how the statistics of connection strength, the heterogeneity of network parameters, and the form of the interaction function shape the network noise and the autocorrelations of the single element if this element has an predominantly oscillatory nature (e.g. a limit-cycle system).

DY 51.8 Wed 17:30 MA 001

Long-lasting desynchronization by coordinated reset stimulation in neuronal networks with spike-timing dependent plasticity — •Justus A. Kromer and Peter A. Tass — Stanford University, Stanford CA, USA

Abnormally strong synchronization of neuronal activity plays an important role in several brain disorders such as Parkinson's disease, epilepsy, and tinnitus. Deep brain stimulation is a therapy that specifically counteracts neuronal synchronization in related brain areas. In contrast to standard high-frequency deep brain stimulation, which aims on the suppression of neuronal activity, coordinated reset deep brain (CR) stimulation is intended to cause overall desynchronization by introducing phase shifts between individual neuronal subpopulations. To this end phase-resetting stimuli are applied to different neuronal subpopulations at different times. This results in a reshaping of the synaptic weights and, for well-chosen stimulation patterns, causes a transition from a pathological state with high synaptic weights and strongly-synchronized neuronal activity to a physiological state with low synaptic weights and desynchronized activity.

Using computer simulations, we study desynchronization by CR stimulation in networks of leaky integrate-and-fire neurons with spike-timing dependent plasticity. We present a novel approach for CR stimulation that significantly increases the field of application. Furthermore, we discuss the robustness of long-lasting desynchronization effects with respect to changes in system parameters such as network connectivity and heterogeneity in neuronal firing rates.

DY 51.9 Wed 17:45 MA 001

Wie klimawirksam ist der Photovoltaik-Zubau in Deutschland ? Verschwiegene Dynamik. — •Nikolaus von der Heydt — Umweltphysik Göttingen - Physik zum Leben - , Landolfshausen

Neue Analysen der weltweit vernetzten Prozessketten zur Herstellung von Si-PV-Anlagen (IEA 2011 bis 2016) ergeben, dass dabei global je kWp etwa 2,6 t CO2eq in die Atmosphäre gelangen, bevor die Anlagen in Deutschland in Betrieb gehen. Danach können sie hier pro Jahr durchschnittlich 475 Kg/kWp vermeiden, indem sie den aktuellen deutschen Strommix ersetzen. Damit dauert es 5,5 Jahre, bis ein jedes Jahr gleicher PV-Zubau eine Kapazität aufgebaut hat, die pro Jahr hier eben soviel CO2 vermeidet wie der Zubau global verursacht. Bis dahin wächst die CO2-Menge in der Atmosphäre an, bei z.B. 6 GWp/a auf 43 Mt. Danach überwiegt die Vermeidung, und nach 11 Jahren ist die CO2-Schuld getilgt. - Wirksamer Klimaschutz erfordert es, die CO2-Last des deutschen Strommix in 10 Jahren auf ca. 100 g/kWh zu senken, z.B. durch Ersatz von Braunkohle durch Windkraft mit Gas-KWK. Dann könnten deutsche PV-Anlagen je kWp nur noch 84 Kg/a vermeiden, und eine konstant wachsende PV-Kapazität könnte erst nach 30 Jahren die jährliche globale Herstellungs-Emission gerade kompensieren. Soll danach die erreichte Kapazität erhalten werden, müsste die bis dahin in der Atmosphäre angesammelte CO2-Menge für immer dort bleiben. Bei z.B. 6 GWp/a wären das 233 Mt. Mit Akkus und Freiland-Aufständerungen verdoppelt sich die Herstellungs-Emission mindestens, das bedeutet die 4-fache angesammelte CO2-Menge. Im Beispiel sind das 932 Mt - die deutsche Jahresemission.

DY 52: Active Matter III (joint session DY/CPP/BP)

Time: Wednesday 15:30–18:45 Location: BH-N 243

DY 52.1 Wed 15:30 BH-N 243

Three-body correlations and conditional forces in suspensions of active hard disks — •Andreas Härtel[1], David Richard[2], and Thomas Speck[2] — [1]University of Freiburg, Freiburg, Germany — [2]Johannes Gutenberg-University Mainz, Mainz, Germany

Self-propelled Brownian particles show rich out-of-equilibrium physics, but while decades of studying the structure of liquids have build up a deep understanding of passive systems, not much is known about correlations in active suspensions. For this reason, we derive an approximate analytic theory for three-body correlations and forces in systems of active Brownian disks starting from the many-body Smoluchowski equation. Via this theory we discuss properties of conditional three-body forces, an effective swimming speed, and pair distributions. We further test and validate our theory using particle-resolved computer simulations. They allow us to discuss the modeling of active Brownian swimmers with nearly hard interaction potentials. We finally define appropriate parameters to describe active systems and discuss them as a basis for further studies of correlations in active suspensions and for an emerging liquid state-theory.

DY 52.2 Wed 15:45 BH-N 243

Giant Kovacs-Like Memory Effect for Active Particles — •Rüdiger Kürsten[1], Vladimir Sushkov[2], and Thomas Ihle[1] — [1]Universität Greifswald — [2]Hochschule für angewandte Wissenschaften München

Dynamical properties of self-propelled particles obeying a bounded confidence rule [1] are investigated by means of kinetic theory and agent-based simulations. While memory effects are observed in disordered systems, we show that they also occur in active matter systems [2]. In particular, we find that the system exhibits a giant Kovacs-like memory effect that is much larger than predicted by a generic linear theory. Based on a separation of time scales we develop a nonlinear theory to explain this effect. We apply this theory to driven granular gases and propose further applications to spin glasses.

[1] Phys. Rev. E 90, 063315 (2014)
[2] Phys. Rev. Lett. 119, 188001 (2017)

DY 52.3 Wed 16:00 BH-N 243

Active Brownian Particles in Crowded Media — •Jonathan Ónody[1], Alexander Liluashvili[1], and Thomas Voigtmann[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt e.V, Köln, Deutschland — [2]Fachgruppe Physik, Heinrich-Heine Universität, Düsseldorf, Deutschland

We investigate the dynamics of model microswimmers (active Brownian particles) evolving at high densities and in the presence of crowding, i.e., in model porous media, making use of the mode-coupling theory of the glass transition (MCT). The microswimmers are modeled by hard disks in two dimensions undergoing both, translational and rotational diffusion. In addition they posses a constant self-propulsion velocity in their direction of orientation. MCT predicts an idealized active-glass transition, and we discuss the features of the slow dynamics emerging close to that transition. The porous background is treated as a frozen disordered density field. We discuss the structure of the resulting theory, distinguishing between connected and disconnected parts of the correlation functions.

1. Liluashvili, A., Ónody, J., and Voigtmann, Th., Mode Coupling Theory for Active Brownian Particles, Phys. Rev. E in press, arXiv:1707.07373 (2017).

2. Krakoviack, V., Mode-coupling theory for the slow collective dynamics of fluids adsorbed in disordered porous media, Phys. Rev. E 75, 031503 (2007).

3. Götze, W., Complex Dynamics of Glass-Forming Liquids - A Mode-Coupling Theory

DY 52.4 Wed 16:15 BH-N 243

Cans and cannots of heat engines with nonequilibrium baths — •stefano steffenoni[1], viktor holubec[2], gianmaria falasco[3], and klaus kroy[2] — [1]Max Planck for the Mathematics in the Science, leipzig — [2]Institute for Theoretic Physics, Leipzig — [3]University of

Luxembourg, Luxembourg

We investigate a heat engine based on a Brownian colloid, confined in a parabolic potential and coupled to an active particles bath. The energetics of the cycle is governed by the variance of the colloid distribution. With a suitable definition of a time-dependent effective temperature, it obeys the same dynamical equation as a passive colloid coupled to a conventional thermal bath. Performance of the active heat engine including maximum efficiency, efficiency at maximum power and maximum efficiency at a fixed power can thus all be understood from ordinary thermodynamics, using the appropriate effective temperature. On this basis, we provide a thorough analysis of recent experiments (Krishnamurty et al. Nat. Phys. 2016) that lead to the spectacular claim that thermodynamic cycles coupled to active baths can surpass the ultimate efficiency of an equilibrium Stirling cycle.

DY 52.5 Wed 16:30 BH-N 243

Dynamics of self-propelled granular particles on a vibrated plate — •Tina Hanselka and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

Screws sliding on a periodically vibrating plate can be used as a very simple model system to examine the motion of self-propelled particles in 2D. We analyze the active Brownian motion a single screw performs, then we explore the self-organization of large groups of particles, focusing on mixtures between active and passive materials, realized by screw nuts of comparable weights.

15 min. break

DY 52.6 Wed 17:00 BH-N 243

Diffusive dynamics of complex colloidal particles in active suspensions of microswimmers — •Florian von Rüling, Francine Kolley, Patricia Dähmlow, Hajnalka Nadasi, and Alexey Eremin — Otto von Guericke University Magdeburg

We report experimental studies on the active motion of puller-type microswimmers Chlamydomonas reinhardtii (C.R.) and the entrainment and the diffusion of complex passive particles in thin capillaries. C.R., self-propelled unicellular alga, swims in the regime of low Reynolds number due to its flagellar motion breaking time-reversal symmetry. Having an eyespot, the alga shows phototactic behaviour. Employing a particle tracking algorithm and polarising microscopy, we explore the enhancement of the diffusion of the sphere- and rod-shaped particles by swimming algae. Furthermore, we demonstrate the effect of the microswimmer-induced flow on the director field of nematic droplets dispersed in the active colloid.

DY 52.7 Wed 17:15 BH-N 243

Self-spinning particles phase separate and move collectively — •Christian Scholz[2,1], Michael Engel[1], and Thorsten Pöschel[1] — [1]Institute for Multiscale Simulation, FAU Erlangen, Germany — [2]Institut für Theoretische Physik 2, HHU Düsseldorf, Germany

We create 3d-printed minimalistic robots that perform self-spinning motion. Binary mixtures of clockwise and counter-clockwise spinning particles phase separate and exhibit collective ballistic motion along the interfaces. We compare our experimental system to Langevin simulations to demonstrate that our macroscopic system is a form of active soft matter. Simulations also allow us to demonstrate that confinement in the system, on long time scales, favors symmetric demixing patterns.

DY 52.8 Wed 17:30 BH-N 243

Entropy production of active particles and for particles in active baths — •Patrick Pietzonka[1,2] and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Germany — [2]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK

Entropy production of an active particle in an external potential is identified through a thermodynamically consistent minimal lattice model that includes the chemical reaction providing the propulsion and ordinary translational noise. In the continuum limit, a unique expression follows, comprising a direct contribution from the active process and an indirect contribution from ordinary diffusive motion. From the corresponding Langevin equation, this physical entropy production cannot be inferred through the conventional, yet here ambiguous, comparison of forward and time-reversed trajectories. Generalizations to several interacting active particles and passive particles in a bath of active ones are presented explicitly, further ones are briefly indicated. [1] P. Pietzonka and U. Seifert, J. Phys. A: Math. Theor. **51**, 01LT01 (2018)

DY 52.9 Wed 17:45 BH-N 243

Binary Mixtures of Active and Passive Particles — •Francesco Alaimo[1,2] and Axel Voigt[1,2,3] — [1]Institut für Wissenschaftliches Rechnen, TU Dresden, Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany — [3]Center for Systems Biology Dresden (CSBD), Dresden, Germany

We use a modification of the Binary Phase Field Crystal model to introduce a continuous approach for binary mixtures of passive and active particles.

This continuous model is used to numerically study different effects that arise in binary mixtures. First, we see how activity promotes crystallization and cluster formation in a passive system, a phenomenon that has been observed experimentally. By varying the relative densities we can observe how passive obstacles influence the dynamics of active particles. Finally, we show how, under specific conditions, a crowded environment can lead to a partial trapping of active particles.

DY 52.10 Wed 18:00 BH-N 243

Phase diagram, capillary waves, and interfacial stiffness of active-passive polymer mixtures — •Jan Smrek, Kostas Daoulas, and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

The active-passive polymer mixtures serve as a model for phase separation of transcriptionally active and inactive DNA strands in nuclei of living cells. Is it possible to distinguish the equilibrium phase separation, driven by chemical differences, from the non-equilibrium one? Here, we study the interfacial properties of the phase separated steady states of the scalar active-passive polymer mixtures. We construct phase diagrams and extract the analogue of the equilibrium critical exponent β governing the density difference. Looking at the interface fluctuations, we find they follow the equilibrium capillary waves spectrum. This allows us to establish a mechanistic definition of the non-equilibrium interfacial stiffness and its dependence on the activity asymmetry. We show how the interfacial width depends on the activity ratio and comment on the finite size effects. Our results show the non-equilibrium steady state behaves in many respects as an equilibrium polymer mixture with LCST.

DY 52.11 Wed 18:15 BH-N 243

High-motility light-driven AgCl Janus microswimmers interacting with passive beads — •xu wang[1], Larysa Baraban[2], Annie T. Phuong Nguyen[2], Jin Ge[1], Vyacheslav Misko[3], Gianaurelio Cuniberti[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [3]Department Fysica, Universiteit Antwerpen, B-2020 Antwerpen, Belgium

Visible light driven nano/micro swimmers are promising candidates for potential biomedical and environmental applications, which have been highlighted in the study of manmade nanao/micro swimmers stimulated by versatile light sources.1-5 To increase the motile speed, Janus polystyrene (PS)/AgCl microswimmers have been developed, which are capable to be actuated and tuned by blue light and achieve a high moving speed with 7 μm/s in pure water. To understand the interaction mechanism between artificial microswimmers and the surrounding environment, with the stimuli of blue light, prepared clusters composed of different numbers of Janus PS/AgCl particles and PS beads are used as active and passive motile objectives for sub-systematic models. The dynamics of a single Janus particle, single Janus particles assemblies, collective behaviours have been investigated and demonstrated both with experimental and simulated results.

DY 52.12 Wed 18:30 BH-N 243

High-motility visible light-driven AgCl Janus microswimmers interacting with passive beads — •Xu Wang[1], Larysa Baraban[2], Annie T. Phuong Nguyen[2], Jin Ge[1], Vyacheslav Misko[3], Gianaurelio Cuniberti[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Dresden University of Tech-

nology, 01062 Dresden, Germany — [3]Universiteit Antwerpen, B-2020 Antwerpen, Belgium

Visible light driven nano/micro swimmers are promising candidates for different applications. However, the previous obtained mean squared displacement (MSD) values are low (up to 200 squared micrometers (10 s)) even under the favorable UV light illumination.[1,2] This is a severe drawback for the applications where the efficient transport of microswimmers is demanded.

We demonstrate AgCl based spherical Janus microswimmers reveal an efficient propulsion under blue (visible) light (λ=450-490 nm)illumination. The proper design of a AgCl based microswimmer can boost the MSD to 3000 squared micrometers (10 s) in pure H2O. We investigate the motion of individual Janus particles as well as their small (3-particles) and large (many particles) clusters. With experimental results and numerical simulations (by Langevin equations), we provide an insight into the collective behavior of the Janus microswimmers surrounded by polystyrene (PS) beads.

1. Angew.Chem.Int.Ed. 2009,48,3308. 2. ChemNanoMat 2017,3,65.

DY 53: Complex Fluids and Soft Matter (joint session DY/ CPP / BP)

Time: Wednesday 15:30–19:15 Location: BH-N 334

DY 53.1 Wed 15:30 BH-N 334

Tactoids and membranes of chiral rod-like particles — •Anja Kuhnhold and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Suspensions of chiral rod-like particles exhibit a rich phase diagram, including isotropic, chiral nematic (cholesteric) and smectic phases. The cholesteric phase is in particular shown by biological materials, such as fd viruses and cellulose nanocrystals [1].

Besides the bulk phases these rod-like particles assemble to objects of various geometries, e.g. tactoids (spindle-shaped droplets), twisted ribbons or colloidal membranes. Those assemblies are either found in the isotropic background phase of the same constituent particles or in mixtures with depletant particles [2]. Shape and structure of the resulting objects are determined by the interfacial tension with the surrounding phase and the elastic constants and chirality of the mesogens. Understanding the relation between molecular parameters, type (and strength) of interactions and final structures is needed to direct the 'engineering' of such systems to certain applications, e.g. sensing, templating.

We use Monte-Carlo simulations to study properties of tactoids and membranes composed of different (model) chiral rod-like particles. As depletants we use Asakura-Oosawa spheres. For the studied system sizes the tactoids are either nematic or smectic and the membranes appear as diverse twisted structures.

[1] J. Lagerwall et al., NPG Asia Materials **6**, e80 (2014).
[2] T. Gibaud, J. Phys.: Condens. Matter **29**, 493003 (2017).

DY 53.2 Wed 15:45 BH-N 334

The dynamics of smectic layer reorganization — •Patricia Dähmlow, Torsten Trittel, Kathrin May, Kirsten Harth, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

Centimeter-sized freely floating smectic bubbles are studied during their relaxation towards equilibrium spherical shape from an initial elongated hose-like one. These bubbles are observed via high-speed optical imaging. The film area of the nanometer thick bubbles decreases linearly with time within a few milliseconds, driven by capillary forces and inhibited by smectic layer reorganization. Compared to soap bubbles, this film area reduction is much slower, since the layer reorganization in smectics strongly dissipates energy.

Due to the surface reduction of the smectic bubble, the thickness of the film increases locally by forming ordered stacks of excess layers (islands). These islands grow until the equilibrium spherical bubble shape is reached. Additionally, we found, that the relaxation time of the bubbles depends on the film thickness. We discuss the limitations of a minimalistic model that captures smectic layer reorganization processes.

DY 53.3 Wed 16:00 BH-N 334

Mechanically induced smectic-C to smectic-A phase transition during the rupture of a thin film — •Torsten Trittel and Ralf Stannarius — Otto-von-Guericke Universität Magdeburg, 39106 Magdeburg, Germany

Mechanically induced phase transitions in condensed matter are quite rare, mostly they occur in the vicinity of the transition temperatures. We demonstrate a transition between liquid crystal mesophases that is induced far from the transition temperature, and involves solely capillary forces. The rupture of bubbles made from liquid crystal (LC) materials is observed with high speed imaging. In the smectic C phase, the LC molecules show a preferential tilt respective to the layers. We show that capillary forces during film rupture can trigger smectic C to smectic A transitions, which rapidly increase the film thickness while reducing the surface area of the films. The effect occurs on a microsecond scale, practically independent of film thickness and temperature.

DY 53.4 Wed 16:15 BH-N 334

Dynamics and rheology of ferronematics — •Gaurav P. Shrivastav and Sabine H.L. Klapp — Institut für Theoretische Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin.

Suspensions of magnetic nanoparticle (MNP) and liquid crystals (LC) show a rich variety of self-assembled structures and have a wide range of applications [1].

Using molecular dynamics (MD) simulations, we study the dynamical and rheological properties of these mixtures. We consider an 80:20 binary mixture of LCs and MNPs and perform MD simulations in NVT ensemble. We find that LC and MNP both show normal translational and rotational diffusive behavior in the isotropic and also in the nematic phase. However, in the nematic phase both species display an increased translational diffusion in the direction parallel to the nematic director.

To characterize the rheological properties of the mixture, we deform the bulk LC-MNP mixture by shearing it with constant shear rates. The stress-strain rate flow curve shows a shear thinning behavior in these mixtures. We also observe that the nematic order of LC and MNP both increases with strain but the degree of ordering in MNPs is higher than in LCs if the quiescent mixture is in the isotropic phase.

References:

[1] S. D. Peroukidis, and S. H. L. Klapp, Phys. Rev. E 92, 010501(R) (2015).
[2] G. P. Shrivastav, and S. H. L. Klapp, in preparation (2018).

DY 53.5 Wed 16:30 BH-N 334

Binary mixture thin film growth: A simulation study — •Eelco Empting, Miriam Klopotek, and Martin Oettel — Universiy of Tuebingen, Germany

We consider a binary lattice model for growth of demixing thin films. In addition to hard-core repulsion, the particles interact via attraction with their nearest neighbors, the strength of which depends on whether particles are of the like species. This system is a generalization of the regular solution theory model and can exhibit demixing and gas-liquid coexistence.

We present a spinodal decomposition diagram, which was obtained by mean-field calculations. We compare kinetic Monte Carlo simulations with expectations from this diagram. In general, deposition into spinodal regions of the phase diagram leads to demixing. With specific microscopic kinetics it is possible to arrest this demixing process. This leads to effects such as (i) kinetically limited demixing close to the surface and (ii) templated growth (repetition of the surface layer).

DY 53.6 Wed 16:45 BH-N 334

Confined Suspensions as Fluidic Hourglasses — Alvaro Marin[1], Henri Lhuissier[2], Massimiliano Rossi[3], and •Christian J. Kaehler[3] — [1]Physics of Fluids, University of Twente, The Netherlands — [2]IUSTI, Marseilles, France — [3]Bundeswehr University Munich, Germany

Objects of different nature are being forced through constrictions all the time: sand in an hourglass, particles in a fluid through a porous medium, blood through a narrowed vessel or people leaving a room in panic. In all these cases it is important to make sure that the system keeps continuously flowing, sometimes even lives are at risk. The case

of particles in a fluid affects porous mediums, filters and membranes, which become unusable when clogged. We use microfluidic devices with a bottleneck of squared cross-section through which we force dilute polystyrene particle solutions with diameters comparable to the bottleneck size and down to one tenth its size. In low friction conditions and at certain opening sizes, we show experimental evidence of perfectly flowing particle system with no detectable clogging events even at its maximum concentration, just as it occurs in dry granular systems. We describe analytically such a transition by modelling the arch formation as a purely stochastic process, which yields a good agreement with the experimental data.

15 min. break

DY 53.7 Wed 17:15 BH-N 334

Phasonic equilibrium in colloidal quasicrystals — •Johannes Hielscher and Sebastian C. Kapfer — FAU Erlangen-Nürnberg, Institut für Theoretische Physik

We study decagonal intrinsic quasicrystals in two dimensions that are supported by a short-range double-minimum pair potential. Spatial correlations of phasonic flips [1], the preference of rational approximants at low temperatures [2], and energetic considerations indicate that a mathematically ideal quasicrystal is not an equilibrium state of this system.

We conduct Monte Carlo simulations of phasonic flips, using a model potential that separates configurational (phasonic) contributions from the influence of continuous (phononic) displacements. Amplitude and extent of collective phasonic excitations depend on temperature, hence also the frequencies of local motifs.

The isolation of the phasonic degrees of freedom enables a separate inspection of thermodynamic properties of these excitations, such as the heat capacity. We discuss how to translate these findings into the thermodynamics of systems governed by physical dynamics.

[1] J. Hielscher, M. Martinsons, M. Schmiedeberg & S. C. Kapfer: *J. Phys.: Cond. Matt.* **29**, 094002 (2017)

[2] A. Kiselev, M. Engel & H.-R. Trebin, *Phys. Rev. Lett.* **109**, 225502 (2012)

DY 53.8 Wed 17:30 BH-N 334

The delocalization transition in a colloidal glass — •Markus Gruber[1], Gustavo Abade[1], Matthias Fuchs[1], Antonio Puertas[2], Nesrin Senbil[3], and Frank Scheffold[3] — [1]U Konstanz, Germany — [2]U Almeria, Spain — [3]U Fribourg, Switzerland

Using microscopic probe particles we can study local transport processes and structural dynamics, especially of dense colloidal dispersions. In order to examine nonlinear phenomena such as shear melting, an external force has to be applied. We focus on the microscopic analogon of shear melting for the probe in a glassy host. The force on the probe is increased until it can break out of its cage and delocalize [1]. This phenomenon will be called the delocalization transition.

Our model system is a spherical probe particle subject to a constant external force in a colloidal suspension of hard spheres around the glass transition. The statistical dynamics of the probe particle can be expressed by the self-part of the van-Hove-function for the probe particles. We use a refined mode-coupling theory (MCT) approach for the self-intermediate scattering function for this calculation.

We find that the critical force is strongly connected to the strength of the local cages. Furthermore, the van-Hove-function exhibits an exponential tail in force direction, which increases in weight and correlation length when approaching the critical force. This indicates strong dynamical fluctuations, which will dominate measurements of active microrheology. These results are compared to molecular dynamics computer simulations as well as experiments on an emulsion glass.

[1] Gruber, Abade, Puertas, Fuchs, PRE 94, 042602 (2016)

DY 53.9 Wed 17:45 BH-N 334

Inhomogeneous bulk phases in fluids with competing interactions — •Daniel Stopper and Roland Roth — Institute for Theoretical Physics, University of Tuebingen, Germany

Using classical density functional theory, we theoretically study colloidal suspensions with so-called competing interactions, where in addition to a hard core interaction a short-ranged attractive force competes with a longer-ranged repulsive force. Remarkably, these kind of interactions can give rise to self-assembly into cluster phases without any external field. In particular, the clusters can form complex non-spherical three-dimensional periodically ordered structures [1,2]. For instance, it is found that the so-called Gyroid-phase can be thermodynamically stable - a structure which for instance is responsible for structural colors in specific types of birds or butterflies. Generally, besides the Gyroid-phase, several further types of structures can be stable including lamellar, cylindrical, or spherical micelles.

[1] Edelmann and Roth, Phys. Rev. E 93, 062146 (2016); [2] Stopper and Roth, Phys. Rev. E 96, 042607 (2017).

DY 53.10 Wed 18:00 BH-N 334

Squeezing bio-capsules into a constriction: deformation till break-up — •Badr Kaoui, Anne Le Goff, and Anne-Virginie Salsac — Biomechanics and Bioengineering Laboratory (UMR 7338), CNRS, Sorbonne Universités, Université de Technologie de Compiègne, Compiègne, France

We study experimentally the deformation and break-up of liquid-filled capsules trapped at an axisymmetric step constriction, and subjected to increasing pressure drops. We considered biological (trout fish eggs) and bioartificial (made of ovalbumin and alginate) ones, with the objective to characterize the transition to break-up. We find that both capsule populations behave as a brittle material. They do not exhibit any plastic deformation prior to break-up. Moreover critical pressure drop exhibits a stochastic behavior as known for the fracture of disordered media. The break-up probability follows a three-parameter Weibull distribution, from which one can deduce the capsule rupture characteristics [A. Le Goff, B. Kaoui, G. Kurzawa, B. Haszon, A.-V. Salsac, Squeezing bio-capsules into a constriction: deformation till break-up, Soft Matter 13, 7644 (2017)].

DY 53.11 Wed 18:15 BH-N 334

Screening in ionic liquids: an analytical approach — •Fabian Coupette and Andreas Härtel — University of Freiburg, Freiburg, Germany

Recent experiments report an unexpected increase of the electrostatic screening length in concentrated electrolytes [*Faraday Discuss.* **199**, 239 (2017)] which, as yet, lacks a theoretical foundation. The screening length can be obtained from the exponential long-range decay of the total correlation between ionic species, which in turn can be extracted from (classical) density functional theory. We propose a new functional for the primitive model of charged hard spheres which accounts for the packing of ions and solvent particles. With this approach, we find a universal behavior of the screening length in three distinct scaling regimes, including a strong increase at high ion concentrations. This increase culminates in a divergence of the screening length above a certain threshold. We validate our predictions by also performing Molecular Dynamics simulations, where we further observe a structural transition relatable to ion clustering close to the divergent regime. The universal scaling behavior matches well the experimental findings, however, differences remain which we will discuss in detail. We conclude that accounting for excluded volume is already inducing a strong increase in the screening length for concentrated systems, but insufficient to utter quantitative expectations for more intricate solvents, for instance polar ones. In this context we finally sketch the incorporation of dipolar interactions into our theory.

DY 53.12 Wed 18:30 BH-N 334

Charge-Scaling Effect on the Dynamics of an Ionic Liquid: A Molecular Dynamics Simulation Study — •Tamisra Pal and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt , Hochschulstraße 6, 64289 Darmstadt, Germany

We investigate the structural and dynamical relaxation processes in several charge-scaled 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][PF6]) room temperature ionic liquids (ILs) using molecular dynamics simulation, to quantify the relevance of the ionic charges on the temperature-dependent structural relaxation, including its dynamic heterogeneity. Charge-scaling provides an innovative way to systematically alter the dynamics of liquids by variation of a single control parameter. The rationale behind the use of reduced partial charges between ± 0.48 to 0.72 e is mainly governed by the charge-transfer mechanism taking place in the hydrogen bond between the imidazolium ring and the anion, along with the polarizability effects that invoked huge interest to better describe the dynamics in ILs. We perform extensive simulations from low temperatures in the viscous regime to high temperature far above the melting point to analyze the dependence of the dynamics on the ionic charges in a detailed manner. To characterize dynamics in terms of activation energies over the whole temperature range, recent studies on molecular glass formers

have shown that E(T) can be split into low temperature cooperative energy E_c(T) and high temperature constant activation energy E_∞. We extend these studies to relate the E_c(T) associated with the collective molecular motion to the dynamical heterogeneity, e.g., to the size of clusters of mobile ions.

DY 53.13 Wed 18:45 BH-N 334

Hydrodynamics of droplet lattices in quasi 2D free-standing liquid crystal films — •Christoph Klopp, Torsten Trittel, Alexey Eremin, Kirsten Harth, and Ralf Stannarius — Otto-von-Guericke Universität Magdeburg

In an experiment on ISS, we prepared nearly regular triangular droplet lattices on free-standing liquid crystal films to investigate the diffusion and vibration dynamics on these lattices [1]. The layered structure in smectic A phases allows the preparation of thin and homogeneous macroscopic films. We record the motion of the droplets and calculate their diffusion characteristics. The experiments are compared to numerical simulations of droplet arrangements assuming specific repulsive interaction potentials. The mean-square displacement of the droplets reveals mobilities in the lattice and information on the strength of the potential.

The study was supported by NASA, DFG and DLR within the OASIS project.

[1] N. A. Clark, A. Eremin, M. A. Glaser, N. Hall, K. Harth, C. Klopp, J. E. Maclennan, C. S. Park, R. Stannarius, P. Tin, W. N. Thurmes, and T. Trittel, Realization of hydrodynamic experiments on quasi-2D liquid crystal films in microgravity, ASR Volume 60, 737-751, 2017

DY 53.14 Wed 19:00 BH-N 334

ROLE OF PORE FORMING TOXINS IN MODULATING THE LIPID DYNAMICS. — •Vadhana Varadarajan[1], Rajat Desikan[2], and Ayappa Ganapathy K[3] — [1]Indian Institute of Science, Bangalore, India — [2]Indian Institute of Science, Bangalore, India — [3]Indian Institute of Science, Bangalore, India

Pore-forming toxins (PFT's) secreted by bacteria are important bacterial virulence factors which oligomerize and spontaneously self-assemble on the mammalian cell membranes. The effect of an alpha PFT and a beta-PFT on saturated and unsaturated mammalian cell membranes are investigated using molecular dynamics simulations. The structure and dynamics of lipids in the vicinity of PFT's are different away from them giving rise to structural and dynamic heterogeneities. We also investigated the role of cholesterol in these systems. Our findings reveal that cholesterol fluidizes the lipid bilayer and the local structure is closely related to the dynamics which also depends on the saturation level of the lipid as well as the hydrophobic mismatch of the lipid bilayer with the PFT's. We also investigated the survival probability of the lipids in the vicinity of PFT which can be used to quantify the lifetime and death of cells. Our study reveals that the beta-PFT is less toxic than alpha-PFT.

DY 54: Statistical Physics of Biological Systems I (joint session BP/DY)

Time: Thursday 9:30–13:00 Location: H 2013

DY 54.1 Thu 9:30 H 2013

Thermodynamic bounds on the ultra- and infra-affinity of Hsp70 for its substrates — •Basile Nguyen[1,2], David Hartich[1], Paolo De Los Rios[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart, Germany — [2]Laboratory of Statistical Biophysics, Institute of Physics, School of Basic Science and Institute of Bioengineering, School of Life Sciences, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

The 70 kDa heat shock protein Hsp70 has several essential functions in living systems, such as protecting cells against protein aggregation, assisting protein folding, remodeling protein complexes, and driving translocation into organelles. These functions require high affinity for nonspecific amino acid sequences that are ubiquitous in proteins. It has been recently shown that this high affinity, called ultra-affinity, depends on a process driven out of equilibrium by ATP hydrolysis. Here, we establish the thermodynamic bounds for ultra-affinity, and further show that the same reaction scheme can in principle be used both to strengthen and to weaken affinities (leading in this case to infra-affinity). We show that cofactors are essential to achieve affinity beyond the equilibrium range. Finally, we consider small GTPases which can benefit from infra-affinity to optimize intracellular signal transduction.

[1] B. Nguyen, D. Hartich, U. Seifert and P. De Los Rios (2017), *Biophys. J.* 113, 362-370

DY 54.2 Thu 9:45 H 2013

A reaction center driven by entropy — •Franz-Josef Schmitt, Zuleyha Yenice Campbell, Mai Vi Bui, and Thomas Friedrich — Technische Universität Berlin, Sekr. PC 14, Straße des 17. Juni 135, 10623 Berlin

The phototrophic cyanobacterium *Halomicronema hongdechloris* contains chlorophyll *a* and *f* in photosystem II. The ratio of Chl *f* to Chl *a* is reversibly changed from 1:8 under illumination with far red light (720-730 nm) to a very low level of Chl *f* under white-light culture conditions. Phycobiliproteins exhibit highly efficient excitation energy transfer (EET) to Chl *a* and from there to Chl *f* within 200 ps apparent transfer time if *H. hongdechloris* grown under far red light is illuminated with 630 nm laser radiation which is absorbed by phycobilisomes. However excitation energy localized on Chl *f* shows long lifetime of more than 1 ns. Questions arise about composition of the reaction center and possible primary charge separation driven by Chl *f*. Our Simulations and thermodynamic considerations suggest that the time- and wavelength-resolved ps fluorescence data can be explained assuming light-induced far red-shifted traps of excitation energy localized on Chl *f* in the light harvesting antenna while the large majority of Chl *a* is strongly coupled to these Chl *f* traps driving the uphill EET from Chl *f* to Chl *a* by entropic force.

DY 54.3 Thu 10:00 H 2013

Shape of pinned polymer loops in an external force field — •Wenwen Huang[1], Yen Ting Lin[2], and Vasily Zaburdaev[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Los Alamos National Laboratory, New Mexico, USA

We studied the shapes of pinned polymer loops subjected to a constant external force field. We show that the polymer density profile can be calculated analytically in agreement with the simulation results. Moreover, we calculated the distribution of gyration radius and found it to vary non-monotonically with the strength of the external force field: the distribution is broader for moderate forces and more narrow for strong and weak forces. Furthermore, we analyzed the gyration tensor of the polymer loop characterizing its overall shape and in particular two parameters called asphericity and the nature of asphericity. These parameters, along with the gyration radius, can be used to quantify experimental data.

DY 54.4 Thu 10:15 H 2013

The labyrinth-like shapes of nasal cavities arise from physical and geometrical constraints — •David Zwicker[1,2], Rodolfo Ostilla-Mónico[2], Daniel E. Lieberman[2], and Michael P. Brenner[2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Harvard University, Cambridge, USA

Although the nasal cavity is vital for heating and humidifying inhaled air in all vertebrates, its shape varies widely across animals. To understand this variability, we here connect nasal geometry to its function by theoretically studying the airflow and the associated scalar exchange that describes heating and humidification. We show that optimal geometries, which have minimal resistance for a given exchange efficiency, are narrow with a uniform gap width. Our prediction for the gap width matches measured values over a large range of animal sizes. Moreover, we show that geometric constraints imposed by the head can be satisfied with the observed labyrinth-like geometries, which perform almost as well as the optimal shapes without the constraints. Taken together, our theory explains the geometric variations of natural nasal cavities quantitatively and we hypothesize that the trade-off between high exchange efficiency and low resistance to airflow is the main driving force shaping the nasal cavity.

DY 54.5 Thu 10:30 H 2013

Cell polarization in elliptical geometry: how does C. Elegans determine its first axis? — •Raphaela Gessele, Jacob Halatek, and Erwin Frey — Department of Physics, Ludwig-Maximilians-Universität München, 80333 Munich, Germany

Cell polarity defines axes that guide cell differentiation and division. In the single cell state of the Caenorhabditis Elegans embryo, PAR protein patterns determine the anterior-posterior axis which further guides the first cleavage. Experiment and theory have indicated that mutual binding inhibition of (anterior) aPAR and (posterior) pPAR proteins is the key mechanism of polarity maintenance by the PAR reaction-diffusion network. Strikingly, our analysis of the reaction-diffusion dynamics in (elliptical) cellular geometry shows that mutual inhibition alone does not lead to a stable polarity along the long (anterior-posterior) axis of the cell but generically favors polarity by aPAR and pPAR protein domains aligned with the short axis. We find that the geometry adaption of the patterning process depends on an intricate interplay between attachment-detachment dynamics on the one hand, and cytosolic reactivation on the other hand. Our findings show that the local ratio of membrane surface to cytosolic bulk volume is the main geometric cue to which patterns adapt. Furthermore, an inactive phase after membrane detachment can switch the preferred polarity axis - The decisive parameter for switching is the diffusion length of the inactive phase. In conclusion, our studies reveal the crucial role of geometry for self-organized pattern formation. Geometry should be explicitly considered in models for intracellular pattern formation.

DY 54.6 Thu 10:45 H 2013

A Spheroidal Squirmer in Shear Flow — •Kai Qi[1], Elmar Westphal[2], Gerhard Gompper[1], and Roland G. Winkler[1] — [1]Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Jülich Centre for Neutron Science, Forschungszentrum Jülich, D-52425 Jülich, Germany

Squirmers are generic models for microswimmers like bacteria and algae. The behavior of a spheroidal squirmer [1, 2] in shear flow is studied by hydrodynamic simulations via the multiparticle collision dynamics [3] approach. Due to the elongated shapes of spheroids, alignment along the shear direction is observed for both passive spheroidal colloids and squirmers in the weak shear flow. When the shear rate exceeds a critical value, alignment changes from the shear to the vorticity direction. The alignment transition reveals a clear dependence on the hydrodynamic dipole of the swimmer's flow field. Pullers with a large positive force-dipole coefficient exhibit gradual variations of the alignment direction, whereas abrupt changes are found for pushers with a large negative coefficient. Comparison between elongated and spherical squirmers reveals a significant shape dependence of their behaviors in shear flow.

[1] M. Theers, E. Westphal, G. Gompper, and R. G. Winkler, Soft Matter **12**, 7372 (2016).

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

[3] G. Gompper, T. Ihle, D. M. Kroll, and R. G. Winkler, Adv. Polym. Sci. **221**, 1 (2009).

15 min. break

Invited Talk DY 54.7 Thu 11:15 H 2013

Protein Pattern Formation: Rethinking Nonlinear Dynamics — •Erwin Frey — Ludwig-Maximilians-Universität München, München, Germany

Protein pattern formation is essential for spatial organization of many intracellular processes like cell division, flagellum positioning, and chemotaxis. More generally, these systems serve as model systems for self-organization, one of the core principles of life. We present a rigorous theoretical framework able to generalize and unify pattern formation for quantitative mass-conserving reaction-diffusion models. Within this framework, separation of diffusive mass redistribution on the level of conserved species provides a general mathematical procedure to decompose complex reaction-diffusion systems into effectively distinct functional units, and to reveal the general underlying bifurcation scenarios. We apply this general framework to a range of specific intracellular pattern forming protein networks, and show how it facilitates the identification of general self-organisation principles.

DY 54.8 Thu 11:45 H 2013

Self-organised length oscillations of cellular protrusions — Mareike Bojer[1,2], •Isabella Graf[1], and Erwin Frey[1] — [1]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Munich, Germany — [2]present address: Department of Physics, Technische Universität München, Garching, Germany

We consider a stochastic non-equilibrium model which is inspired by the interplay of directed transport and diffusive motion of molecular motors in growing and shrinking cellular protrusions like filopodia. Based on this model we investigate the effect of finite diffusion in a half-closed geometry and show that it can lead to temporal patterns in the form of oscillating system length. We examine the dynamics of the system length in terms of the growth rate of the protrusion and identify two different limits: For small growth rate, the system length changes very stochastically and our analytic prediction, using a so-called adiabatic assumption, agrees well with the result from numerical simulations. For larger growth rate, however, temporal patterns occur. More concretely, we observe quasi-periodic changes in length in a parameter regime where motor mixing (diffusion) is slow compared with the shrinkage dynamics. We provide an intuitive picture for the origin of this pattern-forming mechanism which relies on the closure of the system at the dynamic end of the protrusion and the resulting particle conservation.

DY 54.9 Thu 12:00 H 2013

Force sharing between elastically coupled molecular motors — •Mehmet Can Ucar and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14476 Potsdam, Germany

Molecular motors are nano-scale machines that drive many essential processes within the living cell such as the organization of the mitotic spindle, the powering of flagella and cilia, and the long-distance transport of cellular cargos. These motor proteins frequently work in teams of multiple motors and can collectively generate large forces, but the underlying mechanism of force generation and force sharing remains controversial. Here we address this question by introducing a new model for cargo transport by elastically coupled molecular motors. For a system of two identical motors acting against an antagonistic motor or an optical trap, we find that motors share the generated forces almost equally among the members of the same team. The model furthermore provides a new explanation for observed forces in different in vitro studies.

DY 54.10 Thu 12:15 H 2013

Statistical inference of bacterial chemotaxis strategies — •Maximilian Seyrich[1], Zahra Alirezaei[2], Carsten Beta[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam, Germany

Bacteria like *E. coli* move with alternating runs and tumbles. Modern imaging techniques provide a high-throughput access to these run-and-tumble trajectories. However, good tumble recognition analysis is still a bottleneck and needs to set a-priori threshold parameters. We present a high-throughput inference technique, which allows to infer all swimming parameters of the bacterium without such a need.

We set up a random-walk model that describes runs and tumbles as a stochastic process of the bacterium's swimming direction and speed extending our previous work [1]. The dynamics of the swimming direction is described by enhanced rotational Brownian motion during tumbling, while thermal and shot noise together with a relaxational drift analogously to an Ornstein-Uhlenbeck process govern the speed dynamics. In order to infer the relevant swimming parameters, moments and autocorrelation functions are calculated for our model and matched to the ones determined from experimental trajectories. We first show that our method identifies the classical bacterial chemotaxis strategy of *E. coli*, i.e., the tumble rate decreases when swimming along the chemical gradient. We also find evidence that a fast subpopulation of *E. coli* reduces its mean tumble angle in this direction.

[1] O. Pohl *et al.*, PLoS Comp. Biol. **13**, 1 (2017).

DY 54.11 Thu 12:30 H 2013

Chemoattractant induced transient adaptation in the oscillatory cytoskeleton of motile amoeboid cells. — •Jose Negrete JR[1,2], Alain Pumir[3,4], Christian Westendorf[4], Marco Tarantola[4], Eberhard Bodenschatz[4,5,6], and Carsten Beta[7] — [1]Max Planck Institute for the Physics of Complex Systems, Dres-

den, Germany — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [3]École Normale Supérieure de Lyon, Lyon, France — [4]Max Planck Institute for Dynamics and Selforganization — [5]University of Göttingen, Göttingen, Germany — [6]Cornell University, Ithaca, USA — [7]University of Potsdam, Potsdam, Germany

Dictyostelium discoideum presents oscillatory actin polymerization cycles which amplitude is mostly given by noise. We investigate the transient response on the actin polymerization activity in Dictyostelium discoideum induced by a short pulse of cAMP. The stimulation induces a transient response, of reduced amplitude and frequency, which time duration is stochastic and varies between cells. To model the observed actin behavior, we extend the description of noisy oscillator by introducing an inhibitory variable that acts as a timer for the transient phase.

DY 54.12 Thu 12:45 H 2013

Evolution of carrying capacity and extinction of populations in a stochastic system — •Hye Jin Park[1], Yuriy Pichugin[1], Weini Huang[2], and Arne Traulsen[1] — [1]Max Planck Institute for Evolutionary Biology, Plön, Germany — [2]Barts Cancer Institute, London, United Kingdom

Once a mutant emerges in the population, new interactions are drawn between types, which may lead to changes in the population size. Using the game theory, we implement this population dynamics in a stochastic system. Since interactions between types are described by a game payoff matrix, the emergence of a mutant is interpreted as extending the payoff matrix. New equilibria can emerge by the change of the payoff matrix. If the population settles to a new equilibrium state, the population size changes. We examine the change of population size in time and quantify the extinction risk by the mean time to extinction.

DY 55: Focus: Emergent phenomena in driven quantum many-body systems (joint session DY/TT)

In the past years, driven quantum many-body systems have been demonstrated to offer a huge playground for emergent states of matter. These range from light-induced switching of phases in solids and laser-modified chemical reactions via Floquet topological states in photonic crystals to artificial gauge fields in optical lattices and Floquet time crystals in many-body localized systems. The goal of the proposed session Emergent phenomena in driven quantum many-body systems is to bring together distinguished scientists from a variety of fields who work on driven quantum systems from different perspectives, both theoretically and experimentally, to stimulate interdisciplinary discussions and guide future research directions. For the general audience, this is an opportunity to gain a broad overview of a growing research field with great potential and many open questions.

Coordinator: France Manghi (Modena)

Time: Thursday 9:30–11:30 Location: EB 107

Invited Talk DY 55.1 Thu 9:30 EB 107

Nuclear and electronic dynamics in ultrafast photoinduced charge separation — •Carlo Andrea Rozzi — CNR-NANO, Modena, Italy

The sub-ps dynamics of photoinduced charge separation is studied in several prototypical photovoltaic materials by combining TDDFT and molecular dynamics simulations. The results are validated against high time resolution pump-probe spectroscopy, and ultrafast electron diffraction. The role of coherent coupling between electronic and nuclear degrees of freedom is shown to be of key importance in triggering charge delocalization and transfer both in covalently bonded molecules[1] and non-bonded bulk heterojunctions[2]. The possible exploitation of our findings in order to design and synthesize novel molecular scaffolds[3] for photovoltaic applications is discussed. Further work in progress on ultrafast photoexcitation of polymer-copolymer aggregates and perovskites is presented.

[1] C. A. Rozzi et al., Nat. Comm 4, 1602 (2013) [2] S. Falke et al., Science 344, 1001 (2014) [3] S. Pittalis et al., Adv. Func. Mat. 25, 2047 (2015) [4] G. M. Vanacore et al., arXiv:1801.03731

Invited Talk DY 55.2 Thu 10:00 EB 107

Theory of pump-probe spectroscopy: Ultrafast laser engineering of ordered phases and microscopic couplings — •Michael Sentef — Max Planck Institut für Struktur und Dynamik der Materie (CFEL), Hamburg

Intense femtosecond laser pulses, spanning a large range of photon energies from the X-ray to the THz regime, allow for controlled excitations ("pump") and monitoring ("probe") of the nonequilibrium dynamics of all the relevant microscopic degrees of freedom in solids. The field of ultrafast materials science is currently evolving towards ultrafast laser engineering of nonthermal phases of matter with novel properties. I will discuss recent theoretical progress in understanding these diverse phenomena from microscopic models and nonequilibrium simulations. I will show examples of light-enhanced superconductivity in an electron-phonon system from classical nonlinear phononics [1] and laser-controlled order competition between superconductivity and charge-density waves [2]. I will discuss laser engineering of microscopic couplings in graphene [3] based on quantum nonlinear phononics [4]. Finally, I will show ab initio time-dependent density functional theory results for laser-engineered Hubbard U in NiO [5].

[1] M. A. Sentef et al., Phys. Rev. B 93, 144506 (2016). [2] M. A. Sentef et al., Phys. Rev. Lett. 118, 087002 (2017). [3] E. Pomarico et al., Phys. Rev. B 95, 024304 (2017). [4] M. A. Sentef, Phys. Rev. B 95, 205111 (2017). [5] N. Tancogne-Déjean et al., arXiv:1712.01067.

This work was supported by Deutsche Forschungsgemeinschaft through the Emmy Noether Programme (SE 2558/2-1).

DY 55.3 Thu 10:30 EB 107

Transient dynamics in an excitonic insulator: Fast computation of nonequilibrium Green's functions — •Riku Tuovinen[1], Denis Golež[2], Michael Schüler[2], Martin Eckstein[3], and Michael Sentef[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany — [2]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [3]Department of Physics, University of Erlangen-Nürnberg, 91058 Erlangen, Germany

A standard approach to nonequilibrium many-body problems is the Keldysh Green's function technique [1]. Information about the studied system, e.g. photoemission spectra etc., is encoded into the Green's function. To access this, we have to consider coupled integro-differential equations (Kadanoff-Baym equations), whose efficient solution is not trivial [2]. The Generalized Kadanoff-Baym Ansatz (GKBA) offers a simplification by decomposing the two-time-propagation of the Green's function into the time-propagation of a time-local density matrix [3]. We discuss the time-propagation method à la GKBA and present some benchmark simulations against the full solution of the Kadanoff-Baym equations, concentrating on a simple model for an excitonic insulator [4]. We investigate the dynamics of competing orders and how the balance between them could be controlled by laser driving.

[1] G. Stefanucci and R. van Leeuwen, Nonequilibrium many-body theory of quantum systems, CUP (2013) [2] A. Stan et al., J. Chem. Phys. 130, 224101 (2009) [3] P. Lipavský et al., Phys. Rev. B 34, 6933 (1986) [4] D. Golež et al., Phys. Rev. B 94, 035121 (2016)

DY 55.4 Thu 10:45 EB 107

Entanglement growth and thermalisation after a spa-

tially inhomogeneous quench — Maximilian Schulz[1,2], •Chris Hooley[1], Roderich Moessner[2], and Frank Pollmann[3] — [1]SUPA, University of St Andrews, UK — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Technische Universität München, Germany

We consider a system of spinless fermions in a strong optical lattice plus a harmonic trap and uncorrelated disorder. We subject them to a quantum quench that consists of an instantaneous displacement of the trap centre.

In [1] we presented an analysis of the behaviour of the non-interacting version of the problem. We observe that (a) even weak disorder strongly breaks the parity symmetry of the clean problem, qualitatively changing the nature of the infinite-time steady state, and (b) the approach to this long-time state is extremely slow, since it involves the fermions' tunnelling across a broad 'Bragg-forbidden' region.

Here we show that the ingredients in the above study also present a way to realise slow logarithmic entanglement growth as usually observed in many-body localized systems without disorder and even without interactions. We present evidence for this by a time-evolving block decimation and exact diagonalization analysis of the interacting and non-interacting cases.

[1] M. Schulz, C.A. Hooley, and R. Moessner, Phys. Rev. A. 94, 063643 (2016).

DY 55.5 Thu 11:00 EB 107

Creating a superfluid by kinetically driving a Mott insulator — Gregor Pieplow, Fernando Sols, and •Charles Creffield — Universidad Complutense, Madrid, Spain

We study the effect of time-periodically varying the hopping amplitude (which we term "kinetic driving") in a one-dimensional Bose-Hubbard model, such that its time-averaged value is zero. By using Floquet analysis, we derive a static effective Hamiltonian in which nearest-neighbor single-particle hopping processes are suppressed, but all even higher-order processes are allowed. Unusual many-body features arise from the combined effect of non-local interactions and correlated tunneling. At a critical value of the driving, the system passes from a Mott insulator to a superfluid formed by two quasi-condensates with opposite nonzero momenta. A many-body cat state combining the two macroscopically occupied momentum eigenstates emerges even with hard-wall boundary conditions. This work shows how driving of the hopping energy provides a novel form of Floquet engineering, which enables atypical Hamiltonians and exotic states of matter to be produced and controlled.

DY 55.6 Thu 11:15 EB 107

Time evolution, dynamics and control of edge states in laser-driven graphene nanoribbons — •Matteo Puviani[1] and Andrea Bertoni[2] — [1]Università degli Studi di Modena e Raggio Emilia, Modena, Italy — [2]CNR Institute of NanoSciences - S3, Modena, Italy

An intense laser field in the high-frequency regime drives carriers in graphene nanoribbons out of equilibrium and creates topologically-protected edge states. Based on a solution of the Floquet Hamiltonian we have studied these states in different regimes of intensity and polarization. We show that the time-dependent band structure contains many unconventional features that are not captured by considering the Floquet eigenvalues alone. By analyzing the evolution in time of the state population we have identified regimes for the emergence of time-dependent edge states responsible of charge oscillations across the ribbon. Furthermore, we show that they exhibit a robust dynamics also in the presence of very localized lattice defects, which is characteristic of topologically non-trivial behaviour. We eventually reveal how it is possible to control them applying an electrostatic potential barrier or creating a Quantum Point Contact, making them promising candidates for flying qubits architectures.

DY 56: Complex Contagion Phenomena I (Focus Session, joint SOE/DY/BP/SNPD) (joint session SOE/DY/BP)

Contagion processes are stochastic dynamical systems that are ubiquitous in natural and engineered systems and their fundamental understanding is of crucial importance for prediction and control of large-scale system behavior. A classical example of a contagion process is the spread of infectious diseases. In addition, in recent years, there has been also an increased scientific interest in so-called social contagion phenomena, which is largely fueled by the rise of digital communication in online social platforms. New challenges that arise due to the digital transformation of communication can be addressed by developing new concepts like collective risk perception.

(Session organizers and chairs: Philipp Hövel, Pawel Romanczuk, and Jonathan Donges)

Time: Thursday 9:30–13:15 Location: MA 001

Invited Talk DY 56.1 Thu 9:30 MA 001

Epidemic threshold on temporal networks — •Vittoria Colizza — Inserm, Paris, France

Our understanding of communicable diseases prevention and control is rooted in the theory of host population transmission dynamics. The network of host-to-host contacts along which transmission can occur drives the epidemiology of communicable diseases, determining how quickly they spread and who gets infected. A large body of epidemiological, mathematical and computational studies has provided a number of insights into the understanding of the process and the identification of efficient control strategies. The explosion of time resolved contact data has however opened the stage to new challenges. What are the structural and temporal aspects, and possibly their non-trivial interplay, that are critical for disease spread? To answer this question, I will introduce the infection propagator approach, a theoretical framework for the assessment of the degree of vulnerability of a host population to disease epidemics, once we account for the time variation of its contact pattern. By reinterpreting the tensor formalism of multi-layer networks, this approach allows the analytical computation of the epidemic threshold for an arbitrary time-varying network of host contacts, i.e. the critical pathogen transmissibility above which large-scale propagation occurs. I will apply this framework to a set of empirical time-varying contact networks and show how it can be used to test different intervention strategies for infection prevention and control in realistic settings.

Invited Talk DY 56.2 Thu 10:00 MA 001

Critical regimes driven by recurrent mobility patterns of reaction-diffusion processes in networks — •Jesus Gomez-Gardenes — University of Zaragoza, Spain

Reaction-diffusion processes have been widely used to study dynamical processes in epidemics and ecology on networked metapopulations. In the context of epidemics, reaction processes are understood as contagions within each subpopulation (patch), while diffusion represents the mobility of individuals between patches. Recently, the characteristics of human mobility, such as its recurrent nature, have been proven crucial to understand the phase transition to endemic epidemic states. Here, by developing a framework able to cope with the elementary epidemic processes, the spatial distribution of populations and the commuting mobility patterns, we uncover three different critical regimes of the epidemic incidence as a function of these parameters. Interestingly, we show a regime of the reaction*diffussion process in which, counter-intuitively, mobility detriments the spreading of the disease. We analytically determine the precise conditions for the emergence of any of the three possible critical regimes in real and synthetic networks.

Invited Talk DY 56.3 Thu 10:30 MA 001

Phase Transitions in Cooperative Coinfections — •Peter

Grassberger[1], Li Chen[2], Fakhteh Ghanbarnejad[3], and Weiran Cai[4] — [1]Juelich Research Center, Juelich, Germany — [2]Northwestern Polytechnical University, Xi'an, Shaanxi, China — [3]Technische Universität Berlin, Berlin, Germany — [4]Technische Universität Dresden, Dresden, Germany

We study the spreading of two mutually cooperative diseases on different network topologies, with two stochastic versions of an SIR type model. Cooperativity can lead to hybrid spreading/extinction transitions, which show at the same time typical signatures both of first order (discontinuous) and second order (continuous) phase transitions. Details depend strongly on the underlying network(s), but also on some details of the algorithms.

As a rule, first order and hybrid transitions occur on networks with few short but many long loops, while continuous transitions are found when there are either many short or few long loops. The latter happens on 2-d lattices, while the former is typical for high-dimensional regular lattices or Erdős-Rényi networks. In three dimensions, the behavior is most rich, and a zoo of different first order / second order mixtures are observed.

15 min. break

Invited Talk DY 56.4 Thu 11:15 MA 001

Linear and nonlinear scenarios of societal change — •Andrzej Nowak — University of Warsaw, Poland

We argue that is that rapid social changes occur rapidly in an abrupt and nonlinear manner resembling a phase transition. Societies in the midst of rapid change are characterized by dual realities corresponding to the new and the old, and the change occurs as the islands of the new expand at the expense of the islands of the new. The central notion is that social influence processes play a pivotal role in promoting social change. Dynamic Theory of Social Impact, which is based on numerous experiments, describes social influence of a group of sources on the target. The findings are based on computer simulations of the theory and confirmed by empirical data collected during the societal transitions that occurred in Poland in the late 1980s and early 1990s. We discuss the dynamics associated with rapid transitions in a society*s norms and attitudes, potential for rapid reversals and role of history is social dynamics.

Invited Talk DY 56.5 Thu 11:45 MA 001

Collective Sensing and Decision-Making in Animal Groups: From Fish Schools to Primate Societies — •Iain Couzin — Dept. of Collective Behaviour, Max Planck Institute for Ornithology & Chair of Biodiversity and Collective Behaviour, University of Konstanz, Konstanz, Germany

Understanding how social interactions shape biological processes is a central challenge in contemporary science. Using an integrated experimental and theoretical approach I will address how, and why, animals exhibit highly-coordinated collective behavior. I will demonstrate new imaging technology that allows us to reconstruct (automatically) the dynamic, time-varying networks that correspond to the visual cues employed by organisms when making movement decisions. Sensory networks are shown to provide a much more accurate representation of how social influence propagates in groups, and their analysis allows us to identify, for any instant in time, the most socially-influential individuals within groups, and to predict the magnitude of complex behavioral cascades before they actually occur. I will also introduce a new fully-immersive Virtual Reality environment for freely-moving animals, and investigate the coupling between spatial and information dynamics in groups. Finally I will reveal the critical role uninformed, or unbiased, individuals play in social networks effecting fast and democratic consensus decision-making in collectives, including with experiments involving schooling fish and wild baboons.

DY 56.6 Thu 12:15 MA 001

Quantitative assessment of import risks for emergent infectious disease outbreaks — •Olga Baranov[1] and Dirk Brockmann[1,2] — [1]Robert Koch-Institut, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Germany

During the last decade outbreaks of emergent pathogens that potentially pose a risk of global dissemination have increased in number and magnitude. When new outbreaks occur, one of the key challenges is a quantitative assessment of the situation, especially concerning global spread. To this end, sophisticated computational models have been developed incorporating exact situation details, disease parameters and demographics. One of the key problems is that highly detailed models are difficult to gauge, because of the initial lack of parameters, substantially impacting the applicability of even the most sophisticated models. We propose an alternative approach for estimating relative import risk from network topology and outbreak origin. It is based on the assumption that during the initial outbreak phase, global import risk is determined by a low dispersal count regime. In this regime disease specific data play only a minor role. Using world aviation network, we demonstrate how import risk at any location can be inferred. We show that this method can be used to compute an airports dissemination profile as a function of outbreak location and how outbreaks in different regions lead to a different subset of key airports. Our method is fast and not limited to a particular type of infectious disease. It can be used as an initial risk assessment tool for public health researchers and policy makers that need to address a real world scenario.

DY 56.7 Thu 12:30 MA 001

How to compete in a multi-pathogen system? — Francesco Pinotti[1], •Fakhteh Ghanbarnejad[2], Philipp Hövel[2], and Chiara Poletto[1] — [1]Sorbonne Universités, UPMC, INSERM, IPLESP UMRS 1136, Paris, France — [2]Institute of Theoretical Physics, TU Berlin, Berlin, Germany

In an ecological system pathogens often need to share their host with other pathogens, and therefore compete for the resources with different spreading strategies. Both cooperative and competitive interactions in bacterial infections have been observed. These two mechanisms have been studied separately in the majority of cases and non-trivial dynamical effects can be expected to arise from their combination. In this work, we study two strains competing with each other for host resources in the presence of a third pathogen cooperating with both of them. We first treat dynamics in a homogeneously mixed population by means of mean-field theory and stability analysis. We study the impact of cooperation on the outcome of the two-pathogen competition, which can be quantified in terms of dominance of one competing pathogen or the co-circulation of both of them. We show that the presence of a third cooperating pathogen can alter the outcome of competition as it may favor the more cooperative pathogen over the more infectious one. We then consider more complex contact structures among hosts and perform computer simulations to study the evolution of the diseases.

DY 56.8 Thu 12:45 MA 001

Defining the scope: A context specific approach to identifying key airports during a pandemic — •Clara Jongen[1,2], Olga Baranov[2], and Dirk Brockmann[1,2] — [1]Humboldt-Universität zu Berlin, Germany — [2]Robert Koch-Institut Berlin, Germany

Human transportation and mobility networks play an important role in the global spread of infectious diseases. Network theory is one of the key methods to understand the nature of these phenomena. In this context, a family of node and link centrality measures has been devised to identify network elements that facilitate the spread and thus require particular attention in the development of containment strategies. However, most centrality measures are not context sensitive, e.g. they do not account for the location of an outbreak. Using the example of disease dynamics on the global air-transportation network we introduce the concepts of node *scope* and *confluence*. These quantities are context dependent centrality measures that are designed to account for the initial outbreak location. We show that scope and confluence can strongly depend on regional aspects of an outbreak and can therefore be adapted to specific outbreak scenarios. We show that each airport is characterized by a node specific scope and confluence profile as outbreak locations are varied. Scope and confluence also permit to address what outbreak locations are particularly threatening to specific nodes in the network. Our method can be used as an assessment tool for understanding global disease dynamics and permit a fast yet specific assessment of an airport's role in global disease dynamics.

DY 56.9 Thu 13:00 MA 001

Comparison of Control Strategies for the Spread of *Bovine Viral Diarrhea*: A Stochastic Agent-Based Model — •Jason Bassett[1], Pascal Blunk[1], Thomas M. Isele[1], Hartmut H. K. Lentz[2], Jörn Gethmann[2], Philipp Hövel[1,3], and Franz J. Conraths[2] — [1]TU Berlin, Berlin, Germany — [2]Friedrich Loeffler Institute, Greifswald, Germany — [3]BCCN, Berlin, Germany

Bovine Viral Diarrhea (BVD) is an important cattle disease due to its global prevalence and its economic implications [1]. In this work we have developed a stochastic agent-based model to describe the spread

of BVD in Thuringia through trade mediated contacts of animals. The agents act at the level of the animal, the herd or the farm on a network of farms connected according to a supply and demand managing system, while the BVD dynamics are based on a model by [2]. We initialise the simulation according to a realistic farm size distribution for Germany and the state of Thuringia, and compare the results of the simulation with demographic and endemic data solely for the state of Thuringia. We also run the simulation for different parameter settings (scenarios) including vaccination strategies and currently implemented or considered regulations. Finally, we present and discuss some network analysis results on the simulated network [3].

DY 57: Talk S. Egelhaaf

Time: Thursday 9:30–10:00 Location: BH-N 243

Invited Talk DY 57.1 Thu 9:30 BH-N 243

Anomalous Diffusion due to Crowding or External Potentials — •Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Diffusion is one of the most fundamental processes in physics. Classical Brownian motion implies a mean squared displacement that grows linearly with time. In many situations, however, deviations from the linear time dependence are found. The time dependence becomes nonlinear and the diffusion anomalous, e.g., upon increasing the particle concentration, adding obstacles or imposing an external potential. We experimentally investigate different situations where anomalous diffusion is observed. First, the effect of crowding is studied. The motion of small colloidal tracers is followed in the presence of concentrated colloidal particles, which represent the host matrix. Since this matrix retains some mobility, it slowly rearranges and hence the large particles act as mobile obstacles. The effect of the obstacle mobility on the tracer dynamics is systematically investigated in another experiment. The obstacles are exposed to an external potential created by a light field which allows us to tune the obstacle mobility. In the next step, the effects of crowding and of the external potential are combined. Both, crowding and an external potential, slow down the dynamics. However, their combination leads to a non-monotonic dependence on particle concentration. In all these experiments, the different parameters can be varied systematically in a broad range and quantitative data on the single-particle level are obtained. This allows for a detailed characterization of the observed anomalous diffusion.

DY 58: Chimera states: symmetry-breaking in dynamical networks (joint session DY/SOE)

Time: Thursday 10:00–13:00 Location: BH-N 128

DY 58.1 Thu 10:00 BH-N 128

Optimal design of the Tweezer control for chimera states — •Iryna Omelchenko[1], Oleh E. Omel'chenko[2], Anna Zakharova[1], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Weierstrass Institute, Berlin, Germany

Chimera states are complex spatio-temporal patterns which consist of coexisting domains of spatially coherent and incoherent dynamics in systems of coupled oscillators. In small networks, chimera states usually exhibit short lifetimes and erratic drifting of the spatial position of the incoherent domain. We introduce a tweezer feedback control scheme which can effectively stabilize and fix the position of chimera states in small systems [1]. We analyse the action of the tweezer control in small nonlocally coupled networks of Van der Pol and FitzHugh-Nagumo oscillators, and determine the ranges of optimal control parameters. We demonstrate that the tweezer control scheme allows for stabilization of chimera states with different shapes, and can be used as an instrument for controlling the coherent domains size, as well as the maximum average frequency difference of the oscillators.

[1] I. Omelchenko, O. E. Omel'chenko, A. Zakharova, M. Wolfrum, and E. Schöll, Phys. Rev. Lett. **116**, 114101 (2016).

DY 58.2 Thu 10:15 BH-N 128

Asymmetric frequencies in symmetric oscillator networks — •Diemut Regel[1,2] and Marc Timme[1,2] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Goettingen — [2]Chair for Network Dynamics, Center for Advancing Electronics (cfaed) and Institute for Theoretical Physics, TU Dresden, 01062 Dresden

The emergence of collective order fundamentally underlies the function of dissipative dynamical systems. Certain symmetries such as a continuous translation symmetry or a discrete permutation symmetry constitute common conditions to enable dynamical ordering processes. Homogeneous changes to local system properties do not affect such symmetries. Here we report that homogeneously decreasing the entirely local self-interactions in symmetrically pulse-coupled oscillator networks may remove constraints common in all oscillator networks coupled continuously in time and thereby enable increased disorder during collective transient dynamics. Moreover, the persistent long-term dynamics may exhibit asymmetrically disordered average frequencies despite the system being entirely symmetric. We explain and systematically evaluate this anomalous phenomenon of collective network dynamics.

DY 58.3 Thu 10:30 BH-N 128

Chimeras in a minimal oscillator network and its thermodynamic counterpart — •Sindre W. Haugland[1,2], Felix Kemeth[1,2], and Katharina Krischer[1] — [1]Physik-Department, Nonequilibrium Chemical Physics, Technische Universität München, James-Franck-Str. 1, D-85748 Garching, Germany — [2]Institute for Advanced Study - Technische Universität München, Lichtenbergstr. 2a, D-85748 Garching, Germany

A network of nonlinear oscillators can exhibit chimera states, the coexistence of synchronized and desynchronized oscillation, for uniform parameters and symmetrical coupling. In the case of nonlinearly coupled Stuart-Landau oscillators, chimera states form spontaneously from generic initial conditions even when the coupling is purely global.

Here, we start by considering a minimal model of only four globally coupled Stuart-Landau oscillators, identifying a multitude of chimera and related states with a varying degree of symmetry, as well as the specific bifurcations in which these states are created and destroyed. Some of these states are also found to be co-stable. By systematically increasing the ensemble size, we subsequently trace how the minimal states develop and identify which of them give rise to the already known macroscopic chimera states.

DY 58.4 Thu 10:45 BH-N 128

Symmetry-Broken Amplitude- and Phase-Locking in Two Identical Symmetrically Coupled Stuart-Landau Oscillators — •André Röhm and Kathy Lüdge — Institut für Theoretische Physik, TU Berlin

In the model system of two instantaneously and symmetrically coupled identical Stuart-Landau oscillators we demonstrate that there exist stable solutions with symmetry-broken amplitude- and phase-locking. Similar to Chimera States, these states are a simple and approachable example of symmetry-breaking in oscillatory systems. They are characterized by a non-trivial fixed phase and amplitude relationship between both oscillators, while simultaneously maintaining perfectly harmonic oscillations of the same frequency. This is despite the fact, that we do not employ a symmetry-breaking coupling. These states have potential applications as bistable states for switches in a wide array of coupled oscillatory systems.

While some of the surrounding bifurcations have been previously described, we present the first detailed analytical and numerical description of these states and present analytically and numerically how they are embedded in the bifurcation structure of the system, arising both from the in-phase as well as the anti-phase solutions. The de-

pendence of both the amplitude and the phase on parameters can be expressed explicitly with analytic formulas. As opposed to previous reports, we find that these symmetry-broken states are stable, which can we can show analytically.

DY 58.5 Thu 11:00 BH-N 128

Experimental observation of spiral wave chimeras in coupled chemical oscillators — •Jan Frederik Totz[1], Julian Rode[1], Mark Tinsley[2], Kenneth Showalter[2], and Harald Engel[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]West Virginia University, Morgantown, USA

In 2002, studying synchronization of nonlocally coupled oscillators, Kuramoto and coworkers made a remarkable observation: Although both the natural frequency of the individual oscillators as well as their coupling among each other were identical, for certain initial conditions some oscillators became phase-synchronized while others do not [1]. The discovery of this counterintuitive state, named chimera state, triggered an increasing number of studies on partial synchronization. I will present a versatile setup based on optically coupled catalytic micro-particles [2], that allows for the experimental study of synchronization patterns in very large networks of relaxation oscillators under well-controlled laboratory conditions. In particular I will show our experimental observation of the spiral wave chimera, predicted by Kuramoto [2]. This pattern features a wave rotating around a spatially extended core that consists of phase-randomized oscillators [3].

[1] Kuramoto in Nonlinear Dynamics and Chaos, CRC Press (2002)

[2] Taylor et al. PCCP (2015)

[3] Totz et al. Nature Physics (2017)

15 min. break

DY 58.6 Thu 11:30 BH-N 128

Chimera states in multi-strain epidemic models with temporary immunity — •Philipp Hövel[1,2], Larissa Bauer[1], Jason Bassett[1], Yuliya Kyrychko[3], and Konstantin Blyuss[3] — [1]TU Berlin — [2]BCCN Berlin — [3]University of Sussex

We investigate a time-delayed epidemic model for multi-strain diseases with temporary immunity [1]. In the absence of cross-immunity between strains, dynamics of each individual strain exhibits emergence and annihilation of limit cycles due to a Hopf bifurcation of the endemic equilibrium, and a saddle-node bifurcation of limit cycles depending on the time delay associated with duration of temporary immunity. Effects of all-to-all and non-local coupling topologies are systematically investigated by means of numerical simulations, and they suggest that cross-immunity is able to induce a diverse range of complex dynamical behaviors and synchronization patterns, including discrete traveling waves, solitary states, and amplitude chimeras. Interestingly, chimera states are observed for narrower cross-immunity kernels, which can have profound implications for understanding the dynamics of multi-strain diseases.

Reference: [1] L. Bauer, J. Bassett, P. Hövel, Y. N. Kyrychko, and K. B. Blyuss, CHAOS **27**, 114317 (2017).

DY 58.7 Thu 11:45 BH-N 128

Chimera states in brain networks: empirical neural vs. modular fractal connectivity — •Teresa Chouzouris[1], Iryna Omelchenko[1], Anna Zakharova[1], Jaroslav Hlinka[2,3], Premysl Jiruska[4], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Institute of Computer Science, Czech Academy of Sciences, Pod Vodarenskou vezi 2, 18207 Prague, Czech Republic — [3]National Institute of Mental Health, Topolova 748, 250 67 Klecany, Czech Republic — [4]Institute of Physiology, Czech Academy of Sciences, Videnska 1083, 14220 Prague, Czech Republic

The interplay of synchrony and asynchrony in complex brain networks is an important aspect in studies of both brain function and disease. Motivated by its potential application to epileptology, we analyse and compare the collective dynamics of FitzHugh-Nagumo neurons in complex networks with two topologies: an empirical structural neural connectivity derived from diffusion-weighted magnetic resonance imaging and a mathematically constructed network with modular fractal connectivity [1]. We qualitatively simulate the dynamics of epileptic seizures and study the influence of the removal of nodes on the network synchronizability, which can be useful for applications to epileptic surgery.

[1] T.Chouzouris, I. Omelchenko, A. Zakharova, J. Hlinka, P. Jiruska, and E. Schöll, Chimera states in brain networks: empirical neural vs. modular fractal connectivity. arXiv:1710.08219 (2017).

DY 58.8 Thu 12:00 BH-N 128

Chimera State in Neuron Populations with Dynamical Synapses — Ali Calim[1], Philipp Hövel[2], Mahmut Özer[3], and •Muhammet Uzuntarla[1] — [1]Department of Biomedical Engineering, Bulent Ecevit University, 67100 Zonguldak, TURKEY — [2]Institut für Theoretische Physik, Technische Universitat Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [3]Department of Electrical-Electronics Engineering, Bulent Ecevit University, 67100 Zonguldak, TURKEY

Current literature on Chimera state in neuronal populations mostly discusses the topic with dynamical system arguments which does not provide information about potential concrete biological reasons giving rise to emergence of Chimera in neural medium. With this motivation, our aim is to investigate the influence of short-term synaptic plasticity (STP) on Chimera state in a non-locally coupled network of spiking Morris-Lecar neurons. We first show that Chimera state can appear in population with static synapses (non-plastic) in case of either weak synaptic strength or sparse connectivity between neurons. When there exists strong synaptic strength and dense connectivity, the whole population exhibits synchronized behavior. But, we found that optimal levels of synaptic depression and facilitation at chemical synapses can induce Chimera and Multi Chimera states in such strongly and densely coupled neural populations. Notably, to the best our knowledge, we here show for the first time the existence of Chimera state with Morris-Lecar model neurons.

DY 58.9 Thu 12:15 BH-N 128

Synchronization of chimera states in two-layer networks of nonlocally coupled chaotic maps — •Galina Strelkova[1], Andrei Bukh[1], Eckehard Schöll[2], and Vadim Anishchenko[1] — [1]Saratov State University, Saratov, Russia — [2]Technical University of Berlin, Berlin, Germany

We explore numerically synchronization effects and their dynamical and statistical properties in two different two-layer networks of nonlocally coupled chaotic maps. The first network is represented by two coupled one-layer networks of nonlocally coupled identical logistic maps with a control parameter detuning. The second two-layer network we study is made of two coupled one-layer networks of nonlocally coupled chaotic Henon and Lozi maps. We show that both two-layer networks under consideration can demonstrate the phenomena of external and mutual synchronization of various complex spatiotemporal structures, including different chimera states. We quantify the identity of synchronous structures by calculating the cross-correlation coefficient. In the synchronization regime this characteristic is very close to 1. We also show that the synchronization phenomena in the considered two-layer networks are observed within a finite region in the parameter space. To illustrate this we construct the synchronization regions for synchronized chimera structures in the plane of two control parameters of the considered networks.

DY 58.10 Thu 12:30 BH-N 128

Impact of noise on the lifetime of chimera states and spatio-temporal intermittency in ensembles of nonlocally coupled chaotic oscillators — •Nadezhda Semenova[1], Galina Strelkova[1], Vadim Anishchenko[1], and Anna Zakharova[2] — [1]Department of Physics, Saratov State University, 83 Astrakhanskaya Street, Saratov 410012, Russia — [2]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

We describe numerical results for the dynamics of networks of nonlocally coupled chaotic oscillators. It has been demonstrated that elements in amplitude chimera clusters are characterized by a nonstationary dynamics. This process looks like nonperiodic switchings between amplitude and phase chimeras. It has been shown that in autonomous ensembles, the nonstationary regime of switchings has a finite lifetime and represents a transient process towards a stationary regime of phase chimera. Our numerical studies have shown that a single noise perturbation of the ensemble elements in the nonstationary regime can increase the lifetime (duration) of this mode and even revive the amplitude chimera. If single noise perturbations are introduced into the network elements constantly in certain time intervals, then the transient process can be observed for an infinite time. However, has been established that the noise source, which is constantly acting on the

ensemble with the phase chimera, does not induce new regimes and structures and leads only to noisy snapshots. The stationary phase chimera regime turns out to be stable towards noise perturbations.

DY 58.11 Thu 12:45 BH-N 128

Chimera states in networks of logistic maps with hierarchical connectivities — •Alexander zur Bonsen, Iryna Omelchenko, Anna Zakharova, and Eckehard Schöll — Institut für Theoretische Physik, Technische Universität Berlin, Germany

Chimera states are complex spatiotemporal patterns consisting of coexisting domains of coherence and incoherence. We study networks of nonlocally coupled logistic maps and analyze systematically how the dilution of the network links influences the appearance of chimera patterns. The network connectivities are constructed using an iterative Cantor algorithm to generate fractal (hierarchical) connectivities. Increasing the hierarchical level of iteration, we compare the resulting spatiotemporal patterns. We demonstrate that a high clustering coefficient and symmetry of the base pattern promotes chimera states, and asymmetric connectivities result in complex nested chimera patterns.

A. zur Bonsen, I. Omelchenko, A. Zakharova, and E. Schöll, *Chimera states in networks of logistic maps with hierarchical connectivities.* arXiv:1711.03287 (2017)

DY 59: Microswimmers II (joint session DY/CPP/BP)

Time: Thursday 10:00–13:15 Location: BH-N 243

DY 59.1 Thu 10:00 BH-N 243

Dynamical density functional theory for swarms of active microscopic circle swimmers — Christian Hoell, Hartmut Löwen, and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

The study of self-propelled particles and active microswimmers is an intensely growing field. However, mostly straight-propelling objects are addressed. In contrast to that, typical real objects are imperfect and show persistently bent trajectories, as investigated in the present case.

Recently, we introduced a first dynamical density functional theory to describe swarms of straight swimming microswimmers suspended in a fluid [1]. The theory includes all basic ingredients, namely, self-propulsion, hydrodynamic as well as steric interactions between the swimmers, and confinement by external potentials. We have now extended this theory to statistically characterize the collective behavior of microscopic circle swimmers [2].

To illustrate the statistical consequences of circle swimming [2], we consider confinement by a spherical trap. While straight-swimming objects tend to push outward against the confining barriers and only by spontaneous symmetry breaking collectively move around the trap, circle swimmers show a deterministic tendency of rotating around the confinement. An increasing tendency of circle swimming leads to localization of the swimmer density in the center of the trap. We have investigated both pusher- and puller-type swimming mechanisms.

[1] A. M. Menzel et al., *J. Chem. Phys.* **144**, 024115 (2016).
[2] C. Hoell et al., *New J. Phys.* in press (2017).

DY 59.2 Thu 10:15 BH-N 243

Memory-induced transition to persistent rotational motion for active colloids in viscoelastic media — •Narinder Narinder[1], Clemens Bechinger[1,2], and Juan Ruben Gomez-Solano[1] — [1] *2.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany* — [2] *Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany*

Life in nature is strongly conjoined with viscoelastic fluids, such as human blood and mucus. Thus, understanding the behavior of artificial microswimmers [1] in such fluids holds the potential for applications such as targeted drug delivery and cargo transport. Motivated by this, we study the dynamics of active colloids in a viscoelastic fluid. Investigating the fluid in the linear rheological response regime, with the increase in propulsion speed, a strong enhancement of the rotational diffusion of the particles is observed [2]. Further increase in the propulsion velocity of the particles leads to the emergence of a new behavior, in which particles describe well defined circular trajectories. Characterization of these orbits, reveals a non-linear dependence of the angular speed on the propulsion speed. We propose that these circular trajectories, absent in Newtonian fluids, originate from a persistent torque acting on the particles which stem from the strong coupling of particles directed motion to microstructural relaxation of the fluid.

[1] J. R. Gomez-Solano et al., Sci. Rep. 7, 14891 (2017).
[2] J. R. Gomez-Solano et al., Phys. Rev. Lett. 116, 138301 (2016).

DY 59.3 Thu 10:30 BH-N 243

Mesoscale turbulence in active suspensions subjected to orienting external fields — •Henning Reinken[1], Sebastian Heidenreich[2], Markus Bär[2], and Sabine H. L. Klapp[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [2]Mathematische Modellierung und Datenanalyse, Physikalisch-Technische Bundesanstalt, Berlin, Germany

Active fluids show a variety of self-sustained non-equilibrium phenomena. An intriguing example is the emergence of a turbulent state in bacterial suspensions, denoted as mesoscale turbulence [1]. Recent publications have shown that a fourth order field theory for the collective microswimmer velocity describes the main features of mesoscale turbulence, including the emergence of a typical vortex size [2,3]. This theory couples the polar order parameter of the microswimmers to the solvent velocity and can be derived from a microscopic Langevin model including hydrodynamic and steric interactions via the Fokker-Planck equation [3,4]. In this work, we extend the theory towards the impact of orienting external fields (e.g. for magnetotactic bacteria or gravitactic algae cells). Using linear stability analysis and weakly nonlinear analysis, we investigate the influence of such external fields on the emerging structures. In addition, we verify our results via numerical solution of the equations.

[1] M. Marchetti et al., Rev. Mod. Phys. **85**, 1143 (2013).
[2] J. Dunkel et al., New J. Phys. **15**, 045016 (2013).
[3] S. Heidenreich et al., Phys. Rev. E **94**, 020601(R) (2016).
[4] H. Reinken et al., in preparation.

DY 59.4 Thu 10:45 BH-N 243

Cluster formation of microswimmers with individually controlled motility — •Tobias Bäuerle[1], Andreas Fischer[2], Thomas Speck[2], and Clemens Bechinger[1] — [1]Universität Konstanz, Germany — [2]Johannes Gutenberg Universität Mainz, Germany

One of the most interesting aspects of microswimmers is their ability to form dynamical clusters even in the absence of long-ranged interactions. Previous experiments and simulations have demonstrated the occurrence of phase separation into large clusters and a dilute gas phase when the density and motility of the particles is sufficiently high. In contrast to previous studies, where the particle motility was kept constant in space and time, in our experiments we are able to control the motility of each single microswimmer depending on its surrounding, e.g. the local density and configuration of microswimmers. Using a light-activated system, such individual motility control is achieved by a feed-back system consisting of a rapidly scanned laser beam and a real-time particle detection algorithm. By introducing appropriate interaction-rules we demonstrate that formation of clusters can occur already at very small particle densities and that their shape and density can be modified by small variations in the interaction rules.

DY 59.5 Thu 11:00 BH-N 243

Optimal decision making for sperm chemotaxis in the presence of noise — •Justus A. Kromer[1], Steffen Märcker[2], Steffen Lange[3], Christel Baier[2], and Benjamin M. Friedrich[3] — [1]Stanford University, Stanford CA, USA — [2]TU Dresden, Dresden, Germany — [3]cfaed/TU Dresden, Dresden, Germany

Navigating agents such as biological cells rely on noisy sensory input. In cells performing chemotaxis, such noise arises from the stochastic binding of signaling molecules at low concentrations. We theoretically address the classic problem of chemotaxis towards a single target. As application example, we study chemotaxis of marine sperm towards the egg. Recent experiments revealed that these cells are able to dynamically switch between slow and fast chemotactic steering. The benefit of this decision making remains open.

We reveal an inherent coupling between the speed of chemotactic steering and the strength of directional fluctuations that result from the amplification of noise in the chemical input signal. This implies a trade-off between slow, but reliable, and fast, but less reliable steering. By formulating optimal navigation in the presence of noise as a Markov decision process, we show that dynamic switching between slow and fast steering substantially increases the probability to find the egg. This decision making is most beneficial, if chemical signals are above detection threshold, yet signal-to-noise ratios of gradient measurements are low. This situation generically arises at intermediate distances from the egg, thus defining a 'noise zone' that cells have to cross.

15 min. break

DY 59.6 Thu 11:30 BH-N 243

Crowd localisation and cohesion of micro-swimmers with perception-dependent motility — •Francois Lavergne, Hugo Wendehenne, and Clemens Bechinger — Department of Physics, University of Konstanz, 78464 Konstanz, Germany

The origin of crowd formation and cohesion in natural contexts remains an important question of collective dynamics, especially in the absence of taxis, communication, confinement, or attractive forces between the individuals. In this work, we show that the mere variation of the motility depending on the perception of other individuals is enough to induce such behaviour. We introduce a long-range indicator of crowd perception that only assumes the ability of an individual to count others within its vision cone. When this quantity exceeds a certain threshold for a given individual, its velocity is increased. This simple rule is applied in an experiment involving photo-responsive colloidal micro-swimmers, whose velocities can be individually varied by live-tuning the intensity of laser spots directed onto them. We observe that initially very dilute ensembles of these micro-swimmers localise into isolated groups, with virtually empty surroundings in unbound space, in sharp contrast with the long-time diffusive behaviour expected in the case of a constant motility. These groups remain cohesive, despite the activity of individuals within them and the absence of alignment, due to a kinetic stabilisation mechanism stemming from the modulation of the motility upon the non-reciprocal perception.

DY 59.7 Thu 11:45 BH-N 243

Maximum in density heterogeneities of active swimmers — •Fabian Jan Schwarzendahl and Marco G. Mazza — Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Suspensions of unicellular microswimmers such as flagellated bacteria or motile algae exhibit spontaneous density heterogeneities at large enough concentrations. Based on the relative location of the biological actuation appendages (i.e. flagella or cilia) microswimmers' propulsion mechanism can be classified into two categories: (i) pushers, like E. coli bacteria or spermatozoa, that generate thrust in their rear, push fluid away from them and propel themselves forward; (ii) pullers, like the microalgae Chlamydomonas reinhardtii, that have two flagella attached to their front, pull the fluid in and thereby generate thrust in their front. We introduce a novel model for biological microswimmers that creates the flow field of the corresponding microswimmers, and takes into account the shape anisotropy of the swimmer's body and stroke-averaged flagella. We characterize the nonequilibrium phase diagram, as the filling fraction and Péclet number are varied, and find density heterogeneities in the distribution of both pullers and pushers, due to hydrodynamic instabilities. We find a maximum degree of clustering at intermediate filling fractions and at large Péclet numbers resulting from a competition of hydrodynamic and steric interactions between the swimmers. We develop an analytical theory that supports these results. This maximum might represent an optimum for the microorganisms' colonization of their environment.

DY 59.8 Thu 12:00 BH-N 243

Chemotactic interactions in systems of active and passive colloids — •Julian Stürmer[1], Dhruv Singh[2], Maximilian Seyrich[1], Peer Fischer[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]MPI-IS, Heisenbergstr. 3, 70569 Stuttgart, Germany

Self-propelled particles exhibit a variety of self-assembled dynamic structures. In particular, mixtures of active and passive colloids crystallize into 2D clusters as a result of chemotactic interactions [1]. The active colloids represent Janus particles that move while creating sinks in a chemical concentration field. The passive colloids react to the corresponding chemical gradients in form of a diffusiophoretic drift velocity towards the active particles. We model the mixtures using Langevin equations and a diffusion equation for the chemical field extending our approach in [2]. With increasing interaction strength, we observe a gaslike state, an oscillatory and finally a collapsed state. We study the clustering dynamics by quantifying the cluster growth and measuring the cluster velocity as a function of cluster size.

In a similar approach, we model a system of solely active colloids that interact via translational and rotational diffusiophoresis. Here, we take into account the asymmetric character of the Janus particles by including dipole contributions in the chemical concentration field. This asymmetry gives rise to interesting collective phenomena, e.g. the formation of chains that has been observed in recent experiments.

[1] D. P. Singh et al., Adv. Mater. 1701328 (2017)
[2] O. Pohl et al., Phys. Rev. Lett. 112, 238303 (2014)

DY 59.9 Thu 12:15 BH-N 243

Modular microswimmers formed by ion-exchange particles — •Andreas Fischer, Ran Niu, Thomas Palberg, and Thomas Speck — Institut für Physik, Johannes-Gutenberg-Universität Mainz, Germany

Colloidal ion exchange particles generate solvent flow due to a combination of electroosmosis and electrophoresis, which induces long-range attractive interactions between the colloidal particles [1]. These interactions lead to the formation of colloidal "molecules" of varying size and structure. By breaking reciprocality, these molecules can be made active. Depending on their composition, we observe passively diffusing, linearly and circularly moving molecules with different propulsion velocities. We develop a model based on conservative interactions, which makes quantitative predictions about the swimmers' motion that we compare to the experimental results.

DY 59.10 Thu 12:30 BH-N 243

The droplet divisome — Kyle A. Baldwin, Babak Vajdi Hokmabad, and •Corinna C. Maass — MPI für Dynamik und Selbstorganisation Göttingen

Active emulsions of nematic liquid crystals in micellar surfactant solutions are a flexible and well controlled model system for microswimmers, exhibiting a wealth of features like helical swimming, convection driven clustering, chemotaxis and autochemotaxis. Their propulsion is driven by Marangoni stresses caused by self-supporting instabilities in the interfacial surfactant coverage. Generally, such surface tension variations should deform the droplet interface, but we have not seen measurable deviations from a spherical shape for 50μm droplets in Hele-Shaw cells due to strong capillary forces. However, in experiments using squeezed droplets, i.e. larger, more disk-shaped objects in strong two-dimensional confinement, capillary forces are weakened due to an effective switch from areal to line tension and a decrease of the deformable interface to volume ratio. We have observed multipolar Marangoni instabilities, visible deformation during self propulsion and a spontaneous self division cascade for arrested droplets.

DY 59.11 Thu 12:45 BH-N 243

Dynamical arrest in active emulsions — •Babak Vajdi Hokmabad and Corinna C. Maass — MPI für Dynamik und Selbstorganisation Göttingen

Liquid crystal (LC) droplets self-propel in an aqueous surfactant solution due to Marangoni flow at the droplet's interface. This propulsion is sustained by micellar solubilization of the LC phase. The solubilization leads to a secretion of filled surfactant micelles in the trail of the swimming droplet. This causes depletion of empty micelles in the trail and thereby trail avoidance. We have directly imaged the secretion and spreading of the filled micelles by adding fluorescent dye to the LC phase. The decay of the extracted Gaussian profiles in time is consistent with the theoretical diffusive spreading. Using this technique, we are able to visualize the chemotactic interaction of a swimmer with a trail. To study the collective dynamics of this autochemotaxis-dominated system we track individual swimmers in dense droplet ensembles in 2D and 3D. Results show that in a crowded system, a potential landscape is formed with local minima between the trails. We report on dynamical arrest of the swimmers in transient cages formed inside these local minima.

DY 59.12 Thu 13:00 BH-N 243

Active Double Emulsions — •Kyle A. Baldwin, Babak Vajdi

Hokmabad, and Corinna C. Maass — MPI für Dynamik und Selbstorganisation, Göttingen

Active emulsions – solutions containing self-propelling microscopic droplets – display a rich variety of solo and collective swimming behaviours, from self-avoiding helices to collective raft formation, which are strongly influenced by factors such as wall proximity, autochemotaxis, and liquid crystal (LC) structure. Here, we report on the formation and swimming behaviour of active water-oil-water (WOW) double-emulsions; swimming LC oil droplets which carry a secondary inner water droplet. We observe new periodically oscillating swimming modes, and find that shell stability is strongly influenced by nematicity, which inhibits coalescence of the aqueous phases. The utility of these double emulsion swimmers as cargo carriers, and the ability to release this cargo on-demand, makes this system an ideal mechanism for chemical delivery to localised, switchable reaction sites, with prospects for drug delivery.

DY 60: Anomalous Diffusion (joint session DY/BP)

Time: Thursday 10:00–13:15 Location: BH-N 334

DY 60.1 Thu 10:00 BH-N 334

Frequency-dependent Hydrodynamic Interaction Between Two Nanocolloids — •Gerhard Jung and Friederike Schmid — Institut für Physik, Staudingerweg 9, 55128 Mainz

The dynamics of fluids are subject of extensive research since over 300 years. In the second book of the "Principa" Newton investigates the dynamics of viscous fluids to disprove the Cartesian idea that the planetary orbits are created by fluid vortices. Since then this problem has drawn the attention of many great physicists and mathematicians. However, there are still many fundamental questions in the field of fluid dynamics like for example the understanding of hydrodynamic interactions between two particles submerged in a fluid. The first and most basic analytic derivation was published by Oseen describing the interaction between two point particles in a steady-state Stokes flow.

Based on work by Ardekani et al. we extended this approach by considering finite-sized particles in an unsteady compressible flow, described by the linearized Navier-Stokes equations [1]. This theoretical extension enables us to compare results from hydrodynamic theory to molecular dynamics simulations of nanocolloids in a Lennard-Jones fluid. We show that the simulation data agree qualitatively and quantitatively with our theoretical findings. The analytic results can therefore be used to include dynamically consistent hydrodynamic interactions into non-Markovian coarse-grained models.

[1] G. Jung, F. Schmid, accepted by the Journal Physics of Fluids

DY 60.2 Thu 10:15 BH-N 334

Anomalous Diffusion in Complex Dynamical Systems: Diffusing Diffusivity Models — •Rohit Jain and Kizhakeyil L Sebastian — Indian Institute of Science, Bangalore 560012, India

Diffusion inside a crowded, rearranging environment has attracted a lot of attention recently [1]. In such systems, the mean square displacement of diffusing particle remains Fickian obeying $\langle x^2 \rangle \propto T$, yet the distribution of displacements is not Gaussian. Following the work of Chubynsky and Slater [2], we have proposed a class of analytically solvable models where the diffusion coefficient becomes a random function of time [3]. The results obtained with our model are in very good agreement with the simulations of Chubynsky and Slater (see also [4]).

In a different model [5], we have analyzed a case where diffusivity evolves as a Lévy flight process. That is, the distribution of diffusivity decays as power-law of the form $D^{-1-\alpha}$ with $0 < \alpha < 1$, for large D. The distribution of displacements with this model is found to be a Lévy stable distribution with a time dependent width. With this model, the dynamics is Brownian at short times and superdiffusive at long times.

References:

[1] Wang et. al., Proc. Natl. Acad. Sci. U.S.A., **106**, 15160 (2009).
[2] Chubynsky and Slater, Phys. Rev. Lett. **113**, 098302 (2014).
[3] Jain and Sebastian, J. Phys. Chem. B **120**, 3988 (2016).
[4] Chechkin et. al., Phys. Rev. X **7**, 021002 (2017).
[5] Jain and Sebastian, Phys. Rev. E **95**, 032135 (2017).

DY 60.3 Thu 10:30 BH-N 334

First-passage properties of Gaussian interfaces — •Markus Gross — MPI-IS Stuttgart / Uni Stuttgart

Fluctuating interfaces are relevant in various circumstances, such as liquid phase separation, nanofluidics, or surface growth. An effective description of the interfacial dynamics is provided by the Edwards-Wilkinson and the stochastic Mullins-Herring equations, corresponding to non-conserved and conserved dynamics. Despite the Gaussian nature of these models, their first-passage properties are highly nontrivial due to the presence of long-range correlations along the interface. We study here the full spatio-temporal evolution of an interface until it reaches a given maximum height for the first time. Analytical predictions, obtained within weak-noise theory, are contrasted to results of numerical Langevin simulations of the first-passage problem. It is shown the averaged profile shape is accurately captured by weak-noise theory, but the time evolution (specifically, the dynamic exponent) is not. The latter can instead be accounted for within a reduced model based on a fractional Brownian walker, which describes the anomalous diffusion of a tagged monomer of the interface as it approaches an absorbing boundary.

References: M. Gross, arXiv:1708.03466, 1708.03467

DY 60.4 Thu 10:45 BH-N 334

Sinai type diffusion in Gaussian random potentials with decaying spatial correlations — •Igor Goychuk[1], Vasyl O. Kharchenko[2], and Ralf Metzler[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Institute of Applied Physics, Natl. Acad. Sci. Ukraine, Sumy, Ukraine

Logarithmic subdiffusion is usually associated with random force disorder and non-stationary potential fluctuations whose root mean squared amplitude grows with distance. We show that such Sinai type diffusion also universally emerges at sufficiently low temperatures in stationary Gaussian random potentials with spatially decaying correlations, known to exist in a broad range of physical systems. Combining results from extensive simulations with a scaling approach we elucidate the physical mechanism of this unusual subdiffusion. In particular, we explain why with growing temperature and/or time a first crossover occurs to standard, power-law subdiffusion and then a second crossover occurs to normal diffusion with a disorder-renormalized diffusion coefficient. Interestingly, the initial, nominally ultraslow diffusion turns out to be much faster than the universal de Gennes-Bässler-Zwanzig limit of the renormalized normal diffusion, which realistically cannot be attained at sufficiently low temperatures and/or for strong disorder. The ultraslow diffusion is also shown to be non-ergodic and it displays a local bias phenomenon. Our simple scaling theory not only explains our numerical findings, but also has a predictive character.

Funded by the DFG, Grant GO 2052/3-1

DY 60.5 Thu 11:00 BH-N 334

Random diffusivity from stochastic equations: two models in comparison for Brownian yet non-Gaussian diffusion. — •Vittoria Sposini[1,2], Aleksei V. Chechkin[1,3], Flavio Seno[4], Gianni Pagnini[2], and Ralf Metzler[1] — [1]Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany — [2]Basque Center for Applied Mathematics, 48009 Bilbao, Spain — [3]Akhiezer Institute for Theoretical Physics, 61108 Kharkov, Ukraine — [4]INFN, Padova Section and Department of Physics and Astronomy 'G.Galilei', University of Padova, 35131 Padova, Italy

Recently a considerable number of systems have been discovered exhibiting a Brownian yet non-Gaussian dynamics, characterised by a linear growth in time of the mean-squared displacement yet a non-Gaussian probability density function of the particle displacement. This behaviour observed in very different physical systems has been interpreted as resulting from diffusion in inhomogeneous environments and mathematically represented through a variability of the diffusion coefficient. Indeed different models describing a fluctuating diffusivity have been studied. Here it is presented a set of stochastic equations describing a time dependent random diffusivity within a broad spectrum of distributions: the class defined as generalised Gamma distribution. Two models for particles spreading in such variable environments are then studied. The first belongs to the class of generalised grey Brow-

nian motion while the second follows from the idea of diffusing diffusivity. We promote these two physical models for the description of stochastic particle motion in complex environments.

DY 60.6 Thu 11:15 BH-N 334

Infinite invariant densities in intermittent systems — •Philipp Meyer[1], Eli Barkai[2], and Holger Kantz[1] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, D 01187, Dresden, Germany — [2]Department of Physics, Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan, 52900, Israel

Dynamical intermittency is known to generate anomalous statistical behaviour of dynamical systems, a prominent example being the Pomeau-Manneville map. The system exhibits waiting times and chaotic bursts. For a wide range of parameters no physical invariant density exists. We show how this regime can be characterised quantitatively using the techniques of infinite invariant densities and the Thaler-Dynchin limit theorem.

We obtain pseudo Brownian motion by summing up the increments created by the map. The output corresponds to stochastic processes like continuous time random walks. We are able to relate infinite ergodic theory with scale invariant transport. Here time average diffusivities are especially interesting, because they depend not only on the joint probability density function but also on the exact definition of the paths during waiting periods.

We also present a nonlinear oscillator, i.e., a physical model in continuous time, whose properties in terms of weak ergodity breaking and ageing have a one-to-one correspondence to the properties of the Pomeau-Manneville map. We see how expectation values exhibit ageing in terms of scaling in time.

15 min. break

DY 60.7 Thu 11:45 BH-N 334

Tempered dynamics from fractional Brownian motion and generalized Langevin equation: Application to lipid molecule diffusion — •Trifce Sandev[1,2,3], Daniel Molina-Garcia[4,5], Gianni Pagnini[4], Aleksei Chechkin[5], and Ralf Metzler[5] — [1]Ss. Cyril and Methodius University in Skopje, Macedonia — [2]RSD, Skopje, Macedonia — [3]MANU, Skopje, Macedonia — [4]BCAM - Basque Center for Applied Mathematics, Bilbao, Basque Country, Spain — [5]University of Potsdam, Germany

Anomalous diffusion is widely observed in many systems. Often, the system shows a crossover from initial anomalous diffusion to terminal normal diffusion. We consider tempered versions of the fractional Brownian motion and the generalized Langevin equation (GLE) to describe this crossover dynamics. For persistent input noise, the former describes the case when an initially superdiffusive particle switches to normal diffusive behavior, while the latter exhibits a subdiffusive to normal diffusive crossover. Both models are characterized by power-law correlations of the driving noise, i.e., tempered fractional Gaussian noise, which is a noise with Gaussian amplitude and power-law correlations with a cutoff at some mesoscopic time scale. In both models we employed either hard (exponential) or soft (power-law) truncation. We show excellent agreement of the analytical results for the mean squared displacement obtained from the GLE with those obtained for the lipid dynamics in simulated model membranes [1].

[1] D. Molina-Garcia, T. Sandev, G. Pagnini, A. Chechkin, and R. Metzler, in preparation.

DY 60.8 Thu 12:00 BH-N 334

Kinetics of an enzymatic reaction under anomalous diffusion - A case study — •Daniela Froemberg and Felix Höfling — Freie Universität Berlin, Department of Mathematics and Computer Science

The interior of biological cells constitutes a crowded environment in which diffusion of organelles or macromolecules is anomalous[1]. Consequently, such heterogeneous conditions also alter the kinetics of the chemical reactions taking place.

Here, we report on simulations of the reaction-diffusion dynamics of an enzyme-catalyzed reaction using a particle-based scheme. The particles diffuse in space and reactions occur with a certain microscopic propensity if the reaction partners are within a prescribed reaction distance. To mimick a crowded environment, we implement the subdiffusion by a fractional Brownian motion.

For anomalous diffusion, it is well-known that the the diffusion coefficient is a function of the lag time. Similarly, the coefficient $k(t)$ of the effective reaction rate can adopt a timescale dependence. Preliminary results from extensive simulations suggest a power law dependence of $k(t)$, slowing down the reaction as compared to the normal diffusive case.

We detail the behavior of $k(t)$, elucidate the role of the subdiffusion parameter, and test for an old prediction originally made for reactions on fractals.

[1] F. Höfling, T. Franosch, Rep. Prog. Phys. 76 (2013) 046602 (50pp)

DY 60.9 Thu 12:15 BH-N 334

Obstructed Motion – from frozen to mobile obstacles — Christoph Zunke, René Hermann, Manuel A. Escobedo-Sanchez, Jörg Bewerunge, •Florian Platten, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Many natural and industrial processes rely on transport through confined spaces. Confinement by obstacles, for example in porous materials or crowded environments, leads to anomalous diffusion. An idealized situation, the diffusion of point-like tracers through the voids between randomly-placed fixed obstacles, is described by the Lorentz model. Beyond a critical obstacle concentration, the obstacles percolate and hence form finite voids that confine the tracers. Thus the tracer motion becomes localized. However, often the obstacles are mobile, e.g., proteins in biological membranes or organelles in cells. We developed a colloidal model system which permits to tune the particle dynamics through the application of a laser light field. It allows us to study the effect of obstacle mobility. If the obstacles are sufficiently mobile, localization of the tracers is avoided and transient subdiffusion is observed.

DY 60.10 Thu 12:30 BH-N 334

Scaled Brownian motion with resetting — •Anna Bodrova[1], Alexei Chechkin[2,3], and Igor Sokolov[1] — [1]Humboldt University, Department of Physics, Newtonstrasse 15, 12489 Berlin, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [3]Akhiezer Institute for Theoretical Physics, Kharkov Institute of Physics and Technology, Kharkov 61108, Ukraine

In the intermittent stochastic processes the dynamics of the system may be interrupted and recommenced at random times from the initial condition. Examples of such processes are found in many fields such as chemistry, biology, ecology and computer science. The time between resetting events may be distributed according to the exponential law or according to the power law. It may be shown that random resetting fundamentally changes the properties of the diffusion process. In the presence of resetting there is a competition between the tendency of diffusive spreading and confinement around the initial state. In our study during the resetting events the particle performs scaled Brownian motion: diffusive motion with time-dependent diffusion coefficient. We calculate mean-squared displacement and probability density function as main characteristics of this process.

DY 60.11 Thu 12:45 BH-N 334

Self-trapping self-repelling random walks — •Peter Grassberger — Juelich Research Center, Juelich, Germany

The model studied in this talk is a seemingly minor modification of the “true self-avoiding walk" (TSAW) model of Amit, Parisi, and Peliti in two dimensions. The walks in it are self-repelling up to a characteristic time T^* (which depends on various parameters), but spontaneously (i.e., without changing any control parameter) become self-trapping after that. For free walks, T^* is astronomically large, but on finite lattices the transition is easily observable. In the self-trapped regime, walks are subdiffusive and intermittent, spending longer and longer times in small areas until they escape and move rapidly to a new area. In spite of this, these walks are extremely efficient in covering finite lattices, as measured by average cover times.

Basically, the phenomenon is due to a delicate balance between two opposite effects of landscape gradients and roughnesses on random walks: While a gradient enhances diffusion, roughness slows it down. Initially, the walker creates a hill by depositing debris, and the hill gradient wins. But the hill surface is also rough. When roughness becomes too large, the walk becomes subdiffusive which increases further the roughness, leading finally to catastrophic trapping.

The phenomenon seems to be described by scaling laws, and some exponent and critical parameter values seem to be simple rationals. In addition, the deposited debris forms (on square lattices and for

some parameter values) non-trivial patterns that suddenly re-arrange at sharp times.

DY 60.12 Thu 13:00 BH-N 334

Non-Gaussian Brownian and viscoelastic diffusion — •Ralf Metzler — Institute of Physics & Astronomy, U Potsdam, Potsdam

Brownian motion as well as viscoelastic anomalous diffusion are stochastic processes driven by Gaussian noise. A growing number of systems is reported in which the mean squared displacement is linear or anomalous, yet the associated probability densities are non-Gaussian. Examples include Brownian motion with exponential probability density for the motion of colloidal beads along tubular structures or in semiflexible polymer networks. Stretched Gaussian shapes along with Brownian motion are seen for the motion of cells on surfaces. Viscoelastic, anomalous motion is observed for submicron tracers in both bacteria and yeast cells. In many systems, at sufficiently long times a crossover to Gaussian behaviour is observed.

In this presentation I will introduce the various observations of non-Gaussian diffusion. In particular, I will report large scale simulations of lipid bilayer systems: in the dilute case viscoelastic and Gaussian diffusion is observed, while in protein-crowded situations stretched Gaussians are observed. This behaviour can, to a good extent, be explained due to geometric constrictions on the motion. I will then introduce a mathematical model for the description of non-Gaussian motion in terms of a stochastically varying diffusion coefficient. In the short time limit this approach is equivalent to the known approach of superstatistics, while at long times a crossover to Gaussian statistics with an effective diffusivity is found.

DY 61: Granular Matter / Contact Dynamics (joint session DY/CPP)

Time: Thursday 10:00–13:00 Location: BH-N 333

DY 61.1 Thu 10:00 BH-N 333

Predicting contact numbers in granular packings — •Matthias Schröter[1], Simon Weis[2], and Gerd Schröder-Turk[3] — [1]Institute for Multiscale Simulation, University Erlangen, Nägelsbachstrasse 49b, 91052 Erlangen, Germany — [2]Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — [3]School of Engineering and Information Technology, Murdoch University, 90 South Street, Murdoch, WA 6150, Australia

The mechanical stability of granular packings depends on the number of contacts its individual particles form with their neighbors. While these contact numbers can be measured using X-ray tomography [1], there are very few theoretical results prediciting this crucial parameter. A major part of the reason why theory lacks behind here is the frictional nature of the contacts [2]; up to now no effective method has been found to handle the inequality given by Coulomb friction. On the other side there is an abundance of experimental data. This raises the question if training an artificial neural network might be more effective to predict contact numbers than asking human experts.

[1] Schaller, Neudecker, Saadatfar, Delaney, Schröder-Turk, and Schröter, Physical Review Letters **114**, 158001 (2015)
[2] Schröter, EPJ Web of Conferences **140**, 01008 (2017)

DY 61.2 Thu 10:15 BH-N 333

Rotator crystals in a granular monolayer — •Simeon Völkel and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

The collective behaviour of vertically vibrated hexagonal disks confined in a horizontal monolayer is investigated experimentally. The disks tend to rotate upon sufficiently strong driving. Additionally, they can arrange in a hexagonal structure, reminiscent of a rotator crystal in equilibrium systems. We investigate the transitions into and out of this non-equilibrium steady state and their dependence on the presence of a wetting liquid. Furthermore we characterize the rotator crystal state using the bond orientational order parameter, parameters coupled with set voronoi diagrams, as well as the distribution of particle orientations. Finally we explore the influence of the disk's shape by varying the number of corners systematically.

DY 61.3 Thu 10:30 BH-N 333

Collisional charging enhances aggregation in granular gases — •Chamkor Singh and Marco G. Mazza — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077, Goettingen, Germany

Since classical antiquity lightnings have been associated with the ashes produced during volcanic activity. It has been long speculated that collisional charging may play a significant role in particle's aggregation in such natural processes, *e.g.*, in the formation of planetesimals during the early stages of the birth of a planet, charging in dust devils, lightnings in thunderclouds, and electric sparks in dunes. We perform molecular dynamic simulations in three dimensions for a dilute, freely-cooling granular gas of viscoelastic particles that exchange charges during collisions. Using percolation theory, we find a stronger power law growth of the average cluster size, $S(t) \sim t^z$, with $z \approx \frac{3}{2}$ in the *collisionally charged* gas than $z \approx \frac{6}{5}$ in the *neutral* case. Remarkably, z is found to be independent of the typical Bjerrum length, or equivalently, of the ratio of characteristic Coulomb to thermal energy. However, this ratio alters the crossover time of the growth. The velocity distribution of the charged viscoelastic particles does not show a relaxation towards Maxwellian within the early stages of aggregation.

DY 61.4 Thu 10:45 BH-N 333

Structural Evolution of Planar Granular Media — •Clara Wanjura[1], Takashi Matsushima[2], Othmar Marti[1], and Rafi Blumenfeld[3,4,5] — [1]Ulm University, Germany — [2]University of Tsukuba, Japan — [3]Inst. of Physics, Chinese Academy of Sciences, China — [4]Imperial College London, UK — [5]Cambridge University, UK

Granular materials are ubiquitous in nature, but continuum models of their macroscale behaviour and properties have proved to be difficult. Particle-scale properties and the structure affect strongly the large-scale behaviour.

Here we study a key characteristic of the structure in two dimensions: the cell-order distribution (COD). We first describe the evolution of the COD by a set of master equations and establish their validity by comparison to simulation data. The structure and the COD evolve mainly by contact making and breaking events. Of these, we identify and quantify 'non-clapping' events as the most relevant to the COD evolution and distinguish these from the less relevant 'clapping' events, which only add noise to the dynamics. The role of the cell order transition rates and their behaviour in the master equations are studied in detail analytically and numerically.

This formalism can be extended to the study of other structural characteristics.

DY 61.5 Thu 11:00 BH-N 333

Optical Properties of Granular Matter — Dominik Kiese, Koray Önder, Sebastian Pitikaris, Matthias Sperl, and •Philip Born — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51147 Köln, Deutschland

Dense packings of hard spheres exhibit strong local ordering, even with lacking long-range order. The point pattern associated with the short-range order of hard sphere packings are shown to exhibit a photonic band-gap, i.e. a complete suppression of wave propagation for wavelengths similar to the center-to-center particle distance [1]. Common center-to-center distances in real granular media are millimetric, and suppression of THz waves reminiscent of development of a photonic bandgap have been observed [2]. We present an experimental study on the evolution of this bandgap with manipulating the structural order in granular packings. Local order in sedimented particle packings is controlled by mixing ratio and size ratio in binary packings. The relation among the bandgap and the structure offers a tool quickly quantify local order and to track structural changes in agitated granular media. We give an outline how to compute the band structure of hard-sphere packings taking into account the full spatial distribution of the dielectric constant.

[1]L. S. Froufe-Pérez et al., Physical Review Letters 117, 053902 (2016).

[2] P. Born. K. Holldack, Review of Scientific Instruments 88, 051802 (2017).

15 min. break

DY 61.6 Thu 11:30 BH-N 333

Aeolian sand sorting and megaripple formation — Marc Lämmel[1], Anne Meiwald[1], Hezi Yizhaq[2], Haim Tsoar[3], Itzhak Katra[3], and •Klaus Kroy[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany — [2]Dpt. of Solar Energy and Environmental Physics, Blaustein Inst. for Desert Research, Ben-Gurion University of the Negev, Israel — [3]Dpt. of Geography and Environmental Development, Ben-Gurion University of the Negev, Israel

Sand is blown across beaches and deserts by turbulent winds. The seemingly chaotic process creates two dominant bedforms: decametre-scale dunes and centimetre-scale ripples, but hardly anything in between. By the very same process, grains are constantly sorted. Smaller grains advance faster, while heavier grains trail behind. Here, we argue that, under erosive conditions, sand sorting and structure formation can conspire to create distinct bedforms in the forbidden wavelength gap between aeolian ripples and dunes. These so-called megaripples are shown to co-evolve with an unusual, predominantly bimodal grain-size distribution. Combining theory and field measurements, we generate a mechanistic understanding of their shape and migration speed, as well as their cyclic aging, renewal, and sedimentary memory, in terms of the intermittent wind statistics. Our results demonstrate that megaripples exhibit close similarities to dunes and can indeed be mechanistically characterised as a special type of ("reptation") dunes.

DY 61.7 Thu 11:45 BH-N 333

Rheology of 3D frictionless spherocylinders — •Dániel B. Nagy[1], Tamás Börzsönyi[1], Philippe Claudin[2], and Ellák Somfai[1] — [1]Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary — [2]Physique et Mécanique des Milieux Hétérogènes, PMMH UMR 7636 ESPCI - CNRS - Univ. Paris-Diderot - Univ. P.M. Curie, Paris, France

The rheology of dense granular matter is an active domain of research and important both from the fundamental and the applied point of view. In the absence of large gradients, a successful approach formulates the constitutive equation as an effective friction μ, dependent only on the dimensionless inertial number I. In our work we used 3D numerical simulations to extend this formalism to frictionless spherocylinders. As in the case of spherical particles, the effective friction is an increasing function of the inertial number. We systematically investigated the dependence of μ on the particle aspect ratio Q, as well as that of the normal stress differences, the volume fraction and the coordination number. We found an interesting non-monotonic behavior of the quasistatic friction coefficient with Q: from the spherical case $Q = 1$, it first sharply increases, reaches a maximum around $Q \approx 1.05$, and then gently decreases until $Q = 3$, passing its initial value at $Q \approx 2$. We provided a microscopic interpretation for this through the analysis of the distribution of dissipative contacts around the particles. For slightly elongated grains the dissipation density is highest in their central cylindrical band, whereas at larger Q this moves to their caps.

DY 61.8 Thu 12:00 BH-N 333

Controlling Segregation and Convection in Vibrofluidised Granular Media — •Christopher Windows-Yule[1,3], Anthony Rosato[2], and David Parker[3] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]New Jersey Institute of Technology, Newark, NJ, USA — [3]University of Birmingham, Edgbaston, Birmingham, UK

The convective and segregative behaviours of granular materials are of great relevance to myriad industrial and natural processes, yet - despite significant research - remain incompletely understood and infamously difficult to control. In this talk, we detail a series of combined experimental and simulational studies in which we elucidate a deep interrelation between these two important phenomena, and novel manners in which this interrelation may be exploited. In particular, we demonstrate manners in which careful manipulation of the geometry and excitation method of a vibrofluidised system may be used to augment, reduce, induce, suppress and otherwise control both convective and segregative phenomena.

DY 61.9 Thu 12:15 BH-N 333

Rheology of Dense Granular Fluids: Theory & Experiment — •Till Kranz[1,2], Olfa Lopez[1], Annette Zippelius[3], Matthias Fuchs[4], and Matthias Sperl[1,2] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Institut für Theoretische Physik, Uni Köln — [3]Institut für Theoretische Physik, Uni Göttingen — [4]Theorie der Weichen Materie, Uni Konstanz

Granular fluids have been found to display a complicated rheology including Newtonian, shear thinning as well as shear thickening regimes. For a continuum description of granular flows, a constitutive equation is required that captures high densities and high shear rates.

We will introduce simple arguments regarding the time and energy scales in the system to explain the different flow behaviors. Newtonian rheology is expected at the lowest densities and shear rates only, shear thinning is related to the granular glass transition [1], and Bagnold scaling [2] is a consequence of hard-core interactions and shear heating. We will show how these constraints can be made quantitative in the framework of *Granular ITT* (Integration Through Transients) [3]. We will present experimental results for the flow behavior measured in a fluidized bed Couette cell that are well described by our theoretical approach.

[1] W. T. Kranz, M. Sperl and A. Zippelius, Phys. Rev. Lett. **104**, 225701 (2010)
[2] R. A. Bagnold, Proc. Royal Soc. A **225**, 49 (1954)
[3] W. T. Kranz, F. Frahsa, A. Zippelius, M. Fuchs and M. Sperl, arXiv:1710.04452, arXiv:1710.04475

DY 61.10 Thu 12:30 BH-N 333

Simulation and modeling of the frustrated packing in a granular system — •Sára Lévay[1], David Fischer[2], Ralf Stannarius[2], Balázs Szabó[3], Tamás Börzsönyi[3], and János Török[1] — [1]Department of Theoretical Physics, BME, Budafoki út 8., H-1111 Budapest, Hungary — [2]Institute of Experimental Physics, Otto von Guericke University, Universitätsplatz 2., D-39106 Magdeburg, Germany — [3]Wigner Research Centre for Physics, Hungarian Academy of Sciences, P.O. Box 49., H-1525 Budapest, Hungary

Optimal packings of uniform spheres is a solved problem in two and three dimensions. The two-dimensional ground state can be easily achieved by simple dynamical processes while in three dimensions this is almost impossible.

In a recent work we have shown that in $2+\varepsilon$ dimensions, achieved by a container in one dimension slightly wider than the spheres, the particles organize themselves in a triangular lattice touching either of the sides of the container. When the system is agitated, it evolves slowly towards the potential energy minimum through metastable states.

We show results of DEM simulations and Monte Carlo models which fit the experiments: The dynamics is local and is driven by the optimization of the volumes of 7-particle configurations and by the vertical interaction between touching spheres. Defects in the triangular lattice play an important role in the dynamics as they act as an activation source and help the compaction. The system behaves neither as a 2D nor as a 3D system. Geometric frustration hinders the global optimum.

DY 61.11 Thu 12:45 BH-N 333

Frustrated packing in a granular system confined in a $2+\varepsilon$ dimensional box — •David Fischer[1], Sára Lévay[2], János Török[2], and Ralf Stannarius[1] — [1]Institute of Experimental Physics, Otto von Guericke University, Universitätsplatz 2, D-39106 Magdeburg, Germany — [2]Department of Theoretical Physics, BME, Budafoki út 8., H-1111 Budapest, Hungary

Packing of spheres in three dimensions necessarily involves geometrical frustration. The locally optimal tetrahedral packing is not space-filling. In contrast, the close-packed equilateral triangular lattice optimizes the packing of disks in a two-dimensional plane both globally and locally.

We show experimentally that inside a container of a width only slightly wider than the diameter of the spheres, the particles organize themselves in a quasi-triangular lattice touching either the front or back wall of the container. Under appropriate agitation (harmonic vertical vibrations) the system can be driven remarkably close to its ground state. Nevertheless, perfect order is practically never reached.

We demonstrate that the system can be described by 13 local 7-particle configurations and that the volume occupied by those configurations plays a key role in the redistribution dynamics of the system. Our studies offer insights into both the influence of geometrical constraints on random granular packing and a descriptive example of frustrated ordering, comparable to order in antiferromagnetic Ising spin models.

DY 62: Coherent Quantum Dynamics (joint session DY/TT)

Time: Thursday 12:00–12:45 Location: EB 107

DY 62.1 Thu 12:00 EB 107

Initial System-Environment Correlations via the Transfer Tensor Method — Maximilian Buser[1,2], •Javier Cerrillo[1], Gernot Schaller[1], and Jianshu Cao[2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, German — [2]Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139, USA

Open quantum systems exhibiting initial system-environment correlations are notoriously difficult to simulate. We point out that given a sufficiently long sample of the exact short-time evolution of the open system dynamics, one may employ transfer tensors for the further propagation of the reduced open system state. This approach is numerically advantageous and allows for the simulation of quantum correlation functions in hardly accessible regimes. We benchmark this approach against analytically exact solutions and exemplify it with the calculation of emission spectra of multichromophoric systems as well as for the reverse temperature estimation from simulated spectroscopic data. Finally, we employ our approach for the detection of spectral signatures of electromagnetically-induced transparency in open three-level systems.

DY 62.2 Thu 12:15 EB 107

Generation of subharmonic oscillations in driven quantum systems — •Onno Renke Diermann — Condensed Matter Theory, IfP Uni Oldenburg

We present an elementary model for the breaking of discrete time translational symmetry. We consider weakly anharmonic quantum oscillators and apply a time-periodic force which couples close-to-resonant energy levels. An appropriate version of the rotating wave approximation then is employed to derive an effective time-independent Hamiltonian describing a quasiparticle in a multi-well potential. The eigenstates of this potential, which extend over all wells, correspond to Floquet states which inherit the period of the driving force, whereas states localized in only one of the wells of the effective potential correspond to wave packets performing subharmonic motion.

DY 62.3 Thu 12:30 EB 107

Topological Qubit: Quantum States in the Sheaf/Scheme Framework — Antonina N. Fedorova and •Michael G. Zeitlin — Russia, 199178, St.Petersburg, V.O. Bolshoj pr., 61, IPME RAS, Mathematical Methods in Mechanics Group

We consider some generalization of the theory of quantum states, which is based on the analysis of long standing problems and unsatisfactory situation with existing interpretations of quantum mechanics. We demonstrate that the consideration of quantum states as sheaves can provide, in principle, more deep understanding of some well-known phenomena. The key ingredients of the proposed construction are the families of sections of sheaves with values in the proper category of the functional realizations of infinite-dimensional Hilbert spaces with special (multiscale) filtrations decomposed into the (entangled) orbits generated by actions/representations of internal hidden symmetries. In such a way, via proper categorification in a general scheme framework, we open a possibility for the exact description of a lot of phenomena like entanglement and measurement, wave function collapse, self-interference, instantaneous quantum interaction, many-worlds, hidden variables, etc. In the companion paper we consider the machinery needed for the generation of a zoo of the complex quantum patterns during Wigner-Weyl-Moyal evolution together with the constructive algebraic control.

DY 63: Statistical Physics of Biological Systems II (joint session BP/DY)

Time: Thursday 15:00–17:15 Location: H 2013

DY 63.1 Thu 15:00 H 2013

Do Predator attacks tune a collective of interacting agents to criticality and why? — •Pascal Klamser[1,2] and Pawel Romanczuk[1,2] — [1]Institute for Theoretical Biology, Department of Biology, Humboldt-Universität zu Berlin — [2]Bernstein Center for Computational Neuroscience, Humboldt-Universität zu Berlin

Based on theoretical considerations it is hypothesized that biological systems self-tune to criticality [1]. Motivated by this, we investigate the collective behavior of self-propelled agents at the phase transition from an ordered (parallel moving agents = *school*) to a disordered movement (*swarm*) and their reaction to a predator. Systematic numerical simulations show that at the phase transition the performance of the predator decreases. However, this decrease is not only caused by a better response of individuals to the predator, but also by complex spatial structures of the collective at the transition. This finding emphasizes the need of explicitly considering spatial models to describe biological systems, e.g. fish swarms. Beside different interaction-networks (voronoi, k-nearest neighbor, visual-field) an evolutionary algorithm was used to check for the relevance of the results.
[1] Mora, T. and Bialek, W. J Stat Phys (2011) 144: 268.

DY 63.2 Thu 15:15 H 2013

Intermittent collective behavior in small groups of gregarious animals — •Luis A. Gómez[1], Richard Bon[2], and Fernando Peruani[1] — [1]Laboratoire J. A. Dieudonné, Université Côte d'Azur, Nice, France — [2]Centre de Recherches sur la Cognition Animale, Université Paul Sabatier, Toulouse, France

Collective behavior of small groups of gregarious animals is our subject of interest. Experiments with small groups of merino sheep showed interesting features like periodicity of moving and resting phases, synchronization of these phases at the individual level, collective stick–slip dynamics and cohesivity of the group around the center of mass. We show some experimental evidence obtained from the tracking of individual sheep that suggests that the no motion phase of the individuals is qualitatively different to the motion phase. In particular, we discover that a refractory period can be associated to the no motion phase. We propose the introduction of a 3-state model in order to describe the experimental observations for several group sizes (2, 3, 4 and 8 individuals) and study the temporal evolution. Although the model is proposed at the individual level, repercussions at the collective level emerge.

DY 63.3 Thu 15:30 H 2013

How a well-adapting immune system remembers — •Andreas Mayer[1], Vijay Balasubramanian[2], Thierry Mora[3], and Aleksandra Walczak[3] — [1]Princeton University, Princeton, USA — [2]University of Pennsylvania, Philadelphia, USA — [3]Ecole normale superieure, Paris, France

The adaptive immune system uses its past experience of pathogens to prepare for future infections. How much can the adaptive immune system learn about the statistics of changing pathogenic environments given its sampling of the antigenic universe? And how should it best adapt its repertoire of lymphocyte receptor specificities based on its experience? Here, to answer these questions we propose a view of adaptive immunity as a dynamic Bayesian machinery that predicts optimal repertoires based on past pathogen encounters and knowledge about typical pathogen dynamics. Two key experimentally observed characteristics of adaptive immunity emerge naturally from this model: (1) a negative correlation between fold change of protection upon a challenge and preexisting immune levels and (2) differential regulation of memory and naive cells. We argue that to explain the benefits of immune memory, antigenic environments need to be highly sparse. We derive experimentally testable predictions about the diversity of the memory repertoire over time in such sparse antigenic environments. The Bayesian perspective on immunological memory provides a unifying conceptual framework for a number of features of adaptive immunity and suggests further experiments.

DY 63.4 Thu 15:45 H 2013

Asymmetric Link detection via a generalized ESABO ap-

proach — •Jens Christian Claussen — Computational Systems Biology, Jacobs University Bremen, Germany

Mutualisms in biological populations are widespread from bacteria to mammals. Mutualistic interactions can be positive (synergistic) or negative. Often even in microbial data the number of available samples is marginally sufficient to allow for detection of interactions, especially for the low-abundance species that may carry important information in clinical context. The recently introduced ESABO method (PloS Comp Biol 13: e1005361 (2017)) utilizes an information-theoretic approach to evaluate binarized abundances and was demonstrated to detect interaction links that were not apparent in the classical correlation analyses. ESABO provides high (resp. low) scores if joint occurence is higher (resp. lower that in surrogate data. As so far, ESABO concludes on negative interactions when co-occurrence is lower than expected. However, this can be due to asymmetric (unidirectional parasitic) interaction in any of two directions, or due to symmetric interactions. Here we generalize the ESABO method to analyze co-abundance data resolving for asymmetry between the interactions.

DY 63.5 Thu 16:00 H 2013

Modelling the Emergence of Robustness and Evolvability in Genotype-Phenotype Maps — •Marcel Weiss[1,2] and Sebastian E. Ahnert[1,2] — [1]Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, UK — [2]Sainsbury Laboratory, University of Cambridge, UK

Genotype-Phenotype (GP) maps play an important role in evolution and their properties fundamentally affect the outcome of evolutionary processes. A striking property found in several GP maps, such as that of RNA secondary structure, is the positive correlation between the robustness and evolvability of phenotypes, meaning that a phenotype can be strongly robust against mutations and at the same time evolvable to a diverse range of alternative phenotypes. By introducing two analytically tractable GP map models that follow the principles of real biological GP maps, we study the characteristics that cause this positive correlation between phenotype robustness and evolvability. We find that it only emerges if mutations can have non-local effects on sequence constraints, highlighting that these effects are likely to be an important feature of many biological GP maps.

Invited Talk DY 63.6 Thu 16:15 H 2013

Out-of-equilibrium response of soft and biological matter to forces and deformation — •Claus Heussinger — Institut für theoretische Physik, Universität Göttingen

In the talk I will give a few examples from our research concerning the complex dynamical response of soft and biological materials to perturbations via forces or deformation. The systems we study are, in general, far from thermal equilibrium. Phenomena will range from the emergence of flow instabilities (shear-banding, rheo-chaos) in complex fluids, over the visco-elasto-plastic behavior of biological cells and their sub-cellular components, to the fluid-to-solid jamming transition in a-thermal granular particles. The goal is to define suitable model systems where the relevant physical mechanisms can be identified and understood. To this end we use different simulation tools going hand in hand with analytical modeling and, whenever possible, experimental verification.

DY 63.7 Thu 16:45 H 2013

Mechanical tuning of synaptic patterns enhances immune discrimination — •Milos Knezevic[1,2] and Shenshen Wang[1] — [1]Department of Physics and Astronomy, University of California Los Angeles, Los Angeles, CA 90095, USA — [2]Institut fur Theoretische Physik, Technische Universitat Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

An immunological synapse is an adhesive intercellular junction that forms between B cells and antigen-presenting cells (APCs) during recognition. This dynamic surface contact is patterned with complementary receptors and ligands on the apposing membranes, thus specifically regulating directed information transfer. Via synapses, B cells use mechanical pulling forces to extract antigen (Ag) from APCs for subsequent processing and presentation. Recent experiments show that, depending on the stage in its life cycle, a B cell exhibits distinct synaptic patterns accompanied with different strength and timing of force usage, which appears to lead to varied stringency of affinity discrimination. Using a minimal model of membrane adhesion, we study how the observed synaptic architectures can originate from normal mechanical forces coupled to lateral organization of mobile receptors, and show how this coupling might affect the efficiency and selectivity of Ag acquisition. We conclude that cytoskeletal forces could play an important role in tuning the synaptic patterns, which in turn enlarges the dynamic range of immune recognition with enhanced discrimination.

DY 63.8 Thu 17:00 H 2013

Specialisation and plasticity in interacting biological populations — Solenn Patalano[1], •Adolfo Alsina[2], Steffen Rulands[2], and Wolf Reik[1] — [1]Babraham Institute, Cambridge, UK — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The structure and dynamics of biological systems are tightly regulated on multiple scales, from transcriptional and epigenetic regulation to population level feedback. While many biological systems are surprisingly robust against environmental fluctuations they, simultaneously, exhibit a remarkable plasticity in response to changes in their environment. Using the social wasp Polistes as an example we combine experimental and theoretical methods to study how a primitive society simultaneously achieves phenotypic specialisation and a remarkable degree of plasticity. After perturbing the society by queen removal, we experimentally follow the relaxation dynamics into the social steady state across scales, from social and behavioural measurements to physiological measurements and detailed molecular characterisations of single wasps. We develop a theoretical framework that explains the emergence of the social structure of Polistes as a result of opposing dynamics on the molecular and the population scales. We show that such dynamics provide a general principle of how both specialization and plasticity can be achieved in biological systems. As well as elucidating mechanisms of epigenetic plasticity in wasps and other biological systems this study shows that the multiscale dynamics in primitive social insects provide a laboratory for non-equilibrium physics.

DY 64: Traffic Dynamics, Urban and Regional Systems (joint session SOE/DY)

Time: Thursday 15:00–16:15 Location: MA 001

DY 64.1 Thu 15:00 MA 001

A planar growing network model for urban street network evolution — •Oliver Weisse and Reik V. Donner — Potsdam Insitute for Climate Impact Research, Potsdam, Germany

Historically grown cities can be at least partially understood as the result of self-organization principles without central planning authority. In order to understand the associated spatial settlement patterns, it is convenient to analyze the associated urban road networks providing the backbone of such cities. Recent work has demonstrated that the topological and geometric properties of such networks exhibit a surprising degree of universality, suggesting that the corresponding structure formation has been governed by relatively general principles.

Here, we propose an evolving planar network model based on a small set of simple rules that model stochastic network growth under local optimization of construction costs and travel efficiency. Specifically, we assume that the growth of cities follows a probability distribution of nodes in a two-dimensional Euclidean space with higher probability in areas where infrastructure already exists. In contrast to other existing models of urban road networks, this growth is recursive and depends on the existing city. Nevertheless, the geometric characteristics of the generated planar networks are statistically similar for sufficiently large cities, implying that they are largely independent of the specific evolution path. Moreover, the observed properties agree well with those of real-world cities.

DY 64.2 Thu 15:15 MA 001

Dynamics of cities' population: relating Zipf's law and urban scaling — •José M. Miotto — LIACS, Universiteit Leiden, Netherlands

The distribution of city sizes in a country is characterized by having a

power-law tail (Pareto), a common feature of large social systems. Proportional effect -each city grows with the same rate- is a well-accepted growth model for cities that explains the emergence of this feature (Gabaix); however, data from cities gathered in historical scale (Italy, 1861-2011) shows important features that cannot be explained by this model. I will introduce a modified growth model where the growth rate of cities scales with city size, and show that this model can (a) reproduce quantitatively the cities' size distribution evolution in time, (b) provide a better null model for the time evolution of the population of single cities and (c) reveal patterns in the dynamics of internal migration.

DY 64.3 Thu 15:30 MA 001

Urban Kaya relation: understanding urban CO2 emissions — Ramana Gudipudi[1], •Diego Rybski[1], Matthias K. B. Lüdeke[1], Bin Zhou[1], Zhu Liu[2,3,4], and Jürgen P. Kropp[1,5] — [1]Potsdam Institute for Climate Impact Research, 14473, Potsdam, Germany — [2]John F. Kennedy School of Government, Harvard University, Cambridge, Massachusetts 02138, USA — [3]Resnick Sustainability Institute, California Institute of Technology, Pasadena, California 91125, USA — [4]Cambridge Centre for Climate Change Mitigation Research, Department of Land Economy, University of Cambridge, 19 Silver Street, Cambridge CB3 9EP, UK — [5]Dept. of Geo- and Environmental Sciences, University of Potsdam, 14476, Potsdam, Germany

Given the strong global urbanization trend, it is crucial to understand whether large urban areas are more emission efficient in comparison to smaller ones. Recent literature on urban scaling properties of emissions as a function of population size led to contradicting results and more importantly lacked an in-depth investigation of the factors leading to such scaling properties. Therefore, in analogy to the well-established Kaya Identity, we developed an urban Kaya relation to investigate different scaling properties of the indicators within the Kaya Identity. Contrary to traditional urban scaling studies which use ordinary least squares regression, we show that orthogonal regression is necessary when complex relations among scaling exponents are to be investigated.

DY 64.4 Thu 15:45 MA 001

The Urban form, quantifying population spatial distribution in cities — •Valerio Volpati and Marc Barthelemy — IPhT, Universite' Paris Saclay, France

In Urban Economics, the different forces playing a role in the development of a city have been described, leading to idealized models of cities such as the von Thunen monocentric model. In real data, the spatial distribution of activities inside cities is often more complicated and non monocentric. Here we study the population spatial distribution inside french cities, and we introduce measures to quantify how much each city is monocentric, polycentric or homogenous. We classify cities according to such measures and discuss how we can revisit classical models of Urban Economics in light of the empirical analysis.

DY 64.5 Thu 16:00 MA 001

Antipersistence of traffic flow explains congestion durations — •Sebastian M. Krause, Lars Habel, Thomas Guhr, and Michael Schreckenberg — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Many highways are running above their capacity and therefore suffer congested traffic. The traffic breakdown from free flow becomes increasingly likely around a critical flow, a critical number of vehicles per minute. Here we discuss congestion durations which are distributed with a power law over three decades, from minutes to hours [1]. This finding suggests a robust mechanism behind it. Using antipersistent stochastic modeling of the traffic flow, we are able to explain the distribution of congestion durations: The traffic flow shows large fluctuations on short time scales which quickly trend back to the mean value. Consequently, it exceeds the critical flow for time spans which are power law distributed.

[1] S. M. Krause, L. Habel, T. Guhr and M. Schreckenberg, 'The importance of antipersistence for traffic jams', EPL 118, 38005 (2017).

DY 65: Talk T. Speck

Time: Thursday 15:00–15:30 Location: BH-N 243

Invited Talk DY 65.1 Thu 15:00 BH-N 243

Towards a thermodynamics of active particles — •Thomas Speck — Johannes Gutenberg-Universität Mainz

I will give a brief overview on the theoretical modeling of autonomous self-propelled particles with directed motion, which colloquially go by the name "active particles". Being driven away from thermal equilibrium, questions like the physical meaning of entropy production arising from breaking time-reversal symmetry and consistency with thermodynamic principles have received increasing attention. I will discuss the situation for active Brownian particles, a minimal model system of active particles combining directed motion with volume exclusion, in the context of stochastic thermodynamics.

DY 66: Poster: Stat. Phys. (Gen., Critical Phen., Biol.)

Time: Thursday 15:30–18:00 Location: Poster A

DY 66.1 Thu 15:30 Poster A

Phase transitions in highly diverse ecosystems — •Mattes Heerwagen and Andreas Engel — Carl-von-Ossietzky Universität Oldenburg, Oldenburg, Deutschland

Ecosystems with many different species and resources are complex systems. Much of our understanding of such ecosystems derives from low-dimensional models with just a few interacting species and a small number of different resources. Nevertheless, most real systems are characterized by a high degree of biodiversity. Recently, Tikhonov and Monasson [1] showed with methods from statistical physics that high dimensional ecosystems may exhibit two phases: a "vulnerable" one with relatively few survivors and, above a critical degree of biodiversity, a "shielded" one in which the competing species cooperate to protect each other from variations in the resource supply and where the number of survivors reaches a maximum. We extend the model of Tikhonov and Monasson to analyse more heterogeneous ecosystems with different types of generalists and specialists. We study the two phases in this more general setting and determine the critical line of the phase transition.

[1] M. Tikhonov and R. Monasson, Collective Phase in Resource Competition in a Highly Diverse Ecosystem, Phys. Rev. Lett. 118, 048103 (2017)

DY 66.2 Thu 15:30 Poster A

The longest increasing subsequence of a sequence problem: A large deviation study — •Jörn Börjes, Hendrik Schawe, and Alexander K. Hartmann — Institut für Physik, Carl von Ossietzky Universität Oldenburg

The longest increasing subsequence (LIS) problem asks for the longest subsequence in which the elements are in sorted order, lowest to highest and part of the given sequence with length n. The elements indices of the sequence do not need to be continuous to become a LIS. There is an exact mapping between a specific polynuclear growth model and the so called LIS problem [1]. This problem is numerically solved by an algorithm with complexity $O(n \log n)$. We study the distribution of the length of the LIS up to the large deviations. We compare our numerical results to the analytically known results. Using specific large-deviation approaches [2], probability distributions can be sampled over a large range of the support, down to probabilities like 10^{-40}.

[1] Satya N. Majumdar and Sergei Nechaev, Phys. Rev. E 69
[2] A.K. Hartmann Phys. Rev. E 65, OSG 202 (2002)

DY 66.3 Thu 15:30 Poster A

Towards a classification of nonequilibrium steady states via invariant manifolds — •Jens Lucht, Prakhar Godara, Marco Giacomo Mazza, and Stephan Herminghaus — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Nonequilibrium steady states (NESS) give rise to nontrivial cyclic probability fluxes that breach detailed balance (DB), and thus it is not clear how to define a potential analog to equilibrium case. We argue that there is a formal way to define such a NESS potential for systems describable by a Fokker-Planck equation. DB in NESS can be restored [1] by mapping the phase space into a parameterized family of non-intersecting cycles containing the invariant manifolds of the corresponding deterministic, dynamical system. Transition rates between neighboring cycles are obtained from the microscopic dynamics, i.e., from the drift and diffusive currents. Since fluxes between cycles obey DB, we can integrate over the set of cycles. We present some evidence that this gives us a nonequilibrium potential which reaches minimum solely for NESS.

[1]: Phys. Rev. E., 2012, 85, 041133

DY 66.4 Thu 15:30 Poster A

Non-Flat Histogram Techniques for Spin Glasses — •Fabio Mueller, Stefan Schnabel, and Wolfhard Janke — Institut fuer Theoretische Physik, Universitaet Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We take into consideration the 3D Edwards-Anderson model with bimodal bond distribution. The spin-glass nature of the model implies that finding ground states is an NP-hard problem. The round-trip times, defined as the time one simulation method needs for a specific disorder realization in order to travel from the ground state to the high energy region and back therefore reflects the ability of the method to solve that specific optimization problem.

Employing different simulation techniques the round-trip time distributions are investigated and the performance of the different methods is compared. The methods taken into consideration are among the most established broad-energy ensemble methods including the parallel-tempering method and, in addition, a specially designed non-flat histogram technique which is shown to outperform the currently existing methods.

DY 66.5 Thu 15:30 Poster A

Self-learning Monte Carlo simulations of classical and quantum many-body systems — •Kai Meinerz and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

The application of machine learning approaches has seen a dramatic surge across a diverse range of fields that aim to benefit from their unmatched core abilities of dimensional reduction and feature extraction. In the field of computational many-body physics machine learning approaches bear the potential to further improve one of the stalwarts in the field * Monte Carlo sampling techniques. Here we explore the capability of *self-learning* Monte Carlo approaches to dramatically improve the update quality in Markov chain Monte Carlo simulations. Such a self-learning approach employs reinforcement learning techniques to learn the distribution of accepted updates and is then used to suggest updates that are almost always accepted, thereby dramatically reducing autocorrelation effects. It can, in principle, be applied to all existing Monte Carlo flavors and is tested here for both classical and quantum Monte Carlo techniques applied to a variety of many-body problems.

DY 66.6 Thu 15:30 Poster A

study ab Initio of the effect of a-Site substitution on the fe1.12te system — •Mir Ali — Computational Physics Laboratory of Materials, Liabes Djillali University of Sidi Bel-Abbes, Algeria

Abstract: In the present work, our aim is to verify the structural, electronic and magnetic properties of both systems Fe1.12Te and *RTX*(R = Fe, X = Te and T = Ni, Co) in the P4/nmm structure. For this task, we use the density functional theory (DFT) as a theoretical tool integrated into wien2k code (Blaha 2001). The solid Fe1 xMxTe (M =Ni, Co) have been synthesized by Kazakov et al.(Chem.Met. Alloys 3, 155*160 2010). They have observed a systematic shift of the lattice parameters for both systems for M = Ni and Co till x = 0.1, then a second phase with the NiAs-type structure appeared when x passes 0.15. Fe1-xNixTe retains its structure in a concentration between x = 0.1 and 0.15, and Fe1-xCoxTe retains its structure when x is between 0.05 and 0.1 (Blaha 2001)[1]. [1].Blaha, P., Schwarz, K., Madsen, G.K.H., Kvasnicka, D., Luitz,J.: WIEN2K,An Augmented Plane Wave plus Local Orbitals Program for Calculating Crystal Properties. Vienna University of Technology, Austria (2001).

DY 66.7 Thu 15:30 Poster A

Wave localization in locally centrosymmetric disordered lattices — •Christian Morfonios[1], Malte Röntgen[1], and Peter Schmelcher[1,2] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg — [2]Center for Ultrafast Imaging, Universität Hamburg

Since the work of Anderson, disorder in a medium is known to generically induce wave localization due to multiple destructive interference, in turn suppressing the transport through a sample. This may be altered by different forms of correlations between the constituents of the disordered medium which typically lead to the delocalization of wave excitations on configuration average, as indicated by various measures. On the other hand, the presence of global centrosymmetry (spatial inversion symmetry) in an otherwise disordered system has recently been argued to enhance the transport efficiency between given sites via delocalized parity eigenstates. Seeing local centrosymmetry - restricted to different subparts of the system - as a particular type of correlation, we address the question of its impact on wave localization and transport properties in one-dimensional tight-binding lattices.

DY 66.8 Thu 15:30 Poster A

Irreversible Markov chains in spin models: Topological excitations — •Ze Lei[1] and Werner Krauth[1,2] — [1]Ecole Normale Superieure, Paris, France — [2]The University of Tokyo, Tokyo, Japan

We analyze the convergence of the irreversible event-chain Monte Carlo algorithm for continuous spin models in the presence of topological excitations.

In the two-dimensional XY model, we show that the local nature of the Markov-chain dynamics leads to slow decay of vortex–antivortex correlations in comparision with the fast decorrelation of spin waves.

We propose an assignment algorithm for pairing vortices and antivortices, and show that the maximum vortex–antivortex distance follows a Fréchet description. The contributions of topological excitations to the equilibrium correlations vary from a dynamical critical exponent $z \sim 2$ at the critical temperature to $z \sim 0$ in the limit of zero temperature.

In the harmonic approximation of spin waves for dimensions higher than 2, we confirm the event-chain algorithm's fast relaxation (corresponding to $z = 0$). Its mixing times however remain much larger than equilibrium correlation times at low temperatures.

We also describe the respective influence of topological monopole–antimonopole excitations and of spin waves on the event-chain dynamics in the three-dimensional Heisenberg model.

We expect that the fast relaxation of phonon modes explains the success of the event-chain algorithm at high densities for particle systems.

DY 66.9 Thu 15:30 Poster A

Occupation time statistics for single molecule dynamics — •Alessio Lapolla and Aljaz Godec — Mathematical Biophysics Group, Max-Planck-Institute for Biophysical Chemistry (Göttingen)

State-of-the art experimental methods nowadays routinely probe dynamical properties of individual molecules, and thereby provide unprecedented insight into biophysical phenomena at low-copy numbers. Yet, despite the consensus about its relevance, a general theory of single molecule dynamics remains elusive.

Namely, most available experimental techniques are limited by short, typically subergodic observation times. As a result, their interpretation cannot rely neither on ensemble statistical mechanics nor ergodic theory. This poses the need for a statistical mechanics of time-averaged observables, explicitly taking into account the fluctuations between different realizations.

In our work we focused on the statistics of occupation time: the fraction of time a random process spends in any given region of configuration space. We obtained rigorous general results for the lower order moments of the occupation time in Markovian dynamics, which go beyond large-deviation theory. To illustrate the predictive power of the theory we provide exact results for a selection of simple diffusive models of single-molecule dynamics.

DY 66.10 Thu 15:30 Poster A

Accounting for the context-dependent effects in the mod-

elling of synthetic genetic circuits — •Johannes Falk[1], Maleen Hanst[2], Heinz Koeppl[2], and Barbara Drossel[1] — [1]Technische Universität Darmstadt, Institut für Festkörperphysik, Germany — [2]Technische Universität Darmstadt, Bioinspired Communication Systems, Germany

Synthetic biology aims at designing modular genetic circuits that can be assembled according to the desired function. When embedded in a cell, a circuit module becomes a small subnetwork within a larger environmental network, and its dynamics is therefore affected by interactions with the environment. The environment not only causes extrinsic noise but also memory effects, which means that the dynamics of the subnetwork is affected by its past states via a memory function that is characteristic of the cellular environment. Using a modification of the Mori-Zwanzig projection formalism, we show how the modifications of the subnetwork dynamics due to the environment can be calculated for stochastic models. In particular, we derive analytical expressions of memory kernels for specific classes of environments that are derived from linear reaction networks. Furthermore, we present computer simulation results showing how the environment can destroy the periodic oscillations displayed by the isolated subnetwork.

DY 66.11 Thu 15:30 Poster A

Effects of a flexible pinning on the statics and dynamics of a thermalized thin sheet — •Josip Augustin Janeš[1,2], Daniel Schmidt[2], Udo Seifert[3], and Ana-Sunčana Smith[1,2] — [1]Institute Ruđer Bošković, Zagreb, Croatia — [2]PULS Group, Department of Physics and Cluster of Excellence: EAM, FAU Erlangen-Nürnberg, Erlangen, Germany — [3]II. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart, Germany

Mechanical characteristics of freely suspended 2D membranes are commonly determined from their fluctuation spectrum. However, this task is significantly more challenging for the case of membranes attached by proteins to underlying scaffolds. Actually, a complete theoretical description of the effect of a pinning on the dynamic correlations in a membrane is still missing. Here we rectify this situation by modelling the spatial and dynamic correlations by several complimentary analytical methods. We construct a complete theoretical framework for the problem in question and validate our approach by obtaining excellent agreement with the explicit Langevin simulations.

DY 66.12 Thu 15:30 Poster A

Superposition of survival curves as a tool for epistasis analysis of longevity interventions — Stefan Nowak[1,2], Johannes Neidhart[1,2,3], •Jonas Rzezonka[1,2], Ivan G. Szendro[1,2], Rahul Marathe[1,2,4], and Joachim Krug[1,2] — [1]Sybacol, Universität zu Köln, Köln, Germany — [2]ITP, Universität zu Köln, Köln, Germany — [3]MBR Optical Systems, Wuppertal, Germany — [4]Department of Physics, IIT Delhi, New Delhi, India

A problem in ageing research is to understand how different factors contributing to longevity should be expected to act in combination under the assumption that they are independent. Standard epistasis analysis compares the extension of mean lifespan achieved by a combination of interventions to the prediction under an additive or multiplicative null model, but neither model is fundamentally justified. Moreover, the target of longevity interventions is not mean life span but the entire survival curve. We formulated superposition principles that predict the survival curve resulting from a combination of two interventions based on the survival curves of the individual treatments, and quantify epistasis as the deviation from this prediction [1]. We test the method on a published data set comprising survival curves for all combinations of 4 different longevity interventions in *Caenorhabditis elegans* [2]. We find that epistasis is generally weak even when the standard analysis indicates otherwise.

[1] Nowak S, Neidhart J, Rzezonka J, Szendro IG, Marathe R and Krug J (2017) bioRxiv https://doi.org/10.1101/147173.
[2] Yen K, Mobbs CV (2010). AGE 32:39-49

DY 66.13 Thu 15:30 Poster A

Reweighting Simulation in and out of Equilibrium — Marius Bause, Tristan Bereau, and •Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

Markov State Models(MSM) are a discrete representation of the kinetics of a given system constructed by course-graining microtrajectories. While frequently applied to equilibrium systems, a protocol for driven steady state systems has not been developed due to loss of dynamic properties like detailed balance. We propose to apply the principle of Maximum Caliber by Jayne's, postulating that the distribution of paths is given by the maximal path entropy encoding a chosen set of prior information. This reduces the computational effort of constructing an MSM by providing new microscopic relations from macrosopic path-ensemble assumptions. Simultaneously the markovian assumption alleviates the combinatorial explosion of microtrajetories. The method is tested on a minimal model under non-conservative forces.

DY 66.14 Thu 15:30 Poster A

Conformational dynamics of growing polymers under non-stationary conditions — •Jörn H. Appeldorn, Ali Malek, and Reiner Kree — Inst. f. Theoret. Physik, Univ. Göttingen, Friedrich-Hund. Pl. 1, 37077 Göttingen

The time scales of conformational evolution of a poylmer chain and of ongoing polymerization reactions may become comparable for living polymers and for biopolymer reactions. In particular this happens under non-stationary conditions, if the polymerization velocity decreases, for example due to depletion of monomers or activators. We extend both the Rouse model and the dynamical model of a semi-flexible chain in the approximation of constant average line tension to include instationary growth with velocities decreasing as $t^{-\gamma}$. We demonstrate and discuss the appearance of well-defined dynamical transitions in a dragged chain and in a chain in homogeneous shear flow, which are signalled by sudden, qualitative changes in conformational or rheological properties as functions of γ.

DY 66.15 Thu 15:30 Poster A

Synaptic Miniature Transmitter Release:Random in Nature or Partly Deterministic? — •Daungruthai Jarukanont — University of Kassel, Kassel

The mechanism of how synaptic terminals release neurotransmitters by spontaneous vesicle fusion is still unclear. *Since the early work of Fatt and Katz (1952), the spontaneous release of neurotransmitters is assumed to be a purely stochastic process that occurs randomly and can be described by Poisson processes. In this work, we investigate the statistical behavior of the miniature excitatory postsynaptic currents (mEPSCs) in mouse Hippocampal neurons, and of the miniature excitatory junctional potentials(mEJPs) in the neuromuscular junctions (NMJ) of Drosophila larvae. We find that, in contrast to the previous assumptions, neither mEPSCs nor mEJPs could be described the Poisson process. Instead, the inter-event interval histograms of the mEPSCs from mouse Hippocampal neurons are well described by inverse-Gaussian distributions, while the inter-event interval histograms of mEJPs in the neuromuscular junctions of Drosophila larvae are well fitted by gamma distributions. Further study and analysis is still needed to understand the mechanism of the spontaneous release of neurotransmitter. However, it is clear from our analysis that the spontaneous release process is partly-deterministic and not random like as is currently assumed.

DY 66.16 Thu 15:30 Poster A

Two Perspectives on the Condensation-Evaporation Transition — •Franz Paul Spitzner[1], Johannes Zierenberg[1,2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig Postfach 100 920, 04009 Leipzig, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany

The particle condensation-evaporation transition is a standard example of a first-order phase transition. In equilibrium, the consideration may be reduced to the coexistence of a homogeneous gas phase and an inhomogeneous phase consisting of a single macroscopic droplet with surrounding vapour. The transition can either be driven by density or temperature – keeping the respective "orthogonal" quantity constant. While this problem can be rigorously treated only at fixed temperature and in two dimensions, a heuristic derivation of the leading-order finite-size scaling behaviour exists that holds for the transition at fixed temperature and at fixed density.

We present how the well known multicanonical method can be adopted to the grand canonical ensemble, allowing us to investigate the condensation-evaporation transition of a 2D Lennard-Jones gas in both regimes. The careful adjustment of simulation parameters and subtle implementation choices will be discussed, in order to provide insight into the method and consistent results that support the existing prediction of the scaling behaviour.

DY 66.17 Thu 15:30 Poster A

Integer quantum Hall transitions on tight-binding lattices

— •Martin Puschmann[1,2], Philipp Cain[1], Michael Schreiber[1], and Thomas Vojta[2] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Department of Physics, Missouri University of Science and Technology, Rolla, MO, United States

We investigate the integer quantum Hall transition in the lowest Landau band of two-dimensional tight-binding lattices for non-interacting electrons affected by a perpendicular magnetic field. Specifically, we consider both simple square lattices, where Landau levels are broadened by random potentials, and random Voronoi-Delaunay lattices in which (topological) disorder is introduced by bonds between randomly positioned sites. Based on a recursive Green function approach, we calculate the smallest positive Lyapunov exponent describing the long-range behavior of the wave function intensities along a quasi-one-dimensional lattice stripe. In both systems, we observe that the critical exponent of the localization length takes a value of $\nu \approx 2.60$. Our critical estimates, thus, coincide with those based on the semi-classical Chalker-Coddington (CC) network model, see e.g. [1]. They do not agree with the reduced critical exponent, $\nu \approx 2.37$, found by Gruzberg et al. in a recently proposed geometrically disordered CC model [2].

[1] K. Slevin and T. Ohtsuki, Phys. Rev. B 80, 041304 (2009)
[2] I. A. Gruzberg et al., Phys. Rev. B 95, 125414 (2017)

DY 66.18 Thu 15:30 Poster A

Full Counting Statistics of the non-equilibrium Dicke model — •Christopher W. Wächtler and Gernot Schaller — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We consider the single-mode Dicke-Hamiltonian coupled to two Markovian bosonic baths at different temperatures. In the thermodynamic limit the closed system untergoes a second order quantum phase transition from a normal phase to a superradiant phase as the atom-field coupling is increased. In this work, we microscopically derive a generalized master equation with counting fields. We use it to describe the non-equilibrium steady state with constant energy or heat flow through the system. By the use of full counting statistics [1] we investigate for finite system size the energy current as well as its higher moments for evidence of the underlying quantum phase transition. Additionally we consider the thermodynamic limit of the system and disspators by means of a Holstein-Primakoff transformation and displaced bosonic modes [2].

[1] M. Esposito *et al.*, Rev. Mod. Phys. 81, 1665 (2009).
[2] C. Emary, T. Brandes, PRE 67, 66203 (2003).

DY 66.19 Thu 15:30 Poster A

Directed negative-weight percolation — •Christoph Norrenbrock, Mitchell Mkrtchian, and Alexander K. Hartmann — Carl-von-Ossietzky Universität Oldenburg, Oldenburg (Germany)

We consider a directed variant of the negative-weight percolation model [1] in a two-dimensional, periodic, square lattice. The problem exhibits edge weights which are taken from a distribution that allows for both positive and negative values. Additionally, in this model variant all edges are directed. For a given realization of the disorder, a minimally weighted loop/path configuration is determined by performing a non-trivial transformation of the original lattice and solving a minimum weight perfect matching problem. For this problem, fast polynomial-time algorithms are available, thus we could study large systems with high accuracy. Depending on the fraction of negatively and positively weighted edges in the lattice, a continuous phase transition can be identified, whose characterizing critical exponents we have estimated by a finite-size scaling analysis of the numerically obtained data. We observe a strong change of the universality class with respect to standard directed percolation, as well as with respect to undirected negative-weight percolation.

[1] Melchert, O. and Hartmann, A. K., New J. Phys. **10** 043039 (2008)

DY 66.20 Thu 15:30 Poster A

Critical exponents from a Landau-like approach — •Sören Sanders — Carl von Ossietzky Universität, Oldenburg, Deutschland

Landau's approach to continuous phase transitions provides an effective theory for the description around the critical point but falls short in correctly establishing non-trivial critical exponents. Using the example of the Mott-insulator to superfluid transition of the Bose-Hubbard model, we derive from the microscopic properties a Landau-like description not restricted by this limitation and correctly reproduce the best known value for the critical exponent β of the XY-universality class.

DY 67: Poster: Active Matter, Microswimmers

Time: Thursday 15:30–18:00 Location: Poster A

DY 67.1 Thu 15:30 Poster A

Topology of active nematics and dimensionality — •Joscha Tabet and Marco G. Mazza — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany

The complex interplay of topology, viscous dissipation, and active motion leads to stunning nonequilibrium behavior in active nematic fluids. We study the effect dimensionality has on these dynamics. Thus far, the research in this area has mostly been limited to different 2D-topologies. By employing a novel model for nematodynamics based on the stochastic rotation dynamics framework we extend this point of view to quasi-2D and full 3D simulations. Our bottom-up approach reproduces the hydrodynamic equations in a computationally efficient way while maintaining statistical fluctuations. We analyze the topology of active nematics and its coupling with the fluid motion. This method opens up new ways to understanding the dynamics of actin filaments in the cell and the cytoskeleton.

DY 67.2 Thu 15:30 Poster A

Active systems learning at the microscale — •Santiago Muiños-Landin[1], Keyan Ghazi-Zahedi[2], and Frank Cichos[1] — [1]Molecular Nanophotonics. University of Leipzig. Institut for Experimental Physics I — [2]Information Theory of Cognitive Systems, Max Planck Institute for Mathematics in the Sciences

Information exchange makes a collectivity stronger. Different species use interactions between members of a group in order to share information optimizing the solution of problems. These interactions usually rely on sensing mechanisms that individuals also use in order to improve their own knowledge in a feedback loop. Such improvements let them evolve in their behavior through decision making or a learning process. Here we propose a microswimmer collective behavior mechanism based on our previous work, where information exchange is possible through the definition of artificial interactions and behavior evolution is reached via reinforcement learning. We combine these two ideas with swarm algorithms to show how intelligent active behavior is possible in a well defined collective of artificial microswimmers.

DY 67.3 Thu 15:30 Poster A

Probability fluxes for self-propelled particles in strong confinement — •Jan Cammann, Fabian Jan Schwarzendahl, Tanya Ostapenko, Oliver Bäumchen, and Marco G. Mazza — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Active Brownian particles, such as bacteria and motile algae frequently encounter boundaries in their natural habitats. Experimental observations suggest that a wide range of microswimmers seem to spend a significant amount of time close to such boundaries as opposed to staying in the bulk. Experiments on individual cells of the model organism Chlamydomonas reinhardtii in strong confinement show that the probability to find the algae near a boundary is increased with curvature. Additionally local gradients in boundary curvature result in probability fluxes not only bound to the wall, but forming loops that can reach into the bulk and have significant influence on the global behaviour. By describing the particles shape as an asymmetric dumbbell with steric wall interactions, we show that confined active Brownian particle simulations can reproduce the experimental results. This minimal model is capable of reproducing the probability distribution in positional space, as well as the fluxes in probability found in experiments with very good agreement.

DY 67.4 Thu 15:30 Poster A

Dynamics of a nematic microswimmer in aqueous surfactant

solution — •Shubhadeep Mandal and Marco G. Mazza — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The study of self-propelled motion of microswimmers in fluidic environments is of paramount importance to understand modern day applications, such as targeted drug delivery and lab-on-a-chip technologies. In this study, we investigate the dynamics of an artificial microswimmer consisting of nematic liquid-crystal droplet in a surfactant solution. Recent experiments have shown that a nematic droplet suspended in an aqueous surfactant solution not only self-propels, but also exhibits curling or helical motion depending on the physical dimensionality. We perform numerical simulations using stochastic rotational dynamics (SRD) to study the interaction between the nematic swimmer and the surfactant solution. An outstanding question regarding the dynamics of self-propel motion of nematic microswimmers that we address here is the coupling of Marangoni flow and nematic director field. Our first goal is to understand the importance of miceller and molecular solubilization towards the genesis of the self-propelled motion of nematic swimmers. The second objective of the present study is to investigate the symmetry breaking phenomenon towards the curling or helical motion of nematic swimmers.

DY 67.5 Thu 15:30 Poster A

Collective Dynamics of Squirmers in Poiseuille Flow — •Shahajhan Sorathiya and Holger Stark — Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany.

Bacteria in microfluidic Poiseuille flow show interesting collective dynamics such as pronounced centerline depletion [1]. We conduct a parametric study using the squirmer microswimmer model and multiparticle collision dynamics by varying squirmer volume fraction (C), the ratio of fluid flow strength (v_f) to squirmer swimming speed (v_0), and squirmer type β.

The most pronounced feature is a global axial polar order, which develops since squirmers collectively swim upstream against the flow. At $v_f/v_0 = 1$ it is highest for neutral squirmers and also increases with volume fraction C. Pushers show the least polar order while the alignment of pullers lies in between. For large flow speeds $v_f/v_0 > 1$, alignment against the flow decreases strongly for all three squirmer types due to the onset of tumbling [2]. In parallel, for $v_f/v_0 = 1$ the axial velocity profiles of pullers and neutral squirmers are directed against the fluid flow, while for $v_f/v_0 = 4$ the profiles of all squirmers are identical and directed with the fluid flow. Finally, the lateral density profiles for neutral and puller squirmers reveal enrichment in the channel center at all speed ratios and $C < 20\%$, while pusher squirmers develop increased density in the center for $v_f/v_0 > 1$.

[1] R. Rusconi, J. S. Guasto, and R. Stocker, Nature Phys. **10**, 212 (2014).
[2] A. Zöttl and H. Stark, Phys. Rev. Lett **108**, 218104 (2012).

DY 67.6 Thu 15:30 Poster A

Mode-Coupling Theory for Active Particles in Shear Flow — •Julian Reichert and Thomas Voigtmann — Deutsches Zentrum für Luft- und Raumfahrt e.V., Linder Höhe, 51147 Köln

We use the Integration through transients formalism to derive a Green-Kubo relation for non-equilibrium transport coefficients of active Brownian hard disks under shear flow, starting from a microscopic kinetic description. This approach has already proven to be successful in calculating the non-equilibrium swim velocities of active Brownian hard disks without shear and uses the Fourier transformed transient non-equilibrium density-density correlation function as an input. The transient density-density correlation function can be approximated by making use of the Mode-coupling theory (MCT) and plays an important role in the context of glass-forming-liquids. MCT has successfully been applied to passive Brownian particles under homogeneous steady shear flows and for active Brownian particles without shear. Our tak is now to combine both theories by what we hope to learn more about the interplay of the intrinsic active forces and the external flow.

References

1. Liluashvili, A., Ónody, J., and Voigtmann, Th., Mode Coupling Theory for Active Brownian Particles, Phys. Rev. E in press, arXiv:1707.07373 (2017).

2. Fuchs, M., Cates, M.E., A mode coupling theory for brownian particles in homogeneous steady shear flow, Journal of Rheology, 53 (957) (2009).

DY 67.7 Thu 15:30 Poster A

Discriminating collective motion mechanisms using correlations and information measures — •Yinong Zhao[1], Zhangang Han[2], Pawel Romanczuk[1], and Cristian Huepe[2,3,4] — [1]ITB, Humboldt-Universität zu Berlin, 10115 Berlin, Germany — [2]School of Systems Science, Beijing Normal University, Beijing 100875, China — [3]CHuepe Labs, 954 West 18th Place, Chicago, IL 60608, USA — [4]Northwestern Institute on Complex Systems and ESAM, Northwestern University, Evanston, IL 60208, USA

Collective motion is an emergent phenomenon observed in a variety of living systems. Although a variety of models have been introduced that can achieve collective motion in the presence of noise, it is still unclear which, if any, of these algorithms is followed by different animal groups.

We consider different measures that use individual heading and are based on correlations and information theory. We show that these measures can discriminate among various minimal models of collective motion. The models include different types of interactions, either metric or topological and based on either relative heading angles or positions. We show that under a high-noise environment, position-based model shows better collective performance than velocity-based model.

Given their ability to discriminate between different simple models, these measures could be used to help infer the underlying mechanism that leads to collective motion in different experimental systems.

DY 67.8 Thu 15:30 Poster A

Collective Motion of Topologically Interacting Particles in Heterogeneous Media — •Parisa Rahmani[1,2], Fernando Peruani[3], and Pawel Romanczuk[2] — [1]Department of Physics, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, Iran — [2]Department of Biology, Institute for TheoreticalBiology, Humboldt Universität zu Berlin, Germany — [3]Laboratoire J. A. Dieudonné, Université de Nice Sophia Antipolis, France

Collective motion of animals is a fascinating phenomenon occurring in bird flocks, fish schools, and other social animals. Modeling of collective motion is a tool for the understanding of the possible evolutionary benefits and costs associated to group living. An important aspect of collective motion is the impact of environmental heterogeneities. Chepizco et. al. [1] showed that in a model based on metric interaction network, there is an optimal noise which maximizes collective motion in the presence of obstacles. But, observations on animal groups revealed that the Voronoi interaction network outperforms the metric one [2]. Therefore, we study emergence and robustness of collective motion in a group of agents interacting with their topological neighbors in heterogenous media. We show that in this case there is no optimal noise. Topological interaction network is much more robust against obstacles, and even in high obstacle densities ordered phases are observed.

[1] O. Chepizhko et. al., Phys. Rev. Lett., **110** (2013), 238101(1-5)
[2] A. Strandburg-Peshkin et. al., Current Biology, **23** (2013), R709-R711

DY 67.9 Thu 15:30 Poster A

Bead-spring modelling of the triangular three-sphere swimmer — •Sebastian Ziegler[1], Jens Harting[2], Alexander Sukhov[2], and Ana-Sunčana Smith[1] — [1]PULS Group, Department of Physics and Cluster of Excellence: EAM, Friedrich-Alexander University Erlangen-Nürnberg, Nägelsbachstr. 49b, Erlangen, Germany — [2]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Fürther Straße 248, Nürnberg, Germany

A customary approach to model mechanical micropropulsion is to impose the swimming stroke. However, with this approach, the hydrodynamic features of the motion are in essence smoothed over and the problem becomes a purely geometrical one. The alternative approach, yet significantly more demanding, is to specify not the swimming stroke itself but the forces which drive the swimming motion. The swimming stroke then emerges in response to the various forces acting in the system. We use this latter approach to study the behaviour of a triangular-shaped bead-spring microswimmer under the influence of external magnetic field under the condition of no net external force and torque. This swimmer evolves in a versatile manner in dependence of its own geometry and its parameters (viscosity of the fluid, spring constant, shape) and exhibits a resonant behaviour for varying driving frequency.

DY 67.10 Thu 15:30 Poster A

Modeling the interaction of magnetically capped colloidal particles — •Anna Eichler-Volf[1], Sibylle Gemming[1,2], Aaron

Tobias Strobel[2], Maximilian Neumann[2], Gabi Steinbach[1,2], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physics, Technische Universitaet Chemnitz, Chemnitz, Germany

Colloidal self-assembly bears significant potential for the bottom-up fabrication of advanced materials and micromechanical structures. For analyzing correlations between the anisotropy at the particle level and the shape of the assembly, simplified theoretical models have been developed to simulate the self-assembly and resulting structures. Here, we concentrate on particles that interact via polar fields, which are intrinsically anisotropic. Additional anisotropy may be introduced by an asymmetric distribution of the polar material, e.g. in a cap. Observed self-assembled structures can be reproduced by models of dipolar spheres, where the dipole is shifted away from the particle center. The three-dimensional model proposed here represents the extended magnetization distribution by a conductive coil enclosed in a hard sphere. The radius of the coil controls the width of the magnetization distribution. The position, or shift, of the coil inside the sphere determines the magnetic asymmetry.

DY 67.11 Thu 15:30 Poster A

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

Particles that constitute active matter are often elongated in shape, as for instance bacteria or active filaments. The shape and stiffness influence both their individual and collective dynamics and pattern formation. Previous work has already revealed many insights into, for example, the spontaneous formation of dynamical structures such as vortices or active turbulence [1,2]. Though it still remains to completely identify the interactions that lead to the emergence of these fascinating phenomena and, in particular, to identify the role of long-ranged hydrodynamic interactions [2].

Here, we present an approach for simulating hydrodynamically interacting elongated microswimmers in a fluid environment using multi-particle collision dynamics. To form microswimmers rods, we rigidly bind overlapping spherical squirmers to each other. The single squirmers propel themselves with an imposed surface flow at their no-slip boundaries [3]. We present first results of our simulation study on the role of hydrodynamic interactions in phases of active matter with elongated constitutes.

[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 67.12 Thu 15:30 Poster A

A path-integral approach to active matter — •Thomas Schindler, Sebastian Kapfer, and Patrick Ketzko — Friedrich-Alexander Universität, Erlangen, Deutschland

The statistical physics of active particles are a rapidly evolving field with many unsolved problems. One of them is the discrepancy of definitions of thermodynamic observables. In equilibrium systems e.g. the pressures, defined via the derivative of the free energy and defined via the force per area on the container of a gas, always yield equivalent results. This is not true for nonequilibrium systems [1]. Here we use a path integral approach where we study an ensemble of one dimensional trajectories in discrete time steps of diffusing particles with drift velocity. These particles mimic active Brownian particles, but from the ensemble we can define a partition function and hence a free energy of the system. The free energy can be written down explicitly and is amenable to numeric evaluation by Markov-chain Monte Carlo methods. The diffusion is modelled by Gaussian transition probabilities between time steps. The direction of the drift is prescribed by an Ising-like spin variable with predefined temporal correlations which models directional diffusion of the particles.

[1] A. P. Solon, Y. Fily, A. Baskaran, M. E. Cates, Y. Kafri, M. Kardar, and J. Tailleur, Nat. Phys. 11, 673 (2015)

DY 67.13 Thu 15:30 Poster A

Multicomponent Systems of Self-Propelled Particles — •Thomas Bissinger and Matthias Fuchs — Universität Konstanz, Fachbereich Physik, 78457 Konstanz

Self-propelled particles (SPPs) have been studied intensely for more than two decades now, with interests ranging from physics to biology and social sciences.

Our work is on the Vicsek model (VM) in 2D, for which we use a generalization to mixtures of particle species. We investigate motility induced phase separation (MIPS) for a binary mixture of SPPs. MIPS occurs when the absolute particle velocity decreases with increasing density, leading to slowly moving clusters with fast particles crossing between clusters.

Besides particle-based numerical simulations, we treated the system theoretically with a generalization of Ihle's phase space approach [1], which utilizes a Chapman-Enskog expansion to arrive at hydrodynamic equations for the binary VM. An alternate approach followed is based on a description by correlation functions.

[1] Ihle, Thomas. "Kinetic theory of flocking: Derivation of hydrodynamic equations." *Physical Review E* **83.3** (2011): 030901.

DY 67.14 Thu 15:30 Poster A

Micro-Swimming with Inertia in Bulk and on Interfaces — •Oleg Trosman[1], Jayant Pande[1], Alexander Sukhov[2], Maxime Hubert[3], Galien Grosjean[3], Nicolas Vandewalle[3], Jens Harting[2], and Ana Sunčana Smith[1] — [1]PULS Group, Department of Physics and Cluster of Excellence: EAM, FAU Erlangen-Nürnberg — [2]HI ERN - Helmholtz-Institut Erlangen-Nürnberg — [3]GRASP, Université de Liège, Belgium

Most theoretical research in the field of micro-swimming from the past few decades addressed the domain of negligible Reynolds number Re, ignoring inertia. For an intermediate range of Re, however, before turbulences arise, the inertial effects become important. In this work we conduct a theoretical study of how this regime emerges, extending the swimmer model by Golestanian and Najafi by inclusion of the beads' masses. After combining the Oseen-Stokes equations for the coupled motion of distant spheres in a fluid with Newton's force-mass relations we obtain a closed-form expression for the velocity of the swimmer with an explicit inertia dependence. This velocity expression compares considerably better to results obtained from lattice-Boltzmann simulations, for intermediately high bead masses or driving forces, than the inertia-free model of Golestanian and Najafi. Furthermore we perform an additional study on the Stokes law alteration for spheres being dragged along a contact surface of two different fluids using lattice-Boltzmann simulations in order to compare our model with with data obtained from an experimental realisation of the Golestanian-Najafi swimmer on fluid-air interface.

DY 67.15 Thu 15:30 Poster A

Collective motion of self-propelled rods with velocity-reversal — •Robert Grossmann[1], Fernando Peruani[1], and Markus Bär[2] — [1]Université Côte d'Azur, Nice, France — [2]Physikalisch-Technische Bundesanstalt, Berlin, Germany

We review progress in the theory of self-propelled rods. In the first part, diffusion properties of rods with velocity reversal are discussed. In particular, we show that their diffusivity is maximal for an optimal rotational noise amplitude. The relevance of this theoretical finding for microbiological systems is corroborated by an explicit comparison to experimental data. The second part addresses collective properties of active rods. At first, a microscopic justification of alignment-interactions with nematic symmetry is presented based on a realistic model for the repulsive interaction of anisotropic rod-shaped particles. Subsequently, the large-scale properties of rods are analyzed within a hydrodynamic theory that can be systematically derived from the microscopic Langevin dynamics via the corresponding mean-field Fokker-Planck equations. Combining analytical methods, numerical continuation and particle-based simulations, the phase-diagram of self-propelled rods is constructed. The rate of velocity reversals turns out to be a central control parameter for the emergent macroscopic pattern-formation. In this regard, our results constitute a proof-of-principle in favor of the hypothesis in microbiology that velocity reversals of bacteria regulates the transitions between various self-organized patterns observed during the bacterial life cycle. [Phys. Rev. E 94 050602 (2016); New. J. Phys. 18 043009 (2016)]

DY 67.16 Thu 15:30 Poster A

Pair Interactions of heat driven Janus particles — •Nicola Söker and Frank Cichos — Molecular Nanophotonics, Institut für Experimentalphysik I, Fakultät für Physik und Geowissenschaften, Universität Leipzig

Heat driven Janus particles as micro swimmers are based on self-thermophoresis, an thus the generation of interfacial flows induced by an optical heating of a hemispherically gold coated polymer par-

ticle. This non-equilibrium process adds even more complexity to a fluctuating hydrodynamic description of the motion and the interactions of such particles with the environment. In this work an ensemble of heat driven 1mu Janus particles in a thin film of water was observe to get statistics of the noise dominated pair interactions between two active Janus particles in the overdamped limit. Those interactions are split into two contributions. At first the additional heat flow from the other particle altering the overall temperature field and hence the thermos-osmotic forces exerted on the fluid at the particle boundary. And second, hydrodynamic effects, mainly the presence of a second swimmer and its constraints on the fluid flow field. The splitting is done by a comparison with another experiment where only the former contribution is present.

DY 67.17 Thu 15:30 Poster A

Modeling of amoeboid swimmer in confined channel — •Swapnil Dalal, Alexander Farutin, and Chaouqi Misbah — Laboratoire interdisciplinaire de physique (LIPHY), CNRS and Université Grenoble Alpes, F-38000 Grenoble, France

Several micro-organisms (Euglena, Eutreptiella Gymnastica), eukaryotic cells (neutrophils, leukocytes, fibroblasts and cancer cells) undergo shape deformation in order to propel themselves. This self propulsion strategy is referred as amoeboid swimming. We study amoeboid swimming by modeling swimmer as deformable body with an inextensible membrane subjected to local distribution of active forces such that total force and torque acting on swimmer vanishes. This instantaneous local distribution of active force used in this study is dependent on the instantaneous swimmer shape. The active forces applied on the swimmer should instigate its locomotion based on its non reciprocal cyclic deformation in the Stokes flow regime. The active forces in this study are described using correlation function obtained using instantaneous local deformation of swimmer and is time independent. This gives rise to autonomous amoeboid swimmer that adapts itself based on surrounding environment. We study effect of confinement on self adapting amoeboid swimmer. Due to shape dependent active forces, the stroke period of swimmer is a function of confinement and it increases with confinement strength. The swimmer velocity exhibits nonmonotonic behaviour as a function of confinement. The swimmer behaviour averaged over one swimming cycle exhibits pusher nature at lower confinement while it shows puller characteristics at higher confinement.

DY 68: Poster: Complex Fluids, Glasses, Granular

Time: Thursday 15:30–18:00 Location: Poster A

DY 68.1 Thu 15:30 Poster A

Shape, Friction and Cohesion in Granular Packings — •Simon Weis[1], Gerd Schröder-Turk[1,2], and Matthias Schröter[3] — [1]Theoretische Physik1, FAU Erlangen, Germany — [2]School of Engineering and IT, Murdoch University, Australia — [3]Institute of Multiscale Simulations, FAU Erlangen, Germany

Friction and adhesive forces are important parameters for the stability of granular packings. We analyze packings of wetting and non wetting spheres of different sizes and triaxial ellipsoids with different aspect ratios. The structural properties of packings are analyzed with respect to the particle's shape, their friction and adhesive forces. Interparticle friction is changed by grinding the particles with different abrasives and by applying liquid and dry lubricants, which also changes adhesive forces. Adhesive forces are changed by adding water with a surfactant to the packing. Various packings with a range of friction coefficients and liquid contents are prepared at various packing fractions by vertical tapping.

To obtain structural properties, the packings are recorded by X-ray tomography and particles as well as liquid clusters are detected. Structural characterization includes mean and local packing fractions, contact numbers as well as (Set-)Voronoi cell anisotropy by Minkowski tensors.

We show that, although friction has an impact on the mechanical characteristics, the analyzed local structural features remain unchanged. The effect of adhesive forces correlates with particle size.

DY 68.2 Thu 15:30 Poster A

Paranusseffekt unter geometrischer Kohäsion — •Barbara Maier[1] und Thomas Grillenbeck[2] — [1]Ignaz-Günther-Gymnasium Rosenheim — [2]FH-Rosenheim University of Applied Sciences

Der Paranusseffekt ist ein Problem, das die Wissenschaft schon seit geraumer Zeit beschäftigt,vor allem weil es noch keine endgültige Lösung für dieses Phänomen gibt und zum anderen bereitet es beispielsweise in der Pharma- und Lebensmittelindustrie viele Probleme, da sich granulare Mischungen auf ihrem Transport immer entmischen. Wie kann man das also verhindern? Tackerklammern bringen aufgrund ihrer sich verhaken den Form jedenfalls schon mal große Vorteile mit sich, denn dadurch wird der Effekt um einen Großteil verlangsamt. Doch wie kann man das alles optimieren oder kann man den Effekt sogar ganz unterdrücken?

DY 68.3 Thu 15:30 Poster A

Light-Driven Reversible Clustering and Separation of Colloids — •Pooja Arya, David Feldmann, and Svetlana Santer — Institute of Physics and Astronomy, University of Potsdam, 14476Potsdam, Germany

We report on colloids that can be reversibly clustered and separated when illuminated with light of different wavelengths. This is possible to achieve when porous colloids are dispersed in a solution containing a photosensitive surfactant. Under illumination with light it undergoes a reversible trans-cis isomerization accompanied by the changes in dipole moment, shape and size. When a solution of photosensitive surfactants is irradiated with focused light, the formation of local hydrodynamic flow at the solid/liquid interface takes place. The phenomenon is known as light-driven diffusioosmosis (LDDO) [1]. Porous particle provides a large area for surfactant to adsorb. When these porous micron-sized silica particles are dispersed in the surfactant solution, they spontaneously cluster at a solid surface. During illumination with blue light, the colloids separate within a few seconds forming equidistant particle ensemble. The long-range hydrodynamic repulsion results in distances between particles (5 micrometer in diameter) up to 80 micrometer. We report on how this process depends on surfactant concentration and irradiation wavelength.

[1] D. Feldmann, S. R. Maduar, M. Santer, N. Lomadze, O. I. Vinogradova, S. Santer *Manipulation of Small Particles at Solid Liquid Interface: Light Driven Diffusioosmosis* Scientific Reports 6 (2016) 36443.

DY 68.4 Thu 15:30 Poster A

Reversed Currents in 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 — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

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]

DY 68.5 Thu 15:30 Poster A

Measuring the buckling of a chain of permanent magnets under load – comparison with the elastica model — •Lucas Bartosch, Ingo Rehberg, and Reinhard Richter — Experimentalphysik 5, Universität Bayreuth

A one-dimensional chain of spherical neodymium-iron-boron magnets responds to mechanical loadings in a manner reminiscent of an elastic rod, which was recently described by introducing an effective magnetic bending stiffness [1]. We are investigating the deformation of such a chain resting on a plain by means of images recorded by a digital camera. The positions of the magnets are extracted utilizing OpenCV for image processing. The distance between the two endpoints of the chain is manipulated via a computer controlled stepper motor. Moreover, the lateral force is recorded with a magnetic insensitive force gauge. We

are investigating the shape of such a macroscopic chain using digital image processing and compare it to the classical elastica model. In this comparison we find sneaky deviations around an ideal course of the spheres, which may be caused by friction in-between the spheres [2].

[1] D. Vella, E. du Pontavice, C. L. Hall and A. Goriely, *Proc. R. Soc. A* **470**, 20130609 (2013).

[2] I. Rehberg, Comment on: "Stability of vertical magnetic chains", by Johannes Schönke and Eliot Fried, *Proc. R. Soc. A* **473**, 20160703 (2017).

DY 68.6 Thu 15:30 Poster A

Why beam hardening is necessary to measure volume fractions in granular packings — •Manuel Baur[1], Norman Uhlmann[2], Thorsten Pöschel[1], and Matthias Schröter[1] — [1]MSS, FAU, Germany — [2]Fraunhofer Institute for Integrated Circuits, Fürth, Germany

We study density waves in a fluidized bed via x-ray radiography. Dense regions in the bed attenuate the x-rays stronger than dilute ones and result in darker gray values. The commonly used Lambert-Beer law, to describe the photon attenuation, is just valid for monochromatic x-ray beams. Industrially used x-ray tubes do not emit a monochromatic beam, but the broad Bremsstrahlung spectrum. In this case the attenuation coefficient depends on the photon energy. High energy photons are attenuated less than weak energy photons. The ratio of high to low energy photons in the spectrum of the x-ray beam increases after transmitting a slab of material - the beam hardens. An understanding of beam hardening is necessary to quantize density fluctuations in a fluidized bed from radiograms. We present a technique to access the x-ray attenuation as a function of transmitted material thickness and show how the transmitted thickness can be deduced from that.

DY 68.7 Thu 15:30 Poster A

Analytical mesoscale modeling of aeolian sand transport — Marc Lämmel and •Klaus Kroy — Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany

The mesoscale structure of aeolian sand transport determines a variety of natural phenomena studied in planetary and Earth science. We analyze it theoretically beyond the mean-field level, based on the grain-scale transport kinetics and splash statistics. A coarse-grained analytical model is proposed and verified by numerical simulations resolving individual grain trajectories. The predicted height-resolved sand flux and other important characteristics of the aeolian transport layer agree remarkably well with a comprehensive compilation of field and wind-tunnel data, suggesting that the model robustly captures the essential mesoscale physics. By comparing the predicted saturation length with field data for the minimum sand-dune size, we elucidate the importance of intermittent turbulent wind fluctuations for field measurements and reconcile conflicting previous models for this most enigmatic emergent aeolian scale.

DY 68.8 Thu 15:30 Poster A

Electro-osmotic pumping for structured coatings — •raheema muhammad aslam, ran niu, and thomas palberg — Institute of Physics, JGU Mainz, Germany

We assemble charged colloidal spheres at deliberately chosen locations on a charged unstructured glass substrate utilizing ion exchange based micro-pumps. The pump uses trace amounts of ions to generate electroosmotic fluid flows. We show experimentally that our pump operates in almost deionized water for periods exceeding 24 h and induces fluid flows in micrometer per second over hundreds of micrometers. This flow displays a far-field, power-law decay which is characteristic of two-dimensional (2D) flow when the system is strongly confined and of three-dimensional (3D) flow when it is not. Experimentally, we systematically explore the control parameters of crystal assembly at and by micro-pumps and the mechanisms through which they depend on the experimental boundary conditions. We demonstrate that crystal quality depends crucially on the assembly distance of the colloids. This is understood as resulting from the competition between inward transport by the electro-osmotic pump flow and the electro-phoretic outward motion of the colloids. Optimized conditions include substrates of low and colloids of large electro-kinetic mobility. Then a sorting of colloids by size is observed in binary mixtures with larger particles assembling closer to the ion exchanger beads. Moreover, mono-sized colloids form defect free single domain crystals which grow outside a colloid-free void with facetted inner crystal boundaries centred on the ion exchange particle.

DY 68.9 Thu 15:30 Poster A

Binary mixtures of helical Yukawa rods studied by Monte Carlo simulations — •Motoya Suzaka, Anja Kuhnhold, and Tanja Schilling — Institute of Physics in University of Freiburg, Freiburg, Germany

Systems composed of chiral rod-like particles have a complex phase diagram. The main phases are isotropic, nematic, smectic and especially the cholesteric phase. To assess such complex phase diagrams, Monte-Carlo(MC) simulations can be applied. As model system we use helical Yukawa rods where the chirality is due to point charges, that are helically wrapped around the surface.

Of special interest for technical application is the cholesteric pitch in the equilibrium state. We started to study monodisperse systems first. But more meaningful for comparisons to experimental systems are studies on polydisperse systems. The simplest kind of a polydisperse system is a binary one. We therefore use binary mixtures with different particle lengths, surface charges or internal pitches. To simulate the equilibrium cholesteric phase we apply MC simulations and special boundary conditions.[1]

[1] A. Kuhnhold and T. Schilling, J. Chem. Phys. 145, 194904 (2016).

DY 68.10 Thu 15:30 Poster A

Percolation and Conductivity of Network of Hard Rods under Mechanical Load — •Arshia Atashpendar and Tanja Schilling — Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany

Electrically conductive, soft nano-composites are of technological interest e.g. as transparent electrodes and as sensors. The dielectric behaviour of these systems under varying mechanical conditions still remains poorly investigated. Thus, in order to better understand the conductivity properties of dispersed conductive nano-particles in an insulating matrix, we use Monte Carlo simulations to study how the structure of the percolating network, the conductivity and the diffusive properties of a system of isotropic hard rods are affected by mechanical load. The conductance between pairs of rods is considered under the assumption that single electron tunneling is the sole dominant process for electrical connectedness.

DY 68.11 Thu 15:30 Poster A

Growth and Interaction of Colloid Nuclei under Microgravity — •Lou Kondic[1], Michael Lam[1], Boris Khusid[1], and William Meyer[2] — [1]NJIT, Newark, NJ, USA — [2]Glenn Research Center, Cleveland, OH, USA

We have developed a model describing the growth and interaction of colloid nuclei. The model is based on a coupled diffusion problem for the solid and liquid phase, combined with the consistent boundary conditions involving osmotic pressure balance, including interfacial tension. The motion of the solidification front is modeled based on the Wilson-Frenkel law. The single nuclei model is validated by considering various asymptotic limits, as well as by comparing the results to ones available in the literature. The multiple nuclei model allows, for the first time, for the careful computational investigation of the interaction between evolving nuclei. The preliminary comparison with and interpretation of data obtained on the International Space Station (available at psi.nasa.gov) as well as ground-based experiments, will be discussed.

Acknowledgment: This project is supported by the NASA Grant NNX16AQ79G.

DY 68.12 Thu 15:30 Poster A

Structure formation in 4M3H/2E1H mixtures at low temeprature — •Jennifer Bolle, Christian Sternemann, Christian Albers, Göran Surmeier, Fatima Mallal, Robin Sakrowski, and Metin Tolan — Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany

Monohydroxy alcohols (MAs) have been scrutinized as a model of hydrogen bonded fluids. These hydrogen bonds are essential for the microscopic structure and dynamics of water, aqueous solutions and alcohols [1]. MAs are supposed to form supramolecular structures via hydrogen bonding in the liquid phase. Dielectric spectroscopy studies suggest ringlike arrangements for 4-methyl-3-heptanol (4M3H) and chainlike structures in 2-ethyl-1-hexanol (2E1H) and indicate a struc-

tural crossover for 4M3H/2E1H mixtures with temperature [2]. We present X-ray diffraction measurements of $(2E1H)_x(4M3H)_{1-x}$ mixtures over a temperature range from 175K to 405K. The results point towards a change of the supramolecular structures indicated by analysis of the first diffraction peak.
[1] Kaatze, U., Behrends, R., and Pottel, R. "Hydrogen network fluctuations and dielectric spectrometry of liquids". In: Journal of Non-Crystalline Solids . (2002), 305(1), 19-28. [2] Bauer, S., Wittkamp, H., Schildmann, S., Frey, M., Hiller, W., Hecksher, T., and Böhmer, R. "Broadband dynamics in neat 4-methyl-3-heptanol and in mixtures with 2-ethyl-1-hexanol". In: The Journal of chemical physics. (2013), 139(13), 134503.

DY 68.13 Thu 15:30 Poster A

Concentration effects on the phase-behaviour and sheared dynamics of rod-like particles — •Pawel Mollenhauer, Henning Reinken, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Deutschland

Already in thermodynamic equilibrium, systems of rod-like particles show an interesting phase behavior, including isotropic–nematic phase coexistence. Driving such a system out of equilibrium by applying a shear flow results in a shift of the isotropic–nematic transition. Furthermore, sheared nematic liquid crystalline systems can show the formation of bands in the gradient and the vorticity direction [1]. These spatial patterns can additionally feature oscillatory orientational motion of the nematic director (e.g. tumbling or wagging) [2].
In this work, we apply the Doi-Hess-theory [3] that couples the tensorial nematic order parameter to the velocity field. In addition, we explicitly include the concentration dynamics using a DFT-approach bridging microscopic and mesoscopic levels [4]. Starting from an already phase-separated system we numerically investigate the spatiotemporal pattern formation under shear. In contrast to earlier works [5], we do not restrict our investigations to stationary states. Instead, we focus on oscillatory states and vorticity banding.
[1] P. Olmsted, Rheol. Acta **47**: 283 (2008).
[2] R. Lugo-Frías et al., Eur. Phys. J. E **39**: 88 (2016).
[3] S. Hess, Tensor for Physics, (2015).
[4] R. Lugo-Frías et al., J. Phys.: Condens. Matter **28**, 244022 (2016).
[5] P. Olmsted et al., Phys. Rev. E **60**, 4 (1999).

DY 68.14 Thu 15:30 Poster A

Elastic turbulence at low Reynolds numbers and its control — •Reinier van Buel, Christian Schaaf, Leander Rolef, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Viscoelastic polymer solutions have remarkable qualities compared to their Newtonian counterparts. Especially at very small scales, such as employed in microfluidic devices, they enhance mixing and heat transfer. This is due to elastic turbulence [1], which bears the same qualities as inertial turbulence. The relevant dimensionless number for viscoelastic fluids is the Weissenberg number, which is the ratio of nonlinear stress to dissipation via linear stress relaxation. Plane Couette flows of viscoelastic fluids have been shown to exhibit an elastic subcritical instability at low Reynolds numbers whereas flows with curved stream lines are linearly unstable. The critical Weissenberg number is related to the curvature of the flow stream lines.

We report here on the onset of elastic turbulence in a two-dimensional Taylor-Couette geometry using numerical solutions of the Oldroyd B model as our constitutive equation. We observe a critical Weissenberg number that demarcates the transition from a stable to an elastic turbulent flow. We characterize the turbulent flow by observing a strong enhancement of flow resistance and a power-law decay of velocity power spectra, which show that the flow is activated on a broad range of temporal scales. Finally, we present first results on controlling the instability by using time-delayed feedback.

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

DY 68.15 Thu 15:30 Poster A

Scalable and fast heterogeneous molecular simulation with predictive parallelization schemes — •Horacio V Guzman, Torsten Stuehn, and Kurt Kremer — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Multiscale and inhomogeneous molecular systems are challenging topics in the field of molecular simulation. In particular, modeling biological systems in the context of multiscale simulations and exploring material properties are driving a permanent development of new simulation methods and optimizing algorithms. In computational terms, those methods require parallelization schemes that make a productive use of computational resources for each simulation and from its genesis. Here, we introduce the heterogeneous domain decomposition algorithm which is a combination of a heterogeneity sensitive spatial domain decomposition with an *a priori* sliding subdomain-walls procedure. The algorithm modeling is presented for dual resolution systems and inhomogeneous binary fluids, in terms of scaling properties as a function of the size of the low-resolution region and the high to low resolutions ratio. We also show the algorithm competences, by comparing it to its initial domain decomposition algorithms and dynamic load balancing schemes. Specifically, two representative molecular systems have been simulated and compared to the heterogeneous domain decomposition proposed in this work. These two systems comprise an adaptive resolution simulation of a biomolecule solvated in water and a phase separated binary Lennard-Jones fluid.

DY 68.16 Thu 15:30 Poster A

A transient amorphous solid formed from low density aqueous charged sphere suspensions — •Ran Niu[1], Sabrina Heidt[1,2], Ramsia Sreji[3], Riande Dekker[4], Maximilian Hofmann[1], and Thomas Palberg[1] — [1]Institute of Physics, Johannes Gutenberg University, D-55099 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, D-55128 Mainz, Germany — [3]Department of Chemistry Physical and Biophysical Chemistry (PC III), Bielefeld University, D-33615 Bielefeld, Germany — [4]Debye Institute for Nanomaterials Science, Utrecht University, NL-3584 CC Utrecht, The Netherlands

We report the formation of a transient amorphous solid formed from charged polymer spheres suspended in thoroughly deionized water at volume fractions of 0.0002-0.01 [1]. From optical experiments, we observe the presence of short-range order and an enhanced shear rigidity as compared to the stable polycrystalline solid of body centred cubic structure. On a density dependent time scale of hours to days, the amorphous solid transforms into this stable structure. We further present preliminary dynamic light scattering data showing the evolution of a second slow relaxation process possibly pointing to a dynamic heterogeneity known from other colloidal glasses and gels. We compare our findings to the predicted phase behaviour of charged sphere suspensions and discuss possible mechanisms for the formation of this peculiar type of colloidal glass [2]. References 1.*T. Palberg, et al. J. Stat Phys. 2016, 074007 (2016). 2.*R. Niu, et al. Sci. Rep. accepted.

DY 68.17 Thu 15:30 Poster A

^{2}H and ^{17}O NMR studies of dynamics of water-ethylene glycol mixtures — •Verena Fella, Dominik Demuth, and Michael Vogel — TU Darmstadt, Condensed Matter Physics, Darmstadt, Germany

Binary water mixtures play an important role in biological as well as technological systems. Particularly water-alcohol mixtures are used in many applications though a complete understanding of their complex dynamical behaviour is still lacking. Here, nuclear magnetic resonance (NMR) experiments prove to be a powerful tool due to isotope selective measurements. ^{2}H NMR is an established method to analyse mixtures by deuterating one component. Unfortunately, selective observation of water in water-alcohol mixtures is hampered by deuteron exchange. Adjei-Acheamfour et al. (J. Chem. Phys., 143, 214201 (2015)) recently investigated ultraslow dynamics in ice with ^{17}O NMR by selective excitation of the central line. This approach yields many new possibilities to explore glass-forming materials. We combine ^{17}O and ^{2}H NMR to analyse a mixture of $H_2{}^{17}O$ and deuterated ethylene glycol (EG-d4) where each component can be measured separately. Correlation times τ in the range from 10^{-10} to 10^{-5} s show a strong coupling between the water and EG dynamics. For the supercooled phase the correlation times exhibit a broad distribution, so that ^{17}O NMR studies at $\tau > 10^{-5}$ s are limited by short spin-lattice relaxation times T_1. However, we show that ^{17}O NMR yields valuable insights into the crystalline phase of water-EG mixtures. In the future this can be exploited to study crystallisation in various aqueous systems.

DY 68.18 Thu 15:30 Poster A

The non-Gaussian parameter and breakdown of the Stokes-Einstein relation in supercooled liquids — •Lawrence Smith and Andreas Heuer — Institut für physikaliusche Chemie

Elementary units of a binary lennard-jones glassformer can be identified through quantitative analysis of its underlying potential energy landscape. These units can be fully understood within the continuous time random walk formalism and are found to contain the complete in-

formation concerning thermodynamics and diffusivity, while displaying finite size effects with respect to relaxation times and spacial correlations [1].

Previous research has shown that it is possible to identify major contributions to the non-Gaussian parameter as arising from the moments of the waitingtime distribution for jumps between metabasins of the potential energy landscape [2].

This work investigates the impact of coupling between these elementary units on spacial heterogeneity. By analysing the non-Gaussian parameter in molecular dynamics simulations as well as in a stochastic model we gain insight into the breakdown of the Stokes-Einstein relation and into the underlying lengthscales at play.

[1] C. Rehwald, A. Heuer, Phys. Rev. E 86, 051504 2012 [1] C. Schroer, A. Heuer, Phys. Rev. Lett. 110, 067801 2013

DY 68.19 Thu 15:30 Poster A

Nachweis des Debye-Prozesses in einem Monohydroxyalkohol mittels depolarisierter Lichtstreuung — •Andreas Helbling, Jan Gabriel, Florian Pabst, Till Böhmer und Thomas Blochowicz — TU Darmstadt, Institut für Festkörperphysik, 64289 Darmstadt

Lange Zeit wurde die Debye-Relaxation, die der langsamste dynamische Prozess in Monohydroxyalkoholen ist und deren Ursprung immer noch nicht vollständig verstanden ist, nur in der dielektriktrischen Spektroskopie beobachtet. Inzwischen konnte er jedoch auch mit anderen experimentellen Methoden, wie z.B. in mechanischen Scherexperimenten [1], nachgewiesen werden. Daher haben wir Photonen-Korrelations-Spektroskopie (PCS) an dem Monohydroxyalkohol 5-Methyl-2-Hexanol (5M2H) mit breitbandiger dielektrischer Spektroskopie (BDS) über einen weiten Temperatur- und Frequenzbereich verglichen. Zum ersten Mal konnten wir dabei den Debye-Prozess in einem Monohydroxyalkohol in der Lichtstreuung nachweisen. Der Vergleich seines Erscheinungsbildes in beiden Methoden erlaubt es uns aktuelle Modelle seines Ursprungs, wie zum Beispiel Rotationsbewegungen von wasserstoffbrückengebundenen Überstrukturen wie Ketten oder Ringe, zu testen.

[1] Gainaru C. et. al., Phys. Rev. Lett. 112, 098301 (2014)

DY 68.20 Thu 15:30 Poster A

Photometric far-field studies on luminescent borate glass ceramics for LED applications — •Juliane Schuppich[1], A. Charlotte Rimbach[1], Peter W. Nolte[2], Franziska Steudel[2], and Stefan Schweizer[1,2] — [1]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

The most common white light emitting diodes (LEDs) are based on a blue-emitting LED chip coated with a yellow-emitting phosphor; the phosphor acts as a frequency-downshifter for a significant part of the blue light to generate white light. Luminescent glasses represent an interesting alternative to the commonly used phosphor/polymer composite due to their higher thermal and chemical stability. The glasses are optically activated by additional lanthanide ion doping. However, since the optical absorption coefficient of the lanthanide ions is low, the as-made glasses are processed to glass ceramics in a subsequent annealing step. The glass ceramics provide a longer optical path length for the incident blue light due to scattering at the grown crystallites in the glass. In this work, photometric far-field studies on europium-doped lithium borate glass ceramics are presented to show the potential of these systems as frequency-downshifter for LED applications. The experimental results are compared with optical simulations to optimize the glass ceramics with respect to lanthanide ion concentration, crystallite size distribution as well as degree of crystallization.

DY 68.21 Thu 15:30 Poster A

Dynamic glass transition in the supercooled liquid and plastic crystal of ethanol — •Yeong Zen Chua[1], Amanda R. Young-Gonzales[2], Ranko Richert[2], and Christoph Schick[1] — [1]Uni Rostock, Institut für Physik and Competence Centre CALOR, Rostock — [2]School of Molecular Sciences, Arizona State Uni, Tempe, Arizona, USA

Ethanol has been widely investigated and is well-known to exhibit a very interesting polymorphism of different solid phases: a fully-ordered (monoclinic) crystal, a (bcc) plastic crystal, a glassy plastic crystal and an ordinary amorphous glass. Physical vapor deposition (PVD) has been used to prepare amorphous glasses of ethanol, which upon heating to higher temperature transforms into the plastic crystal of ethanol. The dynamic glass transition of supercooled liquid of ethanol is successfully measured by AC nanocalorimetry. Preliminary results for the plastic crystal are also presented. With that, the frequency dependency of the dynamic glass transition of the supercooled liquid of ethanol is measured and compared with published dielectric data. Comparison of dielectric data of supercooled liquid of ethanol with AC nanocalorimetric data shows that ethanol exhibits Debye peak, which cannot be observed in AC nanocalorimetry. In previous published dielectric data, the prominent Debye peaks have been mistaken as structural α relaxation. The dielectric data have been re-evaluated and the high frequency wing in the dielectric spectra is identified as the structural α relaxation.

DY 68.22 Thu 15:30 Poster A

Cogging free magnetic gears — Stefan Borgers, Simeon Völkel, Stefan Hartung, Wolfgang Schöpf, and •Ingo Rehberg — Experimentalphysik V, Universität Bayreuth

The coupling of two rotating spherical magnets is investigated experimentally, with particular emphasis on those motions where the driven magnet is phase-locked to the driving one, which is a feature of the so called cogging free couplings. The theory for these experiments is based on pure dipole-dipole interaction. Technical applications of this kind of coupling are foreseeable particularly for small machines.

DY 68.23 Thu 15:30 Poster A

Nanostructured titania templated by amphiphilic diblock copolymer for lithium-ion battery anodes — •shanshan yin, Peter Müller-Buschbaum, and lin song — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Lithium-ion batteries (LIBs) have been widely used in many aspects of modern life. Compared with conventional graphite anodes, titania possesses higher capacity and better operation safety, which makes it a promising substitute to the commonly used graphite anodes. However, problems such as gradual capacity decay and relative high intercalation potential hinder its practical application. It has been reported that nanostructured titania can efficiently improve the electrochemical performance. Therefore, in this work titania nanostructures are prepared via sol-gel synthesis in combination with the amphiphilic diblock copolymer poly(styrene-block-ethylene oxide) (PS-b-PEO) as structure-directing agent. The morphology of the obtained titania nanostructures is studied with optical microscopy (OM) and scanning electron microscopy (SEM), while the optical properties are investigated with UV/Vis spectroscopy and Photoluminescence (PL).

DY 69: Poster: Quantum Systems

Time: Thursday 15:30–18:00 Location: Poster A

DY 69.1 Thu 15:30 Poster A

Nonequilibrium dynamics of laser-excited graphene: ab-initio MD simulations including electron-phonon coupling — •Sergej Krylow and Martin E. Garcia — Universität Kassel, Theoretische Physik II

Graphene attracted a lot of interest in the last decade due to its unique physical properties. Despite intensive research, there are still open questions regarding the response of Graphene to ultrashort laser pulses. In ultrafast electron diffraction experiments, a decay of Bragg peak intensities with two different decay times can be observed. The generation of a few optical phonons, so called SCOPs, which are strongly coupled to the electronic subsystem is believed to play a major role for this effect. However, the origin of the two timescales and the involved dynamics are not fully understood yet. To address this problem, we performed ab-initio molecular dynamic simulations of monolayer graphene immediately after laser excitation. Our results show that the short decay time can be accounted by the generation of the SCOPs and the long decay time to the equilibration of the phonon system. Furthermore, we see two stages in the dynamics of the lattice towards thermal equilibrium. Within the first picosecond after laser excitation mainly high- and mid-frequency phonons are created. Then, on a much longer timescale, the equilibration with low-frequency phonons occurs. Our result clearly suggest that the bottleneck for thermal equilibration in monolayer graphene are the low-frequency phonons.

DY 69.2 Thu 15:30 Poster A

Quantum non-Markovianity: Simulation, Quantification and Thermodynamics — •Philipp Strasberg — Complex Systems and Statistical Mechanics, Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

This poster reviews recent progress in the understanding of non-Markovian open quantum systems from the author's perspective. Markovian embedding strategies, which allow for a convenient treatment of non-Markovian open quantum systems, are reviewed. Their thermodynamic interpretation and potential to understand more realistic heat engines are discussed. Finally, also some easily computable witnesses of non-Markovianity are presented.

DY 69.3 Thu 15:30 Poster A

Multifractal properties of the ground state of the Bose-Hubbard model — Jakob Lindinger, Andreas Buchleitner, and •Alberto Rodríguez — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Staße 3, D-79104 Freiburg, Germany

We study the multifractal properties of the ground state of the one-dimensional Bose-Hubbard model in Fock space. We confirm that the limit of vanishing interaction exhibits non-trivial multifractality in the Fock basis [1]. In order to get access to the multifractal properties at arbitrary values of the interaction strength, we use exact diagonalisation and quantum Monte Carlo simulations (which enable us to reach $L = 30$, corresponding to a Hilbert space of size $\simeq 6 \times 10^{16}$). Our results suggest the existence of non-trivial multifractality in the ground state for a large range of interaction values. We find that an analysis of the generalised fractal dimensions for different densities exposes qualitatively the superfluid to Mott insulator transition. We furthermore explore different methods to quantitatively characterise the transition.

[1] E. Bogomolny. Multifractality in simple systems. Presentation at the conference "Complex patterns in wave functions: drums, graphs, and disorder" at the Kavli Royal Society Centre, UK (2012)

DY 69.4 Thu 15:30 Poster A

Quantum chaos in undoped graphene with long-range coulomb interaction — •Markus Klug[1], Mathias Scheurer[2], and Jörg Schmalian[1,3] — [1]Affiliation: Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]Department of Physics, Harvard University, Cambridge MA 02138, USA — [3]Affiliation: Institute of Solid State Physics, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany

In the context of thermalization, we investigate the ability of electrons in undoped Graphene in the presence of long-range Coulomb interaction to scramble information. We therefore compute the Lyapunov exponent which represents the inverse time scale describing the exponential growth of certain out-of-time order correlation functions for intermediate times. The Lyapunov exponent λ is determined perturbatively to order $\mathcal{O}(1/N)$ where N is the number of fermion flavors. By doing so we are able to investigate the weak $\alpha \to 0$ and strong $\alpha \to \infty$ coupling regime with α being the fine structure constant determining the electron-electron interaction strength. By restoring $N = 4$ in case of graphene, we find in the strong coupling regime an exponent of order of the recently proposed bound, and for weak coupling a linear dependence on the coupling strength. The conducted analysis provides insights into the sensitiveness of out-of-time order correlators towards physical relaxation processes.

DY 69.5 Thu 15:30 Poster A

Including temperature in a wavefunction description of the spin boson model — •Michael Werther[1,2] and Grossmann Frank[1] — [1]TU Dresden, Institut für Theoretische Physik, Zellescher Weg 17, 01069 Dresden — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden

The Davydov Ansatz is an efficient numerical tool for approximate solution of the Schrödinger-equation for different Hamiltonians. In recent works the D1-Ansatz has been successfully applied to different systems like the Holstein model or the quantum Rabi model[1], where it has proven to yield excellent results that are comparable to those of other numerical methods like HEOM or ML-MCTDH.[2]

Here we present how the Davydov Ansatz can be elegantly used to include temperature effects into the spin boson model, even in the strong coupling regime. In a frame in which all system and bath DOFs can be taken into account, we show how the powerful Dirac-Frenkel variational principle can be applied for approximate propagation of the full density matrix. As an outlook we show how numerical instabilities, arising especially from the multi Davydov Ansatz, can be overcome.

[1] M. Werther, F. Grossmann, J. Phys. A: Math. Theor., in press (2017)

[2] L. Chen, R. Borelli, Y. Zhao, J. Phys. Chem. A 121, 8757-8770 (2017)

DY 69.6 Thu 15:30 Poster A

Transport away from resonance channels in 4D symplectic maps — •Franziska Onken[1,2], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

The dynamics of Hamiltonian systems (e.g., planetary motion, electron dynamics in nano-structures, chemical reactions) can be understood by studying the corresponding symplectic Poincaré maps. A central new feature in higher-dimensional systems is the transport in resonance channels. While such channels are usually investigated in frequency space, we visualize the relevant invariant objects in phase space revealing a highly non-trivial geometry. Especially the transport away from the channel is governed by families of hyperbolic 1D-tori and their stable and unstable manifolds. We provide a visualization of a turnstile in higher dimensions and an approach to measure the corresponding transport.

DY 69.7 Thu 15:30 Poster A

GOE-GUE-Poisson crossover in the nearest neighbor spacing distribution of magnetoexcitons — Frank Schweiner, •Patric Rommel, Jeanine Laturner, Jörg Main, and Günter Wunner — Institut für Theoretische Physik 1, University of Stuttgart, Germany

Until now only for specific transitions between Poissonian statistics (P), the statistics of a Gaussian orthogonal ensemble (GOE), or the statistics of a Gaussian unitary ensemble (GUE) analytical formulas for the level spacing distribution function have been derived within random matrix theory. We investigate arbitrary transitions in the crossover between all three statistics. To this aim we propose a fitting formula for the level spacing distribution function depending on two parameters [1]. Recent investigations on the Hamiltonian of excitons revealed that the combined presence of a cubic band structure and external fields breaks all antiunitary symmetries, and thus the nearest-neighbor spacing distribution of magnetoexcitons can exhibit all three statistics depending on the system parameters. Evaluating

the numerical results for magnetoexcitons in dependence on the excitation energy and on a parameter connected with the cubic valence band structure and comparing the results with the formula proposed allows us to investigate the level spacing dynamics in the crossover regime and to distinguish between regular and chaotic behavior as well as between existing or broken antiunitary symmetries. We also investigate the effect of the exciton-phonon interaction on the level statistics [2].

[1] F. Schweiner et al., Phys. Rev. E 96, 052217 (2017).
[2] F. Schweiner et al., Phys. Rev. B 96, 035207 (2017).

DY 69.8 Thu 15:30 Poster A

Signatures of multiple exceptional points in optical microdisk cavities — •Julius Kullig[1,2], Martina Hentschel[1], and Jan Wiersig[2] — [1]Institut für Physik, TU Ilmenau, Ilmenau, Deutschland — [2]Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Deutschland

Optical microdisk cavities can confine light for very long times in extremely small volumes. However, due to radiation and evanescent leakage the optical modes are described by the non-Hermitian dynamics of open systems. One striking signature of this non-Hermitian physics are exceptional points (EPs) in parameter space at which at least two eigenvalues (complex frequencies) as well as their corresponding eigenstates (modes) coalesce.

Exceptional points in microdisk cavities have been shown to be very useful, e.g., for sensing devices. However, in lots of experimental setups EPs are adjusted in a rather fragile way e.g., via external particles or fibre tips.

In our poster we report on EPs formed by adjusting the properties of the cavity itself such as the refractive index profile and/or the boundary shape. Furthermore, we investigate situations where not a single but several EPs occur which is beyond a two-mode scenario of a single EP2 where two modes coalesce.

DY 69.9 Thu 15:30 Poster A

Transport along resonance channels in 4D symplectic maps — •Martin Langer[1], Roland Ketzmerick[1,2] und Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden, Germany — [2]MPI für Physik komplexer Systeme, Dresden, Germany

A distinctive new feature of higher-dimensional systems is the possibility of Arnold diffusion, i.e. chaotic regions in phase space are all interconnected by the Arnold web. We study a designed 4D symplectic map with a regular region embedded in a chaotic sea, i.e. far away from the integrable regime. The model allows for generating specific resonance structures and shows a considerable drift of orbits in the chaotic region near these resonances. We investigate transport phenomena of ensembles of chaotic orbits in the vicinity of these resonances using 3D phase-space slices, frequency analysis, survival time plots, and chaos indicators.

DY 69.10 Thu 15:30 Poster A

Microwave graphs with time-dependent perturbations — •Tobias Hofmann[1], Aimaiti Rehemanjiang[1], Ulrich Kuhl[1,2], and Hans-Jürgen Stöckmann[1] — [1]Fachbereich Physik der Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]Université Côte d'Azur, CNRS, Institut de Physique de Nice, 06108 Nice, France

The study of microwave billiards, where one Parameter depends on time, always has been a challenge. One possible parameter is the coupling to an external channel, which we have specifically in mind here. The difficulties arise from the need to apply perturbations of sufficient strength with frequencies of the order of the mean level spacing, typically of some MHz to be in the interesting regime.
In microwave networks time variations can be achieved by a means of a T junction, where one port is connected to a cable with a changeable terminator. A wave traveling through the cable being reflected at the end and returning to the T junction acquires a phase given by $\Delta\varphi = 2kl + \varphi_{\mathrm{term}}$, where $k = 2\pi\nu/c$ is the wave number, l the cable length and φ_{term} is the reflection phase. The expected periodic variation of the transmission from port 1 to port 2 with frequency ν was experimentally verified. If now the terminator of the cable is replaced by a variable diode, φ_{term} may be changed continuously by means of the diode voltage. Periodic modulations of the transmission with frequencies up to 10 MHz have already been achieved. By applying stochastic time variations also the study of "noisy graphs" [1] become feasible.

[1] D. Waltner, U. Smilansky, *J. Phys.* **A 47**, 355101 (2014).

DY 69.11 Thu 15:30 Poster A

Quantum localization on fractals in absorbing maps — •Konstantin Clauss[1], Martin Körber[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

In chaotic quantum systems with escape a fundamental question concerns the phase-space localization of resonance states. It is known that a semiclassical description of individual states is given by some classical conditionally invariant measure with the same decay rate. It is not known, however, which specific measure is relevant for quantum mechanics. We combine conditional invariance with finite quantum resolution of the classical fractal chaotic saddle leading to a prediction of the corresponding measure. By this the typical phase-space distribution of resonance states for arbitrary decay rates is explained.

DY 69.12 Thu 15:30 Poster A

Frequency splittings in deformed optical microdisk cavities — •Chang-Hwan Yi[1], Julius Kullig[1,2], Chil-Min Kim[3], and Jan Wiersig[1] — [1]Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Postfach 4120, D-39016 Magdeburg, Germany — [2]Institute for Physics, Theoretical Physics II/Computational Physics Group, Technische Universität Ilmenau, Weimarer Straße 25,98693 Ilmenau, Germany — [3]Department of Emerging Materials Science, DGIST, Daegu 711-873, Korea

The frequency splitting of nearly degenerate optical modes in weakly deformed microdisks is investigated. According to a mirror-reflection symmetry of the cavity, the even and odd parity modes are studied. A semiclassical approach of dynamical tunneling (resonance-assisted tunneling) is implemented in order to explain the frequency splitting between clockwise and counterclockwise propagating waves. We deduce semiclassical predictions for the frequency splittings which agree well with full numerical calculations. As a representative deformation of an integrable and non-integrable systems, the ellipse and the quadrupole shapes are examined in detail. Different properties of the frequency splittings following the Dirichlet and dielectric boundary conditions are discussed.

DY 69.13 Thu 15:30 Poster A

Transport in disordered optical systems — •Florian Heyder and Martina Hentschel — Institute for Physics, Theoretical Physics II/Computational Physics Group, Technische Universität Ilmenau, Weimarer Straße 25, 98693 Ilmenau, Germany

It has been shown that electron transport through a quantum point contact in a two-dimensional electron gas leads to branching patterns of the scattered trajectories. We numerically investigate an analogue that is realized by a 2D optical system where light rays experience a correlated refractive index. The results show a branching behavior as well. We further examine the trajectory-statistics in our disordered systems and find, amongst other, a connection between the correlation length of the refractive index and the persistence of the branching.

DY 69.14 Thu 15:30 Poster A

Non-universal behaviour in branched flow — •Philipp Breul and Ragnar Fleischmann — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

When waves propagate in a weakly scattering complex medium they are strongly focused into branch-like structures on length scales much shorter than the mean-free-path. This *branched flow* is a very general phenomenon: wind driven ocean waves, light, sound, conduction electrons, tsunamis and even earth quakes are examples of waves that in a natural environment typically propagate through a complex medium and can exhibit branching.
Often the medium is best described as a Gaussian random field with intrinsic correlations. For a wide range of different functional forms of these correlations the statistics of branched flows have been found to show universal behaviour that only depends on a few characteristic quantities like the variance σ^2 and the integral correlation length ℓ_c of the fluctuations in the medium. For example does the typical length scale ℓ_b of branched flows scale like $\sigma^{-2/3}$. Inspired by the statistical structure of two-dimensional turbulent fields we study branched flows in media with pronounced anti-correlations that lead to vanishing integral correlation length in transverse direction to the flow. We find that such media exhibit strongly non-universal behaviour and the branchinglength scales like $\ell_b \sim \sigma^{-1}$.

DY 69.15 Thu 15:30 Poster A

An analytical approach to extend Fresnel laws to concave shaped interfaces — •Sebastian Luhn and Martina Hentschel — Institute for Physics, Group for Theoretical Physics II / Computational Physics, Technische Universität Ilmenau, Weimarer Str. 25, 98693 Ilmenau

Optical microcavities play an important role in many modern research fields. In particular it is interesting to study the reflection and refraction of beams at the interfaces of these cavities. The reflection of beams is described by Fresnel*s laws which apply to flat surfaces only and need to be corrected for curved interfaces. Since convex interfaces have been studied already, we perform these cor- rections for concave interfaces. We obtain the reflection coefficients by extend- ing the model of transfer matrices to cylindrical interfaces. Additionally we gain a relation between convex and concave Fresnel coefficients.

DY 69.16 Thu 15:30 Poster A

Optical microcavities for nanoparticle sensing — •Jakob Kreismann and Martina Hentschel — Technische Universität Ilmenau, Institut für Physik, Weimarer Str. 25, 98693 Ilmenau

Optical microcavties play an important role in nanophoptonic innovations and applications. Detection of nanoparticles or even single molecules is already a feasible method, for example by employing the resonant frequency shift due to the interaction of the particles with the evanescent field of a whispering gallery mode confined in a micro toroid or a micro sphere resonator. Usually these devices are designed to detect particles that attach on the side wall of the resonator. Here, we investigate a sensing method where particles can attach on the top surface, thereby overcoming the drawback of the small area of the side surface. We compare various, regular and chaotic, cavity geometries. The chaotic dynamics of the Limacon-shaped resonator are crucial to realize a broad field distribution along the top surface[1]. We perform three dimensional FDTD calculations to optimize the geometry by increasing the sensitive area surrounded by the evanescent field and characterize the sensing properties.

[1] J. Kreismann, S. Sinzinger, and M. Hentschel, Phys. Rev. A 95, 011801(R) (2017).

DY 69.17 Thu 15:30 Poster A

Power-law trapping in the volume-preserving Arnold-Beltrami-Childress map — •Swetamber Das[1] and Arnd Baeker[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]TU Dresden, Institut für Theoretische Physik, Dresden

While stickiness and power-law behavior of Poincaré recurrence statistics for two degree-of-freedom systems is well-understood, this remains to be an open problem for higher-dimensional systems. We study such trapping in the Arnold-Beltrami-Childress map which is an example of a three-dimensional volume-preserving system. If two action-like variables of the map are nearly conserved, the phase space displays tubular structures surrounded by a chaotic sea. Trapping occurs around these tubes and is investigated in phase space and frequency space to identify the underlying origin of stickiness and power-law trapping.

DY 69.18 Thu 15:30 Poster A

Mode spacing tuning analysis of a quantum-dash comb laser — •Patrick Fiala[1], Dominik Auth[1], Christoph Weber[1], Abderrahim Ramdane[2], and Stefan Breuer[1] — [1]Institut für Angewandte Physik, Technische Universität Darmstadt, Schlossgartenstraße 7, 64289 Darmstadt, Germany — [2]CNRS Centre for Nanosciences and Nanotechnologies, C2N, Route de Nozay, 91460 Marcoussis, France

Monolithic self-mode-locked (SML) semiconductor lasers (SCLs) based on Quantum Dashs (QDh) offer stable and broad optical mode combs with mode spacings in the Multi-GHz range. In this contribution, we investigate experimentally the impact of time-delayed optical self-feedback (OFB) on the comb spacing tunability of a single-section QDh comb laser. The influence of varying optical feedback strengths and optical feedback delays is validated experimentally and by adapting a stochastic time-domain model.

DY 70: Poster: Flows, Patterns, Delay, Reaction Diffusion

Time: Thursday 15:30–18:00 Location: Poster A

DY 70.1 Thu 15:30 Poster A

Does a wind turbine care about turbulent intermittency? — •Johannes Kruse[1], Bodil Carlsen[2], and Martin Greiner[2] — [1]Georg-August Universität Göttingen — [2]Department of Engineering, Aarhus University, Denmark

Wind turbines operate in the turbulent atmospheric boundary layer and are exposed to highly intermittent wind fluctuations. We aim to clarify whether a wind turbine cares about these strongly non-Gaussian, multi-fractal fluctuations. Wind time series from an offshore site reveal an enlarged correlation time which is significantly larger than the typical turbine response time. A simple relaxation model for the wind-to-power conversion is investigated to quantify how the intermittency in the wind affects the statistical properties of the turbine power output and how this depends on the response time as well as the dynamical noise of the wind turbine. It is found that in particular for offshore wind turbines the intermittency in the wind can have a significant effect on the fluctuations of the wind power generation time series.

DY 70.2 Thu 15:30 Poster A

Optimization of non-contact seals — •Sabine Bogner — Universität Ulm, Institut für Experimentelle Physik

The non-contact seal of interest provides a separation between an upper and a lower chamber that are connected by a shaft. In the lower chamber there is a hydraulic driving and therefore a lot of liquid is present in the chamber. The upper chamber is filled with air that must be kept clean from liquid. Thus, the seal in between the two chambers must on the one hand prevent the liquid in the bottom chamber from flowing to the upper chamber. On the other hand, it must be contact-free in order to prevent friction between the shaft and its surroundings so that it can rotate freely.

In its current state the sealing effect should be reached by a labyrinth like geometry of a partition wall that divides the two chambers in combination with a fan arranged below the partition wall.

To improve the seal the pressure ratios inside the system are measured for different rates of rotation with an experimental setup. Apart from that the path of the penetrating liquid is analyzed both in the system itself and with CFD simulations. Different geometries of the partition wall labyrinth and the leak fan are tested with respect to their influence on the stream of air and liquid.

DY 70.3 Thu 15:30 Poster A

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

We study the shape of a liquid meniscus and the transfer of a liquid film from a bath of Newtonian liquid onto a (moving) plate under the influence of a Rayleigh surface acoustic wave (SAW). This Landau-Levich-type problem is studied with a thin-film equation that combines SAW driving (employed in [1] for wetting liquid) with the standard dragged-film problem for partially wetting liquid [2] to account for SAW driving in the case of partially wetting liquids. We use numerical path-continuation methods [3] to obtain the pertinent bifurcation diagrams that allow us to discuss the occuring qualitative transitions. [1] M. Moronov and O. Manor. J., *Fluid Mech.*, 810:307–322, 2017; [2] M. Galvagno., D. Tseluiko, H. Lopez and U. Thiele, *Phys. Rev. Lett.*, 112:137803, 2014; [3] H. A. Dijkstra et al., *Comun. Comput. Phys.*, 15:1–45, 2014.

DY 70.4 Thu 15:30 Poster A

Rotating turbulent Rayleigh-Bérnard convection at very large Rayleigh numbers — •Marcel Wedi[1,2], Dennis van Gils[3], Stephan Weiss[2], Guenter Ahlers[4], and Eberhard Bodenschatz[2] — [1]Georg-August-Universität Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organisation, Germany — [3]Twente University, Enschede, The Netherlands — [4]University of

California, Santa Barbara, USA

Thermal convection in astro- and geophysical systems is both, highly turbulent and strongly influenced by Coriolis forces caused by the rotation of their celestial body. We aim to study the influence of rotation on the heat transport and the temperature field at very large thermal driving, in the High Pressure Convection Facility (HPCF) in Göttingen. The facility consists of a cylindrical cell with a diameter of 1.10 m and a height of 2.20 m that can be filled with pressurized sulfur hexafluoride (SF_6) of up to 19 bar. The height of the cell and the large density of SF_6 enable us to reach Ra up to 2×10^{15}. The cell is mounted on a rotating table and connected to the non-rotating world via water feed-throughs and slip rings. We can reach Ekman numbers down to 10^{-8} while still keeping the influence of centrifugal forces small. In our poster we show and discuss recent major upgrades of the facility as well as measurements of the heat flux and the temperature field.

DY 70.5 Thu 15:30 Poster A

Dynamics of wetting explored with inkjet printing — •Jonas Landgraf, Simeon Völkel, and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

Experiments on sessile drops require precise volume control. However, to control drop volume without altering the solid-liquid or liquid-gas interfaces is challenging. Here, we propose to use a conventional, low cost inkjet printhead to solve this challenge. Taking advantage of the high repeatability [1] and fine resolution of drop volume (23 picoliter), we investigate the dynamics of a sessile drop sitting on an inclined substrate. In addition, we explore the wetting front propagation in a granular monolayer.

[1] Völkel and Huang, EPJ Web of Conferences, 140, 09035 (2017)

DY 70.6 Thu 15:30 Poster A

Leidenfrost universality: an experimental study — •Olinka J. Ramírez Soto[1], Michiel A.J. van Limbeek[2], and Detlef Lohse[2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, D-37077 Göttingen, Germany — [2]Universiteit Twente, Drienerlolaan 5, 7522NB Enschede, The Netherlands

When a drop is deposited on a hot surface there is a minimum temperature, the Leidenfrost temperature (T_L), at which the drop levitates in its own vapor. The first detailed description of the phenomenon was given 300 years ago by the physicist J. G. Leidenfrost. Since then, a model describing the conditions at which this phenomenon happens has still to be addressed. Previous studies exhibited a linear relation between T_L and T_{sat} (saturation temperature) for a group of hydrocarbons. A similar behavior between the two temperatures for a single liquid at different ambient pressure conditions was also observed. In the present study, the relation between both temperatures was explored.

The Leidenfrost temperature of different organic liquids and water at low and high pressures was obtained by observing the behavior of drops at different surface temperatures. As a first result, a linear relationship was found between T_L and T_{sat} at low pressures for each liquid. For all liquids, these relation differs by a prefactor. From a dimensional analysis with phase transition variables, we defined the parameter $\frac{L}{C_{Pv}}$ to nondimensionalize both temperatures. The collapse of the experimental data with this parameter, including high pressure measurements, reveals the universality of the Leidenfrost temperature.

DY 70.7 Thu 15:30 Poster A

Magnetic wave calming — •Alexandra Fischer, Armin Kögel, and Reinhard Richter — Experimentalphysik 5, Universität Bayreuth, Germany

One of the most prominent hydrodynamic instabilities in nature is the Kelvin-Helmholtz instability [1]: Wind blowing over water causes surface waves, if a critical velocity is surpassed. Here we demonstrate for the first time, that the magnetic susceptibility of a ferrofluid can be exploited in order to calm the waves by applying a magnetic field parallel to the surface. We measure the spatial growth rate, the critical velocity depending on the frequency of the interfacial wave, and the dispersion relation while varying the magnetic field strength. Finally we compare our values to the non viscous theory as put forward by Rosensweig [2].

[1] Hermann v. Helmholtz, Über discontinuierliche Flüssigkeitsbewegungen. *Berl. Ber.* p. 215. (1868).

[2] Ronald E. Rosensweig, *Ferrohydrodynamics* Cambridge University Press, Cambridge (1985).

DY 70.8 Thu 15:30 Poster A

Slip-mediated dewetting of polymer microdroplets — •Joshua McGraw[1,2], Tak Shing Chan[1], Thomas Salez[3], Simon Maurer[1], Michael Benzaquen[3], Elie Raphaël[3], Ralf Seemann[1], Martin Brinkmann[1], and Karin Jacobs[1,4] — [1]Experimental Physics, Saarland University, 66041 Saarbrücken, Germany — [2]Département de Physique, Ecole Normale Supérieure/ Paris Sciences et Lettres (PSL) Research University, CNRS, 75005 Paris, France — [3]Laboratoire de Physico-Chimie Théorique, UMR Gulliver 7083, Ecole Supérieure de Physique et de Chimie Industrielles ParisTech/PSL Research University, 75005 Paris, France — [4]fLeibniz-Institute for New Materials, 66123 Saarbrücken, Germany

Classical hydrodynamic models predict that infinite work is required to move a three-phase contact line. Assuming a slip boundary condition, in which the liquid slides against the solid, such an unphysical prediction is avoided. Here, we present the results of experiments in which a contact line moves and where slip is a dominating and controllable factor. Spherical cap-shaped polystyrene microdroplets, with nonequilibrium contact angle, are placed on solid self-assembled monolayer coatings from which they dewet. The relaxation is monitored using in situ atomic force microscopy. We find that slip has a strong influence on the droplet evolutions, both on the transient nonspherical shapes and contact line dynamics. The observations are in agreement with scaling analysis and boundary element numerical integration of the governing Stokes equations, including a Navier slip boundary condition.

DY 70.9 Thu 15:30 Poster A

Using the Saffman effect to opitmally control colloidal trajectories in inertial microfluidics — •Felix Rühle[1], Christian Schaaf[1], Fredi Tröltzsch[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin — [2]Institut für Mathematik, TU Berlin, Straße des 17. Juni 136, 10623 Berlin

Inertial microfluidics is used for particle sorting and separation in biomedical applications [1]. Here, fluid inertia at intermediate Reynolds numbers drives cross-streamline migration of colloidal particles under Poiseuille flow and eventually lets them reach lateral steady state positions. These stable positions are determined by stable fixed points in the lateral lift-force profiles and can be controlled via the Saffman effect by applying axial forces [2-4].

We determine the lateral lift-force profiles for different external axial forces using lattice Boltzmann simulations [4]. We then interpret this axial force as a control term [4] and use optimal control theory to numerically determine optimal, time-dependent forces in order to steer particles with variable sizes to target positions in a microchannel. We provide the proof of principle that this is indeed possible.

[1] D. Di Carlo, *Lab Chip* **9**, 3038 (2009).
[2] P.G. Saffman, *J. Fluid Mech.* **22**, 385 (1965).
[3] W.Y. Kim and J.Y. Yoo, *Lab Chip* **9**, 1043 (2009).
[4] C. Prohm and H. Stark, *Lab Chip* **14**, 2115 (2014).

DY 70.10 Thu 15:30 Poster A

Magnetophoretic Lab-on-a-Chip system for biomolecular interaction analysis — •Hai Hoang[1], Özge Efendi[2], Meike Reginka[1], Daniela Bertinetti[2], Dennis Holzinger[1], Friedrich W. Herberg[2], and Arno Ehresmann[1] — [1]Institute of Physics, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel — [2]Institute of Biology, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

Lab-on-a-Chip (LOC) systems are promising devices for point-of-care technologies in biomedicine. Using a microfluidic system in combination with a remotely controllable transportation system of functionalized superparamagnetic beads can increase the detection limit of biomarkers (e.g. proteins) in body fluids. In a first step, the green fluorescent protein (GFP) was used as a model protein. For the LOC approach superparamagnetic beads functionalized with a GFP-specific binder are used for directed transport of GFP and GFP accumulation whereby channel design, mixing of fluids by bead movement and flow speed of the GFP-solution perpendicular to the bead movement are taken into consideration. The investigation of the system is done via optical and fluorescence microscopy as well as tracking and image analysis techniques.

DY 70.11 Thu 15:30 Poster A

Adaptability of oxygen supply by vessel dilation — •Felix J. Meigel[1], Peter Cha[2], Michael P. Brenner[2], and Karen Alim[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Harvard University, Cambridge, MA, U.S.A.

Organs in mammals are pervaded by a vascular network, supplying the tissue with oxygen. In the brain, capillaries built a highly interconnected mesh each equipped with small muscles allowing for the constriction and dilation of capillaries. How much control of oxygen supply resides in the active adaptation of capillary diameter? Here, we build a theoretical model for oxygen transport and absorption in a capillary and determine how capillary geometry and network topology affect the control by active adaptation. On the level of an individual capillary, we derive analytically how vessel parameters affect the local change in oxygen supply due to dilation. Within the model we identify a regime of more than linear increase in supply, which we locate in the vasculature of recorded data of a rat brain excerpt. Extending our model to an entire network we statistically quantify the impact of network architecture on changes in supply profiles.

DY 70.12 Thu 15:30 Poster A

Multiple-relaxation-time lattice Boltzmann implementation for shear thinning fluids — •Sebastian Johannes Müller and Stephan Gekle — Juniorprofessur Theoretische Physik, Universität Bayreuth

An important aspect of biofabrication processes is the shear thinning behaviour of polymer solutions used as bioinks. It becomes particularly important considering the forces acting on the flowing cells and the cell deformations during the printing procedure. As the lattice Boltzmann method is a common approach to computational fluid dynamics, we use a multiple-relaxation-time model to implement different models for non-Newtonian fluids in the simulation package ESPResSo. The simplest model, allowing comparison of the simulation results with analytical flow results, is the power-law model for the fluid viscosity. We extend our simulations with enhanced models for non-Newtonian fluids, like the Carreau-Yasuda and the Cross model, which include Newtonian behaviour in the limits of zero and infinite shear-rate.

DY 70.13 Thu 15:30 Poster A

Propulsion and hydrodynamic particle transport of a magnetically driven colloidal ribbon — •Helena Massana-Cid[1], Fernando Martinez-Pedrero[2], Eloy Navarro-Argemí[1,3], Ignacio Pagonabarraga[1,3], and Pietro Tierno[1,3,4] — [1]Departament de Física de la Matèria Condensada, Universitat de Barcelona, E-08028, Barcelona, Spain — [2]Departamento de Química Física I, Universidad Complutense de Madrid, Ciudad Universitaria, E-28040, Madrid, Spain — [3]Universitat de Barcelona Institute of Complex Systems (UBICS), Universitat de Barcelona, E-08028, Barcelona, Spain — [4]Institut de Nanociència i Nanotecnologia, IN2UB, Universitat de Barcelona, E-08028, Barcelona, Spain

We describe a method to trap, transport and release microscopic particles in a viscous fluid using the hydrodynamic flow field generated by a magnetically driven colloidal ribbon. The ribbon is composed by ferromagnetic microellipsoids that assemble perpendicular to each other due to their permanent magnetic moment. We use an external precessing magnetic field to torque the anisotropic particles forming this structure, and the particle rotational motion is rectified into a net translation due to the hydrodynamic coupling with the surface. Non-magnetic particles can be captured or expelled by the hydrodynamic flow field generated by the propelling ribbon. The proposed technique may be used in channel-free microfluidic applications, where precise trapping and transport of functionalized particles via non invasive magnetic fields is required.

DY 70.14 Thu 15:30 Poster A

Does a vesicle migrate to the center or to the periphery in a bounded shear flow? — •Abdessamad Nait Ouhra[1,2], Alexander Farutin[1], Hamid Ez-Zahraouy[2], Abdelilah Benyoussef[3], and Chaouqi Misbah[1] — [1]Grenoble Alpes University, CNRS, LIPhy, Grenoble, France — [2]Mohammed V University, Rabat, Morocco — [3]Hassan II Academy of Science and Technology, Rabat, Morocco

The lateral migration of a suspended vesicle (a model of red blood cells (RBCs)) in a bounded shear flow is investigated numerically at vanishing Reynolds number (the Stokes limit) using a boundary integral method. We explore the relevant dimensionless parameters to study the dynamics and rheology of a vesicle as a function of the viscosity contrast $\lambda = \eta_{in}/\eta_{out}$, where η_{in}, η_{out} denote the inner and the outer viscosities. A vesicle is found to migrate to the centerline or to the wall depending on λ. We found that below a critical viscosity contrast λ_c, the vesicle is centered, and above λ_c, the vesicle can be either centered or off-center depending on initial condition. The equilibrium lateral position of the vesicle exhibits a saddle-node bifurcation as a function of the bifurcation parameter λ, which leads to a surprising acute decrease of the effective viscosity of the suspension at a critical value of viscosity contrast (λ_c). This study can be exploited in the problem of cell sorting out and can help understanding the intricate nature of the rheology of confined suspensions.

DY 70.15 Thu 15:30 Poster A

Nonlinear analysis of coupled dissipative system with a conservation law — •Tobias Frohoff-Hülsmann[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

We investigate the coupled dynamics of a conserved and a non-conserved order parameter field using the generic example of a Cahn-Hilliard equation that is coupled to a Swift-Hohenberg equation. Both equations correspond to gradient dynamics and, here, we employ a coupling that preserves the variational structure. The coupled system is effectively of 8th order and allows for individual and coupled short-scale and long-scale instabilities. We analytically examine the linear and weakly nonlinear behaviour and study the fully nonlinear bifurcation behaviour employing numerical path continuation. The nonlinear results are compared to the results gained with amplitude equations of first and higher orders obtained in the weakly nonlinear limit.

DY 70.16 Thu 15:30 Poster A

Modeling Structure Formation of Twin Polymerization via a reactive Bond Fluctuation Model — •Janett Prehl, Constantin Huster, and Halit Taskin — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

Understanding the structure formation of new chemical processes is a big challenge for the development of new materials as for instance in the case of Twin Polymerisation (TP). The TP is a chemical method to synthesize interesting nano-porous hybrid materials with organic and inorganic domains in the range of 0.5 up to 3nm for further industrial applications.
In order to obtain the key mechanisms of structure formation processes of TP the reactive bond fluctuation model (rBFM) [1] is developed. In comparison to the classic BFM the rBFM can deal with multiple bond vectors instead of only 1 between the beads. The beads represent the monomers and the bond vector can form and cleave. Within reactive Monte Carlo steps of the rBFM the complex reaction mechanism of TP is defined. By doing so, resulting structural properties as for example the amount of bonds per particle (BpP) or the radial distribution function (RDF) are compared with experimental data.
This comparison will help us to find correlations between the structure formation process and morphological properties of emerging materials.
[1] K.H.Hoffmann, J.Prehl, *Reac Kinet Mech Cat* DOI: 10.1007/s11144-017-1303-y

DY 70.17 Thu 15:30 Poster A

Orientation of stripe patterns in small rectangular domains — •Mirko Ruppert, Fabian Bergmann, Lisa Rapp, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, Deutschland

Motivated by recent observations of pattern formation in small systems, we investigate the orientation of nonlinear stripe patterns in small, rectangular domains for different boundary conditions along the domain borders. In addition the orientation of stripe patterns is investigated, when the control parameter is only supercritical in a small domain. We characterize, how the orientation of stripe patterns depends on the aspect ratio G between the length and the width of a domain. We find stable coexistence between stripe pattern of different wavelength and orientations. Orientational transitions take place at different values of G for different boundary condtions as well as in the case of control-parameter variations. This is investigaged by analytical considerations and numerical solutions of the generic Swift-Hohenberg-model.

DY 70.18 Thu 15:30 Poster A

Traveling waves in a chemorepulsive active particle system — •Samuel Grimm, Fabian Bergmann, Lisa Rapp, and Walter

Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

A chemorepulsive active particle system may give rise to a bifurcation to spatially periodic traveling waves (TWs), whereby the density of active particles is conserved. Traveling waves in conserved systems show modified nonlinear dynamics compared to TWs in unconserved systems. The envelopes of these TWs also obey different generic model equations. We compare simulations of the continuum equations for the active particle systems to simulations of reduced generic equations. This comparison allows for the identification of generic properties of TWs in a chemorepulsive active particle system.

DY 70.19 Thu 15:30 Poster A

Oscillatory phase separation in active particle systems — •Andre Förtsch, Lisa Rapp, Fabian Bergmann, and Walter Zimmermann — University of Bayreuth, Bayreuth, Germany

We introduce a model with two types of interacting active particle A and B. We assume A-A attraction, A-B attraction and B-B repulsion. The continuum approximation corresponds to two chemotactically interacting species. This continuum model shows an oscillatory instability. Since the two particle types are conserved, this oscillatory instability leads to oscillatory phase separation. Particle simulations leads to the same scenario. Above the oscillatory onset of phase separation we find traveling clusters in simulations.

DY 70.20 Thu 15:30 Poster A

Stability and Coexistence of Vegetation Patterns in a Reduced Model — •Florian Dietl[1], Fabian Bergmann[1], Lisa Rapp[1], Ehud Meron[2], and Walter Zimmermann[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth — [2]Blaustein Institutes for Desert Research, Ben Gurion University

We analyze a reduced normal form of a vegetation model for water-limited ecosystems [1]. The model has both finite amplitude homogeneous and spatially periodic solutions, as well as superpositions of the different solutions. We investigate the elementary bifurcations between these states in terms of four coupled, spatially independent nonlinear equations, which are obtained from the original model by a Galerkin-truncation. Among other phenomena, we find for the four coupled equations a transition between a homogeneous vegetation state and a hexagonally modulated state. This and other transitions are characterized and analyzed. We also show that the solutions and bifurcations obtained from the four coupled equations agree over a wide range of parameters with the solutions of the full vegetation model.

[1] E. Gilad et al., J. Theor. Biol. 244, 680 (2007)

DY 70.21 Thu 15:30 Poster A

Time-delayed feedback control of oscillatory states in sheared micellar systems — •Benjamin von Lospichl and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

We investigate a rheological model for the shear stress [1], which is suitable to describe the dynamics of elongated micelles under shear. Within the model a link between a structural variable, namely the micellar length, and the mechanical variables (stress and shear rate) is made. Through this connection it is possible to find a great variety of dynamical states ranging from steady shear banding to spatio-temporal oscillatory and chaotic states. To explore the phase space of the model we employ concepts of linear stability analysis and solve the dynamical system numerically in space and time using a Crank-Nicolson algorithm. A key feature of this model is the appearance of a Hopf bifurcation separating a spatio-temporal oscillatory region from a homogeneous region. Motivated by experiments [2], we explore possibilities to manipulate the oscillatory states by applying time-delayed feedback control (TDFC) such that they become stationary. The TDFC is introduced via a Pyragas scheme [3].

[1] S.M. Fielding and P.D. Olmsted, *Phys. Rev. Lett.* **92**, 084502 (2004).

[2] O. Lüthje *et al.*, *Phys. Rev. Lett.* **86**, 1745 (2001).

[3] K. Pyragas, *Phys. Lett. A* **170**, 421 (1992).

DY 70.22 Thu 15:30 Poster A

Delayed feedback control of self-mobile cavity solitons in a wide-aperture laser with a saturable absorber — •Tobias Schemmelmann[1], Felix Tabbert[1], Alexander Pimenov[2], Andrei Vladimirov[2], and Svetlana Gurevich[1,3] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149, Münster, Germany — [2]Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39, D-10117 Berlin, Germany — [3]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstr. 2, 48149 Münster, Germany

We investigate the spatiotemporal dynamics of cavity solitons in a broad area vertical-cavity surface-emitting laser (VCSEL) under the influence of time-delayed optical feedback using a combination of analytical, numerical and path continuation methods. In particular, two types of moving cavity solitons are found, corresponding to slow and fast motion of the localised structure. We show that time-delayed feedback influences the dynamics of both stationary and moving cavity solitons, leading to a complex dynamical behaviour. The delay-induced instabilities range from simple drifting to wiggling dynamics and a combination of both. In addition, our analysis reveals that it is possible to use time-delayed feedback to stabilise intrinsically drifting cavity solitons.

DY 70.23 Thu 15:30 Poster A

Spatiotemporal instabilities of light bullets in passively-mode-locked lasers — •Frederik Edens[1], Julien Javaloyes[2], and Svetlana Gurevich[1] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany — [2]Departament de Física, Universitat de les Illes Balears, C/ Valldemossa km 7.5, 07122 Mallorca, Spain

Recently, the existence of robust three-dimensional light bullets was predicted theoretically in the output of a laser coupled to a distant saturable absorber. We use a generic model of mode-locking that consists in a time-delayed dynamical system, and describe the passively mode-locked laser using the generic Haus partial differential equation. We analyze the stability and the range of existence of these dissipative localized structures in the uniform-field limit and provide guidelines and realistic parameter sets for their experimental observation. We conclude our analysis by the study of the influence of group velocity dispersion on the stability properties of light bullets and show that it may have a profound impact on their dynamics.

DY 70.24 Thu 15:30 Poster A

Modeling of the Chemotatic Response of Amoeboid Cells with a Phase Field Model — •Eduardo Moreno[1], Francesc Font[1], Carsten Beta[2], and Sergio Alonso[1] — [1]Department of Physics, Universitat Politecnica de Catalunya, Barcelona, Spain — [2]Institute of Physics and Astronomy, Universität Potsdam, Potsdam, Germany

Cells are able to polarize and move following gradients of chemical concentrations. The receptors of the cells induce an internal signal which produce the formation of localized regions of the cell with high concentrations of certain biochemicals which drive the locomotion of cells. We apply a phase field for the description of the interior (where the polarization processes evolve) and the exterior of the cells (where the chemicals diffuse) to model the two types of dynamics and the interaction of both environments at the membrane of the cell. We compare the resulting dynamics of the computer models with experiments of the motion of Dictyostelium discoideum following chemical gradients of the chemo-attractant cAMP (cyclic adenosine monophosphate).

DY 70.25 Thu 15:30 Poster A

Diffusion-influenced bimolecular reactions: Beyond the classical Langmuir-Hinshelwood theory — •Yi-Chen Lin[1,2], Won Kyu Kim[1], Rafael Roa[1], and Joachim Dzubiella[1,2] — [1]Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

The study of the Langmuir-Hinshelwood (LH) reaction mechanism is essential to understand bimolecular catalytic reactions [1]. Nevertheless, the classical theory of the LH reaction is restricted in the limit of the surface-controlled case, while the diffusion-controlled limit can be analyzed within the Smoluchowski theory of diffusion [2]. In other words, the coupling of 2D (on the surface) and 3D (in the bulk) diffusion of reactants is neglected. We present a Brownian dynamics simulation model for the diffusion-influenced LH reaction. The effects of the interaction strength ϵ between the sink and the reactants, of the 2D diffusion and of the crowding of the products on the total rates are investigated under the framework of this simulation model. One of the interesting findings is that the monotonicity of the total rate with the increase of ϵ disappears when the crowding of the products is present. The simulations results exemplify a theory, which we also present in

this work on a mean-field level.

[1] Laidler, K. J., Meiser, J. H., and Sanctuary, B. C. *Physical Chemistry*, 4th ed; Houghton Mifflin: Boston, 2002.
[2] Smoluchowski, M. v. *Physik. Z.* **1916**, 17, 557-585.

DY 71: Poster: Noneq. Stat. Phys., Stoch. Thermo, Brownian Dyn.

Time: Thursday 15:30–18:00 Location: Poster A

DY 71.1 Thu 15:30 Poster A

Non-stationary Generalized Langevin Equation for the Crystallization Process — •Philipp Pelagejcev[1], Thomas Voigtmann[3,4], Hugues Meyer[1,2], and Tanja Schilling[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Research Unit in Engineering Science, Université du Luxembourg, L-4364 Esch-sur-Alzette, Luxembourg — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [4]Department of Physics, Heinrich Heine University, Universitätsstraße 1, 40225 Düsseldorf, Germany

We study crystallization from an undercooled melt in the context of non-equilibrium statistical physics. We have recently derived an equation of motion for an averaged observable over a bundle of system trajectories by means of time-dependent projection operator techniques. Here we apply this technique to the analysis of simulation trajectories.

We observed the crystallization process of an undercooled fluid of Lennard Jones particles in a Molecular Dynamics Simulation under constant temperature (where the heat bath is realised with a Nosé-Hoover thermostat). From the sampled size of the largest crystalline cluster in the system, we construct the memory kernel of the Generalized Langevin Equation. We observe significant memory effects, i.e. the process is not described well by a Markovian approximation.

DY 71.2 Thu 15:30 Poster A

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

Systems with hidden degrees of freedom are a common occurrence within the field of stochastic thermodynamics. Because the full dynamics are not accessible in these setups, the total entropy production cannot be measured. Nevertheless, coarse-graining allows one to define an apparent entropy production. Usually this quantity does not fulfill fluctuation theorems of the usual type [1].

We present a simple model for which we can analytically calculate the fluctuation theorems involving the apparent entropy production. For this model we discuss the role of the strength of the coupling between the hidden and observed degrees of freedom and the limit of time-scale separation between them. Our model also serves as a case study on thermodynamic inference.

[1] J. Mehl, B. Lander, C. Bechinger, V. Blickle, and U. Seifert, Phys. Rev. Lett. **108**, 220601 (2012)

DY 71.3 Thu 15:30 Poster A

A minimal model of an autonomous thermal motor — Hans Fogedby and •Alberto Imparato — Department of Physics and Astronomy, Aarhus University, Ny Munkegade, Building 1520 DK-8000 Aarhus C, Denmark

We consider a model of a Brownian motor composed of two coupled overdamped degrees of freedom moving in periodic potentials and driven by two heat reservoirs. This model exhibits a spontaneous breaking of symmetry and gives rise to directed transport in the case of a non-vanishing interparticle interaction strength. For strong coupling between the particles we derive an expression for the propagation velocity valid for arbitrary periodic potentials. In the limit of strong coupling the model is equivalent to the Büttiker-Landauer model for a single particle diffusing in an environment with position dependent temperature. By using numerical calculations of the Fokker-Planck equation and simulations of the Langevin equations we study the model for arbitrary coupling, retrieving many features of the strong coupling limit. In particular, directed transport emerges even for symmetric potentials. For distinct heat reservoirs the heat currents are well-defined quantities allowing a study of the motor efficiency. We show that the optimal working regime occurs for moderate coupling. Finally, we introduce a model with discrete phase space which captures the essential features of the continuous model, can be solved in the limit of weak coupling, and exhibits a larger efficiency than the continuous counterpart.

DY 71.4 Thu 15:30 Poster A

Transitions between superstatistical regimes: validity, breakdown and applications — Petr Jizba[1,2], •Jan Korbel[3,1], Hynek Lavicka[4,5], Martin Proks[1], Vaclav Svoboda[1], and Christian Beck[6] — [1]Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Czech Republic — [2]Institute of Theoretical Physics, Freie Universitaet Berlin, Germany — [3]Department of Physics, Zhejiang University, Hangzhou, P. R. China — [4]Alten Belgium N.V., Brussels, Belgium — [5]Department of Institutional, Environmental and Experimental Economics, University of Economics in Prague, Czech Republic — [6]School of Mathematical Sciences, Queen Mary, University of London, United Kingdom

Superstatistics is a widely employed tool of non-equilibrium statistical physics which plays an important role in analysis of hierarchical complex dynamical systems. Yet, its "canonical" formulation in terms of a single parameter is often too restrictive when applied to complex empirical data. Here we show that a multi-scale generalization of the superstatistics paradigm is more versatile, allowing to address such pertinent issues as transmutation of statistics or inter-scale stochastic behavior [1]. To put some flesh on the bare bones, we provide a numerical evidence for a transition between two superstatistics regimes, by analyzing high-frequency (minute-tick) data for share-price returns of seven selected companies. Salient issues, such as breakdown of superstatistics in fractional diffusion processes or connection with Brownian subordination are also briefly discussed. [1] P.Jizba, J. Korbel, H. Lavicka, M. Proks, V. Svoboda, and C. Beck, Physica A 493, 29-46 (2018)

DY 71.5 Thu 15:30 Poster A

Extreme values of entropy production in an electronic double dot — •Shilpi Singh[1], Edgar Roldan[2], Izaak Neri[2], Ivan Khaymovich[2], Dmitry Golubev[1], Ville Maisi[1], Joonas Peltonen[1], Frank Julicher[2], and Jukka Pekola[1] — [1]Department of Applied Physics, Aalto University, 00076 Aalto, Finland — [2]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Strasse 38, 01187 Dresden, Germany

The second law of thermodynamics implies that in mesoscopic systems entropy increases on average but leaves open the possibility for these systems to transiently absorb heat from their environment when driven out of equilibrium. Fluctuation relations relate the probability to dissipate a certain amount of heat and to absorb the same amount of heat during a fixed time interval and have been confirmed in experiments. Extreme-value statistics of thermodynamic fluxes characterize the most extreme deviations from the average behaviors. Here we report on the experimental measurement of stochastic entropy production and of records of negative entropy in a metallic double dot under a constant external bias to realize nonequilibrium steady state. We find that the cumulative distribution of entropy production's negative record and the mean value at all times obey the infimum law presented in [PRX 7, 011019]. Our work provides general bounds and equalities for the extreme-value statistics of correlated random variables about which not much is known. This may help to understand the statistics of overheating events in single-electronic devices which are relevant for the design of reversible computers near Landauer's limit.

DY 71.6 Thu 15:30 Poster A

Collective power: Minimal model for thermodynamics of nonequilibrium phase transitions — •Tim Herpich, Juzar Thingna, and Massimiliano Esposito — Complex Systems and Statistical Mechanics, Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We establish a direct connection between the linear stochastic dynamics, the nonlinear mean-field dynamics, and the thermodynamic description of a minimal model of driven and interacting discrete oscillators. These exhibit at the mean-field level two bifurcations separating three phases: a single stable fixed point, a stable limit cycle

indicative of synchronization, and multiple stable fixed points. The apparent contradiction with the underlying linear Markovian dynamics which ensures convergence to a unique steady state is resolved via metastability, i.e. the appearance of gaps in the upper real part of the spectrum of the Markov generator. The dissipated work of the stochastic dynamics exhibit signatures of nonequilibrium phase transitions over long metastable times which disappear in the infinite-time limit. Remarkably, it is also reduced by attractive interactions between oscillators. When operating as a work-to-work converter we study the power output and efficiency of our device in the presence of nonequilibrium phase transitions. We find that the maximum power output is achieved far-from-equilibrium in the synchronization regime and that the efficiency at maximum power is surprisingly close to the universal linear regime prediction. Our work builds bridges between thermodynamics of nonequilibrium phase transitions and bifurcation theory.

DY 71.7 Thu 15:30 Poster A

Quantum heat engines and laser cooling: Floquet theory beyond the Born-Markov approximation — •Sebastian Restrepo[1], Javier Cerrillo[1], Philipp Strasberg[2], and Gernot Schaller[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Complex Systems and Statistical Mechanics, University of Luxembourg, Luxembourg

We combine the formalism of Floquet theory, full counting statistics and a collective coordinate mapping to access the dynamics and thermodynamics of a periodically driven thermal machine beyond the conventional Born-Markov approximation. We identify a collective degree of freedom in the reservoir that is included as part of the original system and that is responsible for the strong coupling and non-Markovian effects. The periodicity of our model is exploited using Floquet theory to obtain a master equation for the newly defined supersystem with full counting statistics methods permitting a thermodynamic analysis. The formalism is applied to a thermal machine consisting of a driven two-level system coupled to two reservoirs at different temperatures with one of the couplings considered time-dependent. In the weak coupling non-Markovian regime the thermal machine can act either as a heat engine or a refrigerator. As the coupling is increased, we identify four different operation regimes and see the eventual disappearing of the refrigerator. We observe that the efficiency and coefficient of performance decrease for stronger couplings. Taking the limit of a single reservoir, our model is able to replicate the setup of state preparation in laser cooling of trapped ions.

DY 71.8 Thu 15:30 Poster A

Application of a Jump-Diffusion Model to Solid-Liquid Interfaces in Ionic Liquids — •Mario Udo Gaimann[1], Andreas Baer[1], Nataša Vučemilović-Alagić[1,2], Ana-Sunčana Smith[1,2], and David Matthew Smith[2,3] — [1]PULS Group at the Institute for Theoretical Physics I and EAM, FAU Erlangen-Nürnberg, Germany — [2]Division of Physical Chemistry, Institute Ruđer Bošcović Zagreb, Croatia — [3]Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Ionic liquids possess a range of tunable properties, such as conductivity and low melting points [1]. These properties are desirable for a broad range of applications, most prominently catalysis at solid-liquid interfaces. Ions in vicinity of these interfaces show patterned or layered adsorption. To understand particle movements in and across layers found in these systems, we employ molecular dynamics to study a confined, periodic sample system consisting of hydroxylated sapphire as well as $[C_2Mim]^+$ cations and $[NTf_2]^-$ anions. Common mean-square displacement approaches inherently predict ions' diffusion tensors as a function of location within the pattern incorrectly, as the diffusive limit can not be reached for small displacements. To resolve this problem, we apply a jump-diffusion model as proposed by Liu *et al.* [2], based on introducing virtual boundaries and solving the Smoluchowski equation within these virtual slabs. We then determine the transport coefficients as a function of the distance from the sapphire.

[1] Rogers R D and Seddon K R 2003 *Science* **302** 5646
[2] Liu P, Harder E and Berne B J 2004 *J. Phys. Chem.* B **108** 21

DY 71.9 Thu 15:30 Poster A

Hot Brownian Motion on Short Time Scales — •Alexander Fischer and Frank Cichos — Molecular Nanophotonics, Peter-Debye-Institute, Universität Leipzig

Hot Brownian motion describes the motion of a heated microsphere in a liquid. It is a fundamental issue for thermal non-equilibrium. A temperature field is created around the heated particle decaying with 1/r and a stationary temperature and viscosity field is moving with the particle through the liquid. The non-equilibrium dynamics of the particle now differs from the unheated particles and an effective temperature and viscosity is introduced to describe the system. Here we report on a study of the fluctuations of a heated particle in an optical trap with nanosecond and nanometer resolution. We achieved to measure the accelerated motion and from that the temperature increase of our particles. The first evidence of the changing characteristic time constants on short time scales was detected.

DY 71.10 Thu 15:30 Poster A

Thermophoresis of Charged Colloids in Electrolyte Solutions — •Martin Fränzl and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

In the last decades thermophoresis of colloids was mainly discussed in terms of thermoosmotic pressure. However, in the recent years it has become clear that, for charged systems in an electrolyte solution the thermoelectric or Seebeck effect may provide an additional non-local driving force. In a non-uniform temperature, positive and negative ions, dissolved in water, have the tendency to migrate towards colder regions. However, in general one of the ion species is moving more rapidly, resulting in a thermoelectric field between the hot and the cold boundary. This field can drive charged colloids to the hot or to the cold, depending on the sign of the electrolyte Seebeck coefficient. The present work investigates the thermoelectric effects by locally heating a gold film with a focused laser beam within a colloidal suspension and discusses the resulting colloidal transport.

DY 71.11 Thu 15:30 Poster A

The Lattice Model of Crowding and Trapping in Line with Experiments in Model Membranes — •Mislav Cvitković[1], Marius Glogger[2], Markus Engstler[2], Susanne Fenz[2], and Ana-Sunčana Smith[3] — [1]Ruđer Bošković Institute, Division of Physical Chemistry, CLS Group, Zagreb, Croatia — [2]Universität Würzburg, Biocenter: Department of Cell and Developmental Biology, Germany — [3]FAU Erlangen–Nürnberg, Institute for Theoretical Physics, PULS Group, Germany

Lateral diffusion of proteins in biological membranes is a fundamental process that is, in living cells, affected both by protein crowding and intermolecular interactions. To account for these effects, we use a 2D lattice gas of hard particles that interact with ensemble of randomly localized traps. We characterize the behaviour of the system on all time scales, and provide an explicit expression for the long time diffusion coefficient as a function of relevant system parameters. Furthermore, we analyse traces from single–molecule experiments on GPI–anchored Variant Surface Glycoproteins (VSGs) that were purified from *Trypanosoma brucei* and reconstituted into supported lipid bilayers. VSGs are found to occur in two conformations [Bartossek *et al.*, *Nature Microbiology* 2:1523 (2017)] and their obstructed diffusion in experiment is found to have similar features to those predicted by the lattice gas model in a broad range of concentrations of VSG.

DY 71.12 Thu 15:30 Poster A

Apparent superdiffusion in subdiffusive d-dimensional generalized Lévy walks — •Tony Albers and Günter Radons — Institut für Physik, Technische Universität Chemnitz, Germany

We investigate a generalized Lévy walk [1] type of motion in a d-dimensional space, where the velocities of the flights depend on the durations of the flights in a nonlinear, deterministic way. This model of anomalous diffusion is essentially characterized by two exponents determining the asymptotic decay of the distribution of flight durations and the nonlinear dependence of the flight velocities on the flight durations. We provide analytical results for the asymptotic time dependence of the ensemble-averaged and time-averaged squared displacement and the randomness of the latter characterized by the ergodicity breaking parameter. In this contribution, we focus on a certain region of the two-dimensional parameter space, where the ensemble-averaged squared displacement increases slower than linear (subdiffusion) whereas the time-averaged squared displacement increases faster than linear (superdiffusion). This new kind of ergodicity breaking is studied in detail.

[1] M. F. Shlesinger, B. J. West, and J. Klafter, Phys. Rev. Lett. **58** 1100 (1987)

DY 71.13 Thu 15:30 Poster A

Heterogeneous diffusion in comb-like structures — •Trifce Sandev[1,2,3], Alexander Schulz[4], Holger Kantz[4], and Alexander Iomin[5] — [1]Ss. Cyril and Methodius University in Skopje, Macedonia — [2]RSD, Skopje, Macedonia — [3]MANU, Skopje, Macedonia — [4]MPIPKS Dresden, Germany — [5]Technion, Haifa, Israel

We consider diffusion with a position dependent diffusion coefficient along a backbone in different comb and fractal grid structures. The comb structures consist of main channel (backbone) and trapping fingers. Diffusion along the backbone, which is chosen to be the x-direction, occurs only at $y = 0$, and the fingers play the role of traps. This is a particular example of geometrical traps, where a particle, moving along the backbone, can get trapped inside a finger of the comb, where it diffuses in the y-direction, until it returns by chance to the backbone. Such behaviour of the particle can be described in the framework of the continuous time random walk theory, where the returning probability scales similarly to $t^{-1/2}$, and the waiting times are distributed according $t^{-3/2}$. We present analytical results for the mean squared displacement for the power-law position dependent diffusion coefficient along the backbone. We observe various diffusion regimes, such as subdiffusion, superdiffusion, hyperdiffusion, as well as stochastic localization. Our analytical results are in a good agreement with the numerical analysis of this heterogeneous transport, obtained in the framework of the Langevin equations description [1].

[1] T. Sandev, A. Schulz, H. Kantz, and A. Iomin, Chaos Solitons & Fractals, DOI: 10.1016/j.chaos.2017.04.041 (2017).

DY 71.14 Thu 15:30 Poster A

Time- and ensemble-averages in evolving systems: Brownian particles exposed to random potentials — Jörg Bewerunge, •Florian Platten, Christoph Zunke, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Anomalous diffusion is a ubiquitous phenomenon in complex systems. It is often quantified using timeand ensemble-averages to improve statistics, although time averages represent a non-local measure in time and hence can be difficult to interpret. We present a detailed analysis of the influence of time- and ensemble-averages on dynamical quantities by investigating Brownian particles in a rough potential energy landscape (PEL). Initially, the particle ensemble is randomly distributed, but the occupancy of energy values evolves towards the equilibrium distribution. This relaxation manifests itself in the time evolution of time- and ensemble-averaged dynamical measures. Individual colloidal particles are exposed to a laser speckle pattern inducing a non-Gaussian roughness and are followed by optical microscopy. The relaxation depends on the degree of roughness of the PEL. It can be followed and quantified by the time- and ensemble-averaged mean squared displacement. Moreover, the heterogeneity of the dynamics is characterized using single-trajectory analysis. The results of this work are relevant for the correct interpretation of single-particle tracking experiments in general.

DY 71.15 Thu 15:30 Poster A

Statistical Distribution of the Area Inside Random Walks Which Return to Their Origin — •Vincent Sacksteder — Royal Holloway University of London

We study 2-D random walks, Levy flights, and Levy walks, using both analytical calculations and extensive Monte Carlo simulations. Counting only loops (walks which return to the origin), and examining the area A of these loops, we calculate the probability distribution of A. We find that the loop area distribution is proportional to the inverse of A for ordinary random walks and decreases more rapidly for Levy flights. The loop area distribution calculated here determines the quantum corrections to electrical conductivity in 2-D disordered systems, which are known as weak localization corrections.

DY 72: Poster: Stoch. and Nonl. Dy., Modeling, Compl. Sys.

Time: Thursday 15:30–18:00 Location: Poster A

DY 72.1 Thu 15:30 Poster A

Stochastic Kuramoto oscillators with discrete phase states — •David J. Jörg — Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom

We present a generalization of the Kuramoto phase oscillator model in which phases advance in discrete phase increments through Poisson processes, rendering both intrinsic oscillations and coupling inherently stochastic. We study the effects of phase discretization on the synchronization and precision properties of the coupled system both analytically and numerically. Remarkably, many key observables such as the steady-state synchrony and the quality of oscillations show distinct extrema while converging to the classical Kuramoto model in the limit of a continuous phase. The phase-discretized model provides a general framework for coupled oscillations in a Markov chain setting.

DY 72.2 Thu 15:30 Poster A

Analysis of stochastic bifurcations with phase portraits — •Marc Mendler, Johannes Falk, and Barbara Drossel — Technische Universität Darmstadt, Institut für Festkörperphysik

We propose a new method to obtain phase portraits for stochastic systems, which in many cases give a correct picture of the most likely states of the system. To this purpose, we start with the Fokker-Planck-Equation of a reaction network and separate the dynamics into a convection and a diffusion part. This allows us to draw stochastic phase portraits as vector plots of the convection part, which is also the determining equation for the extrema of the stationary probability density of the system. We apply this method to different example systems, for which the attractors of the deterministic and stochastic model version can differ from each other. We show that noise-induced bistability and oscillations are correctly reproduced in the stochastic phase portrait in these examples, as well as the bifurcations between them.

DY 72.3 Thu 15:30 Poster A

The influence of intrinsic noise on the dynamics of small gene regulation modules — •Lara Becker and Barbara Drossel — TU Darmstadt, Germany

We examine how the intrinsic stochasticity associated with small molecule numbers affects the dynamics of simple two-gene modules in gene regulatory networks. To this purpose, we model the module in terms of a set of chemical reactions for the involved mRNA and protein molecules. We compare the dynamics obtained from deterministic rate equations with the stochastic dynamics obtained from the Master equation. For the deterministic version, we use the generalized modelling approach, which is based on a linear stability analysis of fixed points, in order to obtain the stability diagram that shows the saddle-node and Hopf bifurcations of the system. For the stochastic system, we perform stochastic simulations using the Gillespie algorithm. We also perform various analytical studies of the stochastic system. On the one hand, we calculate the power spectral density of the fluctuations based on the Linear Noise Approximation and show that for the two-gene negative feedback loop oscillatory behaviour can occur for the stochastic model while it cannot for the deterministic model. Furthermore, we calculate stochastic phase portraits in order to explore the parameter range that shows bistability in the deterministic model.

DY 72.4 Thu 15:30 Poster A

Using Neural Networks to Obtain the Dynamics on the Normally Hyperbolic Invariant Manifold of Driven Systems — •Martin Tschöpe, Johannes Reiff, Robin Bardakcioglu, Matthias Feldmaier, Jörg Main, and Günter Wunner — Institut für Theoretische Physik 1 Universität Stuttgart, Deutschland

The semi-classical reaction dynamics in Transition State Theory (TST) for periodically driven systems has been solved numerically in the past. It has been shown that the reaction rate can be determined by integrating a large number of trajectories and analyzing phase space structures.

An alternative way to obtain a reaction rate for these systems might be to analyze the dynamics on the Normally Hyperbolic Invariant Manifold (NHIM) itself. This task is especially challenging, due to the critical properties of such trajectories. Our work will tackle this disadvantage by using neural networks as a tool to stabilize the numerical integration on the NHIM.

DY 72.5 Thu 15:30 Poster A

Dynamics and Phase Space Structure for Reactions with Multiple Saddles — •Johannes Reiff, Robin Bardakcioglu,

Martin Tschöpe, Matthias Feldmaier, Jörg Main, and Günter Wunner — 1. Institut für Theoretische Physik, Universität Stuttgart, Germany

In chemical and physical reactions with time-dependent potentials, an important task is to distinguish products from reactants. In Transition State Theory (TST), this task has been successfully tackled semi-classically for a single potential barrier using Dividing Surfaces (DSs) attached to Normally Hyperbolic Invariant Manifolds (NHIMs). However, when considering multiple time-dependent saddles, it is still unknown whether a recrossing-free dividing surface exists.

We use Lagrangian descriptors and variations thereof to analyze the phase space structure of such multi-saddle systems. In doing so, fractal-like structures are revealed which make the search for recrossing-free DSs and therefore time-dependent reaction rates more challenging.

DY 72.6 Thu 15:30 Poster A

On the dynamics of a periodically driven damped harmonic oscillator coupled to Ising spins — •Paul Zech and Günter Radons — Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

We aim at an understanding of the dynamical properties of a periodically driven damped harmonic oscillator coupled to a system showing complex hysteresis, such as a random field Ising model at zero temperature. In a first step we investigate a simplified model, the harmonic oscillator coupled to independent spins in quenched random local fields. The model is characterized by continuous (position, velocity, phase) and discrete (spin) degrees of freedom, which classifies it as a hybrid system. By applying established methods of dynamical systems theory and time series analysis, such as Poincaré sections, the determination of Kaplan-Yorke and box-counting dimensions, and by Fourier analysis, we show, how in this system chaos emerges. Furthermore we investigate the dynamical behavior of the system for an increasing number of spins. In doing so we are specifically interested in the behavior as the thermodynamic limit is approached. In this limit the system behaves like a driven harmonic oscillator with an additional nonlinear smooth external force, which means, that the hybrid character of the system vanishes.

DY 72.7 Thu 15:30 Poster A

Application of Closed Orbit Theory to Magnetoexcitons in Cuprous Oxide — •Jonathan Luft genannt Philipps, Jörg Main, and Günter Wunner — 1. Institut für Theoretische Physik, Universität Stuttgart, Germany

Highly excited excitons in cuprous oxide can be described as hydrogen-like Rydberg systems. As there are many semiclassical approaches for the description of the hydrogen atom, we want to apply the closed orbit theory to describe the excitons in cuprous oxide. In contrast to hydrogen atoms, describing these excitons is more challenging due to the underlying band structure. Via calculating the classical trajectories of these highly excited excitons and applying closed orbit theory, we are able to determine the semiclassical photoabsorption spectra. The resulting absorption spectra will be compared with experimental results.

DY 72.8 Thu 15:30 Poster A

Dynamics of asymmetrically coupled systems: averaging over qualitatively different systems? — •Domenic Wagner[1] and Jens Christian Claussen[2,1] — [1]INB, Universität zu Lübeck, Germany — [2]Computational Systems Biology, Jacobs University Bremen, Germany

Studying the dynamics of large coupled nonlinear systems with random interactions is a common approach to model the dynamics of a wide range of biological systems. One of the key parameters of stability has been identified in [1] as the asymmetry parameter of the coupling matrix. In [1| the Ljapunov exponent (of trajectories driven by a common noise source) has been investigated including averaging over many different coupling matrices, which however can belong to systems with qualitatively different phase spaces and attraction sets. We investigate specific of these cases including dynamics from evolutionary game theory and neural networks.

[1| L. Molgedey, J. Schuchhardt, H.G. Schuster, PRL 69, 3717 (1992)

DY 72.9 Thu 15:30 Poster A

Stochastic Differential Equations Driven by Deterministic Chaotic Maps: Analytic Solutions of the Perron-Frobenius Equation — •Griffin Williams and Christian Beck — School of Mathematical Sciences, Queen Mary University of London, Mile End Road, E1 4NS UK

We consider discrete-time dynamical systems systems with a linear relaxation dynamics that are driven by deterministic chaotic forces. By perturbative expansion in a small time scale parameter, we derive from the Perron-Frobenius equation the corrections to ordinary Fokker-Planck equations in leading order of the time scale separation parameter. We present analytic solutions to the equations for the example of driving forces generated by N-th order Chebychev maps. The leading order corrections are universal for $N \geq 4$ but different for $N = 2$ and $N = 3$. We also study diffusively coupled Chebychev maps as driving forces.

DY 72.10 Thu 15:30 Poster A

Driven soliton molecule vibrations: Real-time studies of nonlinear behavior — •Felix Kurtz[1], Daniel R. Solli[1,2], Georg Herink[3], and Claus Ropers[1] — [1]IV. Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Department of Electrical Engineering, University of California, Los Angeles, USA — [3]Experimental Physics III, University of Bayreuth, Germany

Many nonlinear systems exhibit solitons, localized excitations balanced by dispersion and nonlinearity, which also can bind together in so-called soliton molecules. Here, we study the behavior of soliton molecules in a mode-locked laser oscillator. By employing the time-stretch dispersive Fourier transform (TS-DFT), we experimentally access the previously hidden internal dynamics of soliton molecules, tracking their pulse separation and relative phase in real-time. A diverse set of dynamical trajectories is observed, including periodic oscillations of the pulse separation and relative phase [1]. Moreover, we actively drive internal vibrations over a range of frequencies and amplitudes. We identify internal resonances of the soliton molecules and detect higher harmonic and subharmonic responses.

[1] G. Herink, F. Kurtz, B. Jalali, D.R. Solli, C. Ropers, *Science* **356**, 50-54 (2017)

DY 72.11 Thu 15:30 Poster A

Magnetic Phenomena in Spiking Neural Networks — •Andreas Baumbach[1], Mihai Petrovici[1,2], Karlheinz Meier[1], and Johannes Schemmel[1] — [1]Heidelberg University, Kirchhoff Institut for Physics, Heidelberg, Germany — [2]University of Bern, Department of Physiology, Bern, Switzerland

Systems close to criticality are always of particular interest. The arguably simplest model known to exhibit critical phenomena is the Ising model for ferromagnetism. Recent work on spiking neural networks developed a description of these biologically inspired networks under poissonian noise input as a Boltzmann machine. As such a description is widely used in neuroscience to effectively describe biological models and data one would expect that all the phenomena known from statistical physics can also be observed in these systems.

This work investigates a simplified model, the Neuralsampling framework introduced by Buesing et al., which we modify to include exponentially decaying interactions (resembling biological interactions) in an Ising-like network. While the global properties, like the unordered phase in the infinite temperature limit and the ordered phase in the zero temperature limit, we show that the phase diagram of this model shows richer phenomena than the classical Ising model. For example it allows a system to pass through multiple phases, rather than only the unordered-ordered transition, while cooling down.

DY 72.12 Thu 15:30 Poster A

Chain and ladder models with two-body interactions and analytical ground states — Sourav Manna[1] and •Anne E. B. Nielsen[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany

We consider a family of spin-1/2 models with few-body, SU(2) invariant Hamiltonians and analytically known ground states related to the Haldane-Shastry (HS) wavefunction. The spins are placed on the surface of a cylinder, and the standard HS model is obtained by placing the spins with equal spacing in a circle around the cylinder. Here, we show that another interesting family of models with two-body exchange interactions is obtained if we instead place the spins along one or two lines parallel to the cylinder axis, giving rise to chain and ladder models, respectively. In this case, the circumference of the cylinder can be changed independently from the other length scales in the sys-

tem, and we use Monte Carlo simulations and analytical investigations to study how the circumference affects the properties of the models. If the circumference is large compared to the other length scales in the system, we find that the two legs of the ladder decouple into two chains with HS-like properties, and if the circumference is small compared to the other length scales the wavefunction reduces to a product of singlets

DY 72.13 Thu 15:30 Poster A

Constant pressure regime in hydraulic fracturing — •Anton Solovev[1,2] and Yuri Petrov[2,3] — [1]Center for Advancing Electronics Dresden cfaed, TU Dresden, Dresden, Germany — [2]St Petersburg State University, St Petersburg, Russia — [3]Institute of Problems of Mechanical Engineering of the RAS, St Petersburg, Russia

Hydraulic fracturing is a process of fracture development and propagating in a brittle medium as a result of pressurized fluid injection.

Our study is based on a one-dimensional local elastic model (the PKN model) in particle velocity formulation. We investigate how a non-stationary component of the influx function affects the hydrofracturing in an impermeable rock formation.

Further, we propose an influx function that results in almost constant maximum pressure inside the fracture. Typically in literature constanst influx is considered instead. However, it produces unbounded growth of pressure and therefore is not always suitable for describing a pumping engine working in a steady regime.

DY 72.14 Thu 15:30 Poster A

Optimal conditions for coupled geological carbon storage and enhanced oil recovery — •Pegah Shakeri[1,2] and Ghasem Zargar[2] — [1]Saarland University, Experimental Physics, Saarbrücken, Germany — [2]Petroleum University of Technology, Ahvaz, Iran

Utilization of anthropogenic carbon dioxide as an enhanced oil recovery agent has been introduced as a practical solution to compensate for the costs of carbon capture and geological storage by the revenues of the produced oil. A series of experimental laboratory work and simulation studies at the reservoir scale were conducted to examine the impact of several reservoir parameters (e.g. rock type, degree of heterogeneity, relative permeability hysteresis, etc.) and different flood schemes and design variables on the performance of coupled CO2 sequestration and enhanced oil recovery (EOR) process. The design of experiment method in conjunction with response surface methodology was employed for sensitivity analysis and optimization purpose. It was concluded that, in general, applying vertical injection and production wells for Water Alternative CO2 Gas injection (WAG) scheme under the miscible condition in less heterogeneous carbonate reservoirs with lower permeability contrast are the most satisfying combination for coupled CO2 sequestration and enhanced oil recovery. It was also observed that hysteresis plays a significant role in CO2 entrapment especially in alternating injection scenarios due to successive imbibition and drainage cycles occurring during the process. High saturation of trapped gas lowers oil relative permeability which leads to a better but slower oil sweep in the reservoir.

DY 72.15 Thu 15:30 Poster A

Local Riemannian geometry of model manifolds and its implications for practical parameter identifiability — •Daniel Lill[1], Jens Timmer[1,2], and Daniel Kaschek[1] — [1]Institute of Physics, Freiburg University — [2]BIOSS Centre for Biological Signaling Studies, Freiburg University

When dynamic models are fitted to time-resolved experimental data, parameter estimates can be poorly constrained albeit being identifiable in principle. This means that along certain paths in the parameter space, the negative log-likelihood does not exceed a given threshold but remains bounded. This so-called practical non-identifiability can only be detected by Monte Carlo sampling or systematic scanning by the profile likelihood method. In contrast, any method based on a Taylor expansion of the log-likelihood around the optimum, e.g., parameter uncertainty estimation by the Fisher Information Matrix, reveals no information about the boundedness at all.

We show that for some dynamic models the information about the bounds of the log-likelihood is already contained in the Christoffel symbols, which are computed from model sensitivities up to order two at the optimum. Assuming constant Christoffel symbols in the geodesic equation, approximate Riemannian Normal Coordinates are constructed. The new coordinates give rise to an approximative log-likelihood, featuring flat directions and bounds similar to that of the original log-likelihood.

DY 72.16 Thu 15:30 Poster A

Investigation of nanofiber mats by statistical examination of AFM images — •Tomasz Blachowicz[1], Tobias Böhm[2], and Andrea Ehrmann[2] — [1]Silesian University of Technology, Institute of Physics - Center for Science and Education, 44-100 Gliwice, Poland — [2]Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, 33619 Bielefeld, Germany

Image processing of pictures from fibers and fibrous materials allows for investigating diverse geometrical properties, such as yarn hairiness, fiber bifurcations, or fiber lengths and diameters. Such irregular sample sets are naturally suitable to statistical examination of the images, using a random-walk algorithm, resulting in the calculation of the so-called Hurst exponent. While previous investigations have proven the appropriateness of this method for examinations of different fibers, yarns and textile fabrics [1-3], a recent study used AFM (atomic force microscopy) images, split into different gray scales, to analyze and quantify differences between various nanofiber mats created from polyacrylonitrile. Besides a strong influence of the nanofiber diameters, a significant impact of the AFM settings became visible, offering an additional optimization tool for AFM measurements.

[1] T. Blachowicz, A. Ehrmann, K. Domino, Physica A: Statistical Mechanics and its Applications 452, 167-177 (2016)

[2] A. Ehrmann, T. Blachowicz, K. Domino, S. Aumann, M. O. Weber, H. Zghidi, Text. Res. J. 85, 2147-2154 (2015)

[3] A. Ehrmann, T. Blachowicz, H. Zghidi, M. O. Weber, Journal of Physics: Conference Series 633, 012101 (2015)

DY 73: Poster: Networks, Chimera, Energy Systems

Time: Thursday 15:30–18:00 Location: Poster A

DY 73.1 Thu 15:30 Poster A

Reconstructing food webs from time series — •Bernd Fernengel[1], Jose Casadiego[2], and Marc Timme[2] — [1]Instituts für Festkörperphysik, Technische Universität Darmstadt, Hochschulstraße 6, 64289 Darmstadt — [2]cfaed - Center for Advancing Electronics Dresden, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden

Feeding relations in food webs (networks of 'who eats whom' in an ecosystem) determine the time evolution of the biomass of each species. Yet, such links are difficult to be measured directly and are often inaccessible. State-of-art approaches rely on time series of biomasses to establish links between species via pairwise statistical dependencies, although these are prone to recover indirect interactions. Here, we extend the Algorithm for Revealing Network Interactions (ARNI) and demonstrate that sufficiently long time series of biomasses reveal the actual topology of food webs. Furthermore, we show that our approach also determines whether a species has a positive or a negative influence on other species, which is crucial given that a single species interacts with both its predators and preys. Finally, we compare the performance of our approach with other benchmarks and discuss scalability for increasing food web sizes.

DY 73.2 Thu 15:30 Poster A

Pattern formation in games of winnerless competition — •Maximilian Voit and Hildegard Meyer-Ortmanns — Jacobs University, Bremen, Germany

We study models of winnerless competition in the framework of evolutionary game theory [1]. We choose the predation rules and rates in a way that yields a network of heteroclinic orbits for the local dynamics at each site of a spatial grid. Moreover we analyze the impact on spatial pattern formation for games with individual sites coupled via diffusion. We then discuss how to choose the rules on the microscopic level in view of desired domains, coalitions, or alliances on a coarse

scale.

[1] D. Labavic and H. Meyer-Ortmanns, Rock-paper-scissors played within competing domains in predator-prey games, J. Stat. Mech., 113402˜1-21 (2016).

DY 73.3 Thu 15:30 Poster A

Statistical mechanics and condensation into multiple states — •Sina Sadeghi and Andreas Engel — Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany

Condensation processes are ubiquitous in a diverse range of physical phenomena. They occur via collective behaviour of systems comprising many identical interacting entities that each of which may be in one of different possible states. Typically, states are filled by a small number of system components. Condensation occurs by definition if one or multiple states are macroscopically occupied such that a non-zero fraction of all components share the same state. In the present work we employ statistical mechanics methods from disordered systems to investigate static properties of condensation in a general framework. We consider the replicator equation with skew symmetric matrices that can describe the dynamics of condensation into multiple states. We show how typical properties of random interaction matrices play a vital role in manifesting the statistics of condensate states. In particular, an analytical expression for the fraction of condensate states in the thermodynamic limit is provided and the result is confirmed by numerical simulations.

DY 73.4 Thu 15:30 Poster A

Understanding pattern formation in climate networks based on aquaplanet simulations — •Frederik Wolf[1,2], Catrin Kirsch[1], and Reik Donner[1] — [1]PIK, Potsdam, Germany — [2]HU, Berlin, Germany

During the recent years, it has been shown that tools from complex network theory can effectively extract spatio-temporal variability patterns from climate data. While a close linkage between classical empirical orthogonal functions and network degree has been analytically demonstrated, the interpretation of other higher-order network measures like betweenness in such climate networks has remained an open problem so far.

Here, we aim to disentangle the information on the underlying climate dynamics provided by various network measures. For this purpose, we study datasets from so-called aquaplanet simulations performed within the TRACMIP coordinated experiment.

We construct network representations based upon the spatial correlation structures of temperature, wind, geopotential height and precipitation fields and perform a detailed study on the resulting patterns exhibited by different topological and spatial network characteristics. Some of the obtained network structures can be linked with mechanisms known from the Earth's climate system, while others are specific to the aquaplanet setup. By systematically investigating similarities and differences, we contribute to a better understanding of pattern formation in climate networks.

DY 73.5 Thu 15:30 Poster A

Maximum entropy method for analysis and design of photonic communication networks — •Tobias Kussel[1], Felix Wissel[2], and Barbara Drossel[1] — [1]Institute for Condensed Matter Physics, Technische Universität Darmstadt, D-64289 Darmstadt, Germany — [2]IP Carrier & Broadband Networks, Deutsche Telekom, Fixed Mobile Engineering Deutschland, D-64295 Darmstadt, Germany

We present a novel approach to analyzing and planning photonic communication networks using concepts from statistical physics and information theory.

Communication networks play a crucial role in modern life infrastructure. When planning and operating such a network, resilience in case of failures as well as costs of infrastructure have to be taken into account. Classical network design algorithms are based on integer linear programming and are located well within the non-polynomial complexity realm.

To achieve a nearly optimal combination of resilience and cost efficiency, we use the topological analysis of neighbourhood graphs and a maximum entropy routing and spectrum assignment strategy. Combining the topological characteristics with the dynamic load properties under maximum entropy distribution we achieve a highly fault resistant as well as cost optimized fiber network.

DY 73.6 Thu 15:30 Poster A

Inhibition as a determinant of activity and criticality in dynamical networks — •Joao Pinheiro Neto[1], Marcus Aloizio Martinez de Aguiar[2], José Antônio Brum[2], and Stefan Bornholdt[3] — [1]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — [2]State University of Campinas, Campinas, Brazil — [3]University of Bremen, Bremen, Germany

Inhibition appears to be a common trait of dynamical networks in nature, ranging from neural networks and biochemical networks, to social and technological networks. We here study the role of inhibition in a representative dynamical network model, characterizing the dynamics of random threshold networks (RTNs) with both excitatory and inhibitory links. We find the balance between excitatory and inhibitory links to be a key parameter in the dynamics. Varying the fraction of inhibitory links has a strong effect on the network's stable population activity A_∞ and sensitivity to perturbation λ. We develop mean-field approximations for A_∞ and λ, and find that the dynamics is independent of degree distribution in the high degree limit. Instead, the amount of inhibition is a determinant of dynamics and sensitivity, allowing for criticality ($\lambda = 1$) only in a specific corridor of inhibition. In a minimal model of an adaptive threshold network we demonstrate how the dynamics remains robust against changes in the topology. This adaptive model can be extended in order to generate networks with a controllable activity distribution and specific topologies.

DY 73.7 Thu 15:30 Poster A

Phase balancing in the Kuramoto model on small networks — •Franz Kaiser and Karen Alim — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Weakly interacting oscillators play a crucial role for transport and timing along a broad range of systems, from biological systems to powergrids and control of autonomous vehicles. In many oscillator networks the interaction is constrained by boundary effects or conservation laws. Among theoretical models used for coupled oscillators on networks, the Kuramoto model stands out due to its tractability and applicability. While research regarding the Kuramoto model has mainly focused on synchronization phenomena, so called phase balanced states are important for constrained systems. An example occurring in nature are the periodically contracting tubes of the network-shaped organism *Physarum polycephalum*. Here, conservation of fluid volume enclosed within the tubular network is prohibiting synchronized contractions. However, very little is known on the structure of balanced states and the networks stabilizing these in Kuramoto's model. Here, we investigate a certain class of networks in which balanced states turn out to be stable and compare them to networks formed by *P. polycephalum*. The structure of this class of networks is highly symmetric, while the underlying graphs are in general neither circulant nor regular. We derive analytical results correctly characterizing the scaling of phase balanced states with increasing number of nodes in a subclass of the networks found. Our findings point out that network architectures that differ from circulant graphs may well support stable phase balanced states.

DY 73.8 Thu 15:30 Poster A

Chimera states in complex networks: interplay of fractal topology and delay — •Jakub Sawicki, Iryna Omelchenko, Anna Zakharova, and Eckehard Schöll — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Chimera states are an example of intriguing partial synchronization patterns emerging in networks of identical oscillators. They consist of spatially coexisting domains of coherent (synchronized) and incoherent (desynchronized) dynamics. We analyze chimera states in networks of FitzHugh-Nagumo oscillators with hierarchical connectivities, and elaborate the role of time delay introduced in the coupling term. In the parameter plane of coupling strength and delay time we find tongue-like regions of existence of chimera states alternating with regions of synchronization. We demonstrate that by varying the time delay one can deliberately stabilize desired spatio-temporal patterns in the system.

DY 73.9 Thu 15:30 Poster A

Avoiding coion trapping in nanoporous supercapacitors — Konrad Breitsprecher[1], •Svyatoslav Kondrat[2] und Christian Holm[1] — [1]Institute for Computational Physics, Stuttgart — [2]Institute of Physical Chemistry, Warsaw

Nanoporous supercapacitor have attracted much attention recently as energy storage devices with remarkable cyclability, and high power and energy densities. However, their use in high frequency applica-

tions might be limited by a relatively slow charging process. In this molecular dynamics simulation study of a slit-pore capacitor system, [1] we focus on the physics and optimization of charge/discharge cycles. We will see that step-voltage charging is slow because the coions become trapped in narrow pores of supecapacitor electrodes. To avoid such trapping, a slow voltage-sweep charging is considered, which allows to accelerate the overall charging process substantially. However, we will demonstrate that a step-voltage, rather than sweeping, is preferable for fast discharging. Based on these results we will propose an optimal charge/discharge cycle.

[1] The effect of finite pore length on ion structure and charging (https://doi.org/10.1063/1.4986346)

DY 73.10 Thu 15:30 Poster A

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

The Vuilleumier machine is a thermodynamic device which can act as both, heat pump and refrigerator. The working principle is based on the gas displacement between three different temperature niveaus by two gas displacers. Thus, no further working pistons are required. We develop a thermodynamic model of the Vuilleumier refrigerator in the context of endoreversible thermodynamics. The model is based on empirical transport laws which enable a simplified description of the complex transport phenomena and flow properties. The influence of several parameters on the cooling performance is studied.

DY 73.11 Thu 15:30 Poster A

Analyzing a Novel Method of Power Control for Internal Combustion Engines — •Andreas Fischer and Karl Heinz Hoffmann — Institut für Physik – Technische Universität Chemnitz – 09107 Chemnitz – Germany

Vehicles are mainly powered by combustion engines. Thus, improving these engines efficiency reduces both their operational cost as well as the emission of greenhouse gases and other pollutants. Within this work a novel approach to control the engine power is analyzed, utilizing a feature rich 1-D engine simulation. It is found that this method promises an efficiency gain of up to 2 percentage points compared to the common power control method while running the otherwise identical engine to drive a medium load (relative to its capability).

DY 74: Annual General Meeting

Time: Thursday 18:15–18:45 Location: BH-N 243

Duration 60 min.

DY 75: Active Matter (joint session BP/CPP/DY)

Time: Friday 9:30–12:00 Location: H 1058

DY 75.1 Fri 9:30 H 1058

Collective cell behavior - a phase field active polar gel model — •Axel Voigt, Simon Praetorius, and Dennis Wenzel — TU Dresden, Institut für Wissenschaftliches Rechnen

We consider a continuum model for collective cell movement. Each cell is modeled by a phase field active polar gel model and the cells interact via steric interactions. We provide a finite element implementation with a parallel efficiency in the number of cells. This is achieved by considering each cell on a different processor and various improvements to reduce the communication overhead to deal with the cell-cell interactions. We demonstrate results for up to 1.000 cells.

DY 75.2 Fri 9:45 H 1058

Statistical physics and hydrodynamics of passive/active mixtures — •Raphaël Jeanneret[1], Arnold Mathijssen[2], and Marco Polin[3] — [1]IMEDEA-UIB, Esporles, Spain — [2]Stanford University, Stanford, US — [3]Warwick University, Coventry, UK

In this talk I will present a series of experimental and theoretical results regarding the dynamics of passive particles in liquid bath of active ones. The active particles act here, via the flows they generate, as localized and erratic sources of momentum for the passive beads leading to non-trivial dynamics. Beyond their exciting features for the physicist, active/passive systems are worth studying quantitatively for applications as diverse as the transport of passive entities in cells, biogenic mixing (i.e. mixing of the ocean by living creatures), virus infection, cargo transport (e.g. drug delivery) or self-assembly (e.g. via motility-induced phase separation). The model system I consider is composed of the motile micro-alga Chlamydomonas reinhardtii, a model organism at numerous levels, and polystyrene beads. I will first show that the effective diffusion of micron-sized beads embedded in homogeneous suspensions of algae is greatly enhanced compared to their thermal counterpart. I will then demonstrate how this coarse-grained dynamics can be understood from the near-field hydrodynamics of the swimming organisms via hydrodynamical entrainment events. Finally I will talk about recent results regarding systems of weakly Brownian colloids in spatially heterogeneous suspensions of algae and show how our findings can be used to induce the spontaneous demixing of the two kinds of particles.

DY 75.3 Fri 10:00 H 1058

Got worms? Collective feeding in C. elegans — •Robert Endres, Linus Schumacher, Serena Ding, and Andre Brown — Imperial College, London, United Kingdom

Collective behaviour, a hallmark of complex living systems, is often studied in groups of large animals or small cells, but less at the mesoscopic scale. Here, we investigate the collective feeding of the nematode C. elegans, known for its easy genetic manipulation and stereotypic worm postures. In this system, small genetic perturbations can lead to strikingly different population-level behaviors. First, we quantified behavioral differences between the 'solitary' lab strain and a 'social' aggregating mutant strain, using fluorescence imaging and many-worm tracking to probe the dynamics inside aggregates. Second, to understand the mechanism of aggregation, we drew on concepts from motility-induced phase transitions and developed a minimal model. Finally, using this model, we investigated the potential benefits of collective feeding to explain the predominance of aggregating strains in the wild.

DY 75.4 Fri 10:15 H 1058

A continuum model to study coordination of tissue growth — •Maryam Aliee, Damir Vurnek, Sara Kaliman, and Ana-Sunčana Smith — Cluster of Excellence: Engineering of Advanced Materials, Friedrich-Alexander-University of Erlangen-Nürnberg

Living organisms represent fascinating and precise structures. It is still a big challenge to understand the mechanisms though which cells interact with each other and the environment to form reproducible patterns. We analyze how tissue growth is controlled by cell properties putting together a theoretical model and quantitative analysis of experiments. We measure carefully growth properties of a single-layered epithelium, cultured MDCK cells. In these experiments a group of several cells grows to a bigger colony. We observe the density of cells increases and a bulk region with a high constant density is established in the center, surrounded by the edge where cell density decreases. Our results demonstrate a gradual transition from an early exponential growth to a non-linear regime when growth speed increases with colony size.

We develop a continuum model to take into account cell mechanics and growth to study dynamics of tissues. We consider balance of cell number and forces for viscoelastic materials modified by active terms coming from cell division and apoptosis. We solve the equations with analytical and numerical methods. Our results show establishment of bulk and edge regions independent of many details. We study how the dynamics of the colony is controlled by cell characteristics and their interactions with surroundings. Remarkably, our model reproduces the nontrivial properties of MDCK growth in different experiments.

DY 75.5 Fri 10:30 H 1058

Synthetic reconstitution of beating cilia — •Isabella Guido, Smrithika Subramani, Christian Westendorf, and Eberhard Bodenschatz — Max Planck Institute for dynamics and self-organization, Göttingen, Germany

Cilia are microscopic hair-like structures that present a rhythmic waving or beating motion and are found on the surface of almost all mammalian cells and on the body of some protozoan organisms. They are used for fluid flow based transport (e.g. removal of pollutants in the trachea) or for the locomotion in viscous fluid environments.

In our work we aim to develop synthetic ciliated systems able to propel themselves or to move fluids across a fixed surface. For this purpose we employ a bottom-up approach for assembling a simple system made of few building blocks adapted from natural cilia, namely microtubules and motor proteins. Using Kinesin-1, a processive motor powered by ATP hydrolysis, we synthesized a system containing MT bundles that are free to move in all planes, deviating from the conventional gliding assay. By binding them to a surface using a suitable anchor system, we are able to observe the microtubules-motor protein system oscillations in a manner that closely mimics ciliary movement.

The issue that we are addressing in our experiments is: how simple is the simplest system that is able to beat?

DY 75.6 Fri 10:45 H 1058

DNA in the cell nucleus is organized similar to an active microemulsion — •Lennart Hilbert[1,2,3], Yuko Sato[4], Hiroshi Kimura[4], Frank Jülicher[1,3,5], Alf Honigmann[2], Vasily Zaburdaev[1,3], and Nadine Vastenhouw[2] — [1]Center for Systems Biology Dresden — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Max Planck Institute for the Physics of Complex Systems — [4]Tokyo Institute of Technology — [5]Center for Advancing Electronics Dresden

Inside cell nuclei, DNA is stored in the form of chromatin. Chromatin is three-dimensionally organized in response to transcription of DNA into RNA. Here, we studied the mechanisms by which transcription organizes chromatin, using experiments in zebrafish embryonic cells and theory. We show that transcription establishes an interspersed pattern of mutually exclusive chromatin-rich domains and RNA-rich domains. Ongoing transcriptional activity stabilizes the interspersed domain pattern by establishing contacts between the RNA and transcribed parts of chromatin. We explain our observations with an active microemulsion model based on two macromolecular mechanisms: (i) RNA/RNA-binding protein complexes and chromatin undergo phase separation, while (ii) transcription tethers RNA/RNA-binding proteins to chromatin and thereby forms amphiphile particles that intersperse the phases. Thus, three-dimensional DNA organization in the cell nucleus is an example of an unconventional, active microemulsion, stabilized by a catalytically active amphiphile that produces one of the emulsified phases.

DY 75.7 Fri 11:00 H 1058

Size increases produce coordination trade-offs in a simple multicellular animal near criticality — Mircea R. Davidescu[1], •Pawel Romanczuk[2,3], Thomas Gregor[4], Corina E. Tarnita[1], and Iain D. Couzin[5,6] — [1]Dept. of Ecology and Evol. Biology, Princeton University ,USA — [2]Institute for Theoretical Biology, Dept. of Biology, Humboldt Universität zu Berlin, Germany — [3]Bernstein Center for Computational Neuroscience, Berlin, Germany — [4]Joseph Henry Laboratories of Physics, Princeton University, USA — [5]Dept. of Collective Behavior, MPIORN, Konstanz, Germany — [6]Dept. of Biology, University of Konstanz, Germany

Based on theoretical arguments from statistical physics, it has been suggested that collective systems in biology should operate close to criticality in order to maximize their susceptibility to external signals [Mora & Bialek, J Stat Phys, 144, 2 (2011)]. Recently, this hypothesis received increased attention in the context of collective behavior in biology. However, it is still rather controversial and up to know most support for it comes from idealized mathematical models and few experimental systems. Here, we will discuss some recent experimental observations of Placozoa (*Trichoplax Adhaerens*), a simple multicellular animal effectively corresponding to a quasi two-dimensional cellular sheet. By combining experimental data with simple mathematical model of Placozoa motion as a collective system, we find that the observed dynamics are indeed consistent with the criticality hypothesis, but as a consequence these simple animals without a central nervous system have to face a fundamental size-coordination trade-off.

DY 75.8 Fri 11:15 H 1058

Harnessing emergence in bacterial populations: From biological mixing to active mechanics — •Anupam Sengupta — Institute for Environmental Engineering, ETH Zurich, Switzerland — Physics and Materials Science Research Unit, University of Luxembourg

At the scale of a single cell, interactions between a bacterium and its micro-environment represent a complex biophysical interface between phenotypic states (free-living planktonic or surface-attached sessile state) and external cues. In this talk I will discuss two recent works where we use experiments and modeling to elucidate how bacterial phenotype cross-talks with immediate micro-environment, and harnesses the emergent physics for biological functions. In the first case, we will see how Chromatium okenii, a 10 μm long purple sulphur bacterium, is capable of mixing over a meter thick layer of water in the Swiss Alpine lake, Lago di Cadagno. By changing the local fluid density, C. okenii is able to trigger convection rolls, creating a sustained well-mixed nutrient layer within an otherwise stratified lake. In the second instance, we will examine emergent geometrical and mechanical properties of a bacterial colony growing on a soft substrate. We show that such an expanding colony self-organizes into a "mosaic" of micro-domains consisting of highly aligned cells, before emerging into an active nematodynamic system. Interestingly, phenotypic traits - motility in the first and growth-induced stresses in the latter - couple with local hydrodynamics, to elicit important ecological functions at scales that can be orders of magnitude higher than single cells.

DY 75.9 Fri 11:30 H 1058

Hydrodynamic theory of aster positioning by motor proteins — •Andrej Vilfan — J. Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

In fertilized egg cells of certain species the male pronucleus is transported to the center of the cell by growing an asymmetric microtubule aster, which then serves as a track for motor proteins carrying vesicles towards the center. Because these vesicles experience a viscous drag in the surrounding cytoplasm, the motors exert the opposite force on the microtubules. The asymmetry of the aster then leads to a net pulling force towards the cell center. Yet hydrodynamic interactions make the understanding of the process difficult.

Here we discuss a coarse-grained approach where we describe the aster as a porous medium and the moving vesicles as sources of an active pressure gradient. In parallel, we use computational models to determine the parameters of the continuum model. For realistic parameters, we show that a significant proportion (10-20%) of the motor force is converted to a pressure gradient and contributes to aster centering. We conclude that vesicle transport in a viscous environment is a surprisingly efficient way of force generation.

DY 75.10 Fri 11:45 H 1058

Active polymer models for the 3D organization of chromosomes — •Johannes Nuebler[1], Geoffrey Fudenberg[2], Maxim Imakaev[1], Nezar Abdennur[1], and Leonid Mirny[1] — [1]Institute for Medical Engineering and Science, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — [2]University of California, San Francisco, Gladstone Institutes, San Francisco, CA 94158, USA

Eukaryotic chromatin is far from being a randomly arranged polymer in the cell nucleus. Rather, a high degree of spatial organization on various length scales is revealed by Hi-C and imaging techniques. We show that the organization on intermediate scales emerges from the interplay of two mechanisms, one active and one passive: first, on the scale of one million basepairs and below, active formation of growing chromatin loops emerges as a general organizational principle throughout the cell cycle. Second, a block-copolymer based phase separation explains chromatin compartmentalization on larger scales. Interestingly, these processes interact: only the interplay of loop extrusion and spatial segregation explains a large number of experimental perturbations, namely removal of the loop extruder cohesin, removal of the cohesin boundary element CTCF and removal of the cohesin unloader Wapl, and it makes specific predictions for variations in the compartmental interaction and topological constraints (bioRxiv: https://doi.org/10.1101/196261).

DY 76: Complex Contagion Phenomena II (Focus Session, joint SOE/DY/BP/SNPD) (joint session SOE/DY/BP)

Session organizers and chairs: Philipp Hövel, Pawel Romanczuk, and Jonathan Donges. See part I of the session for a synopsis.

Time: Friday 9:30–13:15 Location: MA 001

Topical Talk DY 76.1 Fri 9:30 MA 001

Network reconstruction for the prediction of spreading processes — •Diego Garlaschelli — Lorentz Institute for Theoretical Physics, University of Leiden, The Netherlands

Financial contagion is an epidemic-like phenomenon whereby financial distress can propagate across a network of banks connected by credit relationships, possibly leading to the collapse of the entire system. In order to estimate the systemic risk of financial contagion, the knowledge of the entire interbank network is required. However, due to confidentiality issues, banks only disclose their total exposure towards the aggregate of all other banks, and not their individual exposures towards each bank. A similar problem is encountered in epidemiology. Is it possible to statistically reconstruct the hidden structure of a network in such a way that privacy is protected, but at the same time higher-order properties are correctly predicted? In this talk, I will present a general maximum-entropy approach to the problem of network reconstruction and systemic risk estimation. I will illustrate the power of the method when applied to various economic, social, and biological systems. Then, as a counter-example, I will show how the Dutch interbank network started to depart from its reconstructed counterpart in the three years preceding the 2008 crisis. Over this period, many topological properties of the network showed a gradual transition to the crisis, suggesting their usefulness as early-warning signals. By definition, these signals are undetectable if the network is reconstructed from partial bank-specific information.

DY 76.2 Fri 10:00 MA 001

Agent-based modeling of innovation spreading in ancient times — •Natasa Djurdjevac Conrad[1], Luzie Helfmann[1,2], Johannes Zonker[1,2], Stefanie Winkelmann[1], and Christof Schuette[1,2] — [1]Zuse Institute Berlin — [2]Freie Universitaet Berlin

Modeling of spreading processes has gained a lot of attention in the last decades, since these processes play a crucial role in understanding a wide range of real-world systems that span biological, technical, economical and social sciences. However, very little is known about processes/systems that have happened in ancient times, available data is sparse and we can not observe these systems again.

In this talk, we will present an agent-based model for the spreading of the wool-bearing sheep in a population of herders in the Near East and Europe, between 6200 and 4200 BC. In our model, the herders are represented by agents moving diffusively in a geophysical landscape and simultaneously interacting with other agents. The diffusion of the innovation is thus happening on a spatial network that is changing in time, as the connections between the agents are changing in time due to their movements. We will use our model to explore the dynamical properties of the spreading process and to study the qualitative effect of different aspects affecting the speed and spatial evolution of this spreading process.

DY 76.3 Fri 10:15 MA 001

Identifying the source of large-scale outbreaks of infectious disease — Abigail Horn[1] and •Hanno Friedrich[2] — [1]Bundesinstitut für Risikobewertung, Berlin, Germany — [2]Kühne Logistics University, Hamburg, Germany

We study the problem of identifying the source of emerging large-scale disease outbreaks: given a model of the underlying network and reports of illness, determine the outbreak source location. Existing work on the network source identification problem has focused on studying this problem in trees and extending to general network structures in an *ad hoc* manner; this is to assume the contamination travels along a specific set known paths through a network, which may be an unrealistic approximation. In this work we develop a novel, computationally tractable solution that accounts for all possible contagion transmission paths through the network. We formulate a probabilistic model of the contamination transmission process as a random walk on a network and derive the maximum likelihood estimator for the source location. If the temporal dimension of the spreading process is well understood, we also estimate the epidemic start time. We demonstrate the benefits of this approach to source detection through application to various real network and outbreak contexts, including the 2011 STEC outbreak in Germany spread through the food supply network and ongoing outbreaks of cholera in Mozambique spread through human travel, showing significant improvements in accuracy and robustness compared with the relevant state-of-the-art methods.

DY 76.4 Fri 10:30 MA 001

Spreading of multiple pathogens and their evolutionary stable strategies — •Kai Seegers[1], Fakhteh Ghanbarnejad[1], Alessio Cardillo[2], and Philipp Hövel[1] — [1]Institut für Theoretische Physik, TU Berlin — [2]Institut Catalá de Paleoecologia Humana i Evolució Social (IPHES)

Different pathogens usually spread simultaneously in a host population and thus often influence each other. They can either be competitive, e.g. due to cross immunity, or cooperative, e.g. by suppressing the immune system of the host. The latter can lead to unexpectedly large outbreaks [EPL 104, 50001 (2013),Nature Physics 11, 936-940 (2015)] as it has been seen in the Spanish Flu pandemic in the early 20th century and it has been recently on serious warning alarm for co-infection of HIV and tuberculosis or hepatitis, for instance. However cooperation might not always be the best strategy for pathogens to survive, due to death of the host population or enforced countermeasures. Therefore we combine in a novel approach spreading dynamics of different strains of multiple pathogens with evolutionary game theory. We show bistability of strategies in the parameter space and finally discuss the emergence of competition and cooperation of pathogens.

DY 76.5 Fri 10:45 MA 001

Complex Social Contagion of Structural Discrimination — •Gorm Gruner Jensen and Stefan Bornholdt — Institute for Theoretical Physics University of Bremen Otto-Hahn-Allee D-28359 Bremen Germany

One approach within evolutionary game theory study the spreading of contagious behaviors in populations of agents distributed on a graphs. Typically the agents interact in well defined games with their nearest neighbors, and the evolutionary dynamics are implemented by letting agents copying the behavior of their neighbors. Here we demonstrate that this modelling approach can be applied in studying the complex social contagion of structural discrimination. Starting from established models designed to study the evolution of behaviors like cooperation and altruism, we split the agents into groups distinguished only by an observable labels. This generally entails an increased strategy-spaces, as strategies may now be discriminating, ie. imply different behaviors towards agents from different groups. Our model approach is fundamentally different from previous theories of the emergence and persistence of discrimination, which usually rely on on an intrinsic preference for helping your own kind, on games with asymmetric Nash equilibria - like the Hawk-Dove Game, or on self-fulfilling prophecies. We do, however, find a strong connection between the evolutionary stability of discriminating strategies and the strength of the evolution pressure, which indicates that an evolutionary perspective coul be an important compliment to the existing theories.

DY 76.6 Fri 11:00 MA 001

Making rare events happen: prediction and control of network extinction, switching, and other extreme processes. — •Jason Hindes — U.S. Naval Research Lab, Washington D.C., United States of America

Many complex networks must operate in uncertain and dynamic environments. Over long time scales, combinations of random internal interactions and dynamical perturbations can organize to drive a network from one collective state to another. Such noise-induced large fluctuations may be associated with desirable outcomes, such as epidemic extinctions, or undesirable ones, such as switching in collective order, or loss of network synchrony. In this talk I will discuss a general formalism for predicting rare events in networks with internal and external noise, the role of topology in facilitating the most extreme

network events, techniques for optimal network control that leverage uncertainty, and numerical solutions for the aforementioned when explicit formulas are unknown. Along the way, I will consider many examples: from epidemic dynamics to opinion formation and synchronization of coupled oscillators.

15 min. break

DY 76.7 Fri 11:30 MA 001

Complex contagion in social media — •Philipp Lorenz[1], Jonas Braun[2], and Philipp Hövel[1] — [1]Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Department of Physics, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany

Spreading processes on a network of individuals can be described either under the assumption of independent interaction with equal transmission rates, like the classic SIS/SIR models (simple contagion) or one can take the structure of an individual's neighborhood into account (complex contagion). A very interesting model is sociologically inspired and includes the relative threshold of a node's surrounding required to change its state to infected (convinced). For the online world, especially social platforms, which became the stage of opinion spreading, these models have to be extended. We propose two extensions of the classical threshold model:

- Reposting, the state of a node can be multiple infected (convinced) changing the binary state variable to an integer.
- Recovery, a saturation of exposure, introducing a second threshold that turns nodes into a recovered (immune) state.

We investigate the interplay of these ingredients, separated and in combination with respect to the spreading dynamics and the role of initiators by the quantitative comparison of various scenarios.

DY 76.8 Fri 11:45 MA 001

Flockworks: A class of dynamic network models for face-to-face interactions — •Benjamin F. Maier[1,2] and Dirk Brockmann[1,3] — [1]Robert Koch-Institut, Nordufer 20, 13353 Berlin — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin — [3]Institut für Theoretische Biologie, Humboldt-Universität zu Berlin, Philippstr. 13, 10115 Berlin

Studying the dynamics of face-to-face interaction networks is essential for a better understanding of contact mediated processes, contagion processes, and disease spreading. In many studies regarding social systems, networks are reconstructed using time averages in which links reflect an interaction likelihood, although this measures serves as a qualitative feature from which network properties are computed. During the last years a significant effort was made to resolve this issue by developing algorithms to analyze dynamic processes on the actual time-dependent contact patterns of social systems. However, there is still a lack of simple dynamic network models generating temporal networks of typical behaviour observed in real systems.

We introduce a class of minimal dynamic network models that naturally yield group formation and are easy to control with a small number of parameters. We discuss a variety of properties of those models and show that they reflect the character of real-world temporal data as well as the properties of dynamic processes on this data remarkably well, up to the prediction of epidemic curves.

DY 76.9 Fri 12:00 MA 001

Cooperation vs. defection in an evolutionary ecological framework — •Felix Köster and Fakhteh Ghanbarnejad — Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

In this work, we first extend the CGB model [1] by considering each pathogen has two different strategies: cooperation or defection. Then we analyse the fundamental properties of the interacting contagious processes in a well-mixed population, i.e. homogeneous mean field approximation. Altering parameters we discover new discontinuous phase transitions for which we investigate the multi-stability shift in the phase diagram. We show also qualitatively same results by stochastic simulations. Furthermore, an evolutionary game is introduced to mimic conditions, which force agents to adept their strategies by minimizing their payoff. This study improves our understanding of the natural dynamics of species populations in an evolutionary ecological framework

[1] L. Chen, F. Ghanbarnejad, D. Brockmann "Fundamental properties of cooperative contagion processes"; New J. Phys. 19, 103041(2017)

key words; SIS, interacting dynamics, co-infection, complex contagions, discontinuous transitions

DY 76.10 Fri 12:15 MA 001

Effective Distances for Epidemic Spreading — •Andreas Koher[1], Flavio Iannelli[2], Igor M. Sokolov[2], and Philipp Hövel[1] — [1]Technische Universität Berlin — [2]Humboldt Universität zu Berlin

The analysis of global epidemics revealed that physical distances can hardly be used to forecast the arrival time of the first infected person. Instead, recent results on the global air traffic network suggest that network based measures, so called effective distances correlate well with actual detection times.

We compare numerical simulations on the global air traffic network with different measures that are based on shortest distances, parallel paths and the recently proposed random walk effective distance [1]. Furthermore, we extend the latter and propose an effective distance that is based on non-backtracking walks. This simple diffusion model allows to consider the directed nature of epidemic spreading and relates the hitting probability to the infection arrival time.

[1] F. Iannelli, A. Koher, D. Brockmann, P. Hövel, and I.M. Sokolov, Effective distances for epidemics spreading on complex networks, Phys. Rev. E 95, 012313 (2017).

DY 76.11 Fri 12:30 MA 001

Modeling of Behavioral Cascades in Fish Schools — •Pawel Romanczuk[1,2], Matt Grobis[3], Bryan Daniels[4], Winnie Poel[1,2], Colin Twomey[5], and Iain Couzin[6,7] — [1]Institute for Theoretical Biology, Dept of Biology, Humboldt Universität zu Berlin, Germany — [2]Bernstein Center for Computational Neuroscience, Berlin, Germany — [3]Dept. of Ecology and Evol. Biology, Princeton University, USA — [4]ASU-SFI Center for Biosocial Complex Systems, Arizona State University, USA — [5]Dept. of Biology, University of Pennsylvania — [6]Dept. of Collective Behavior, MPIORN, Konstanz, Germany — [7]Dept. of Biology, University of Konstanz, Germany

Recently, it was shown that the spreading of stereotypical escape behavior (startle) in fish schools corresponds to a complex contagion process [1]. Here, we will discuss the modeling of such behavioral cascades using an extension of the generalized contagion model proposed by Dodds & Watts [2]. In particular, using networks extracted from experimental data, we will identify and discuss parameter regions providing best agreement with experimentally observed cascades. Furthermore, we will apply our modeling ansatz to new experiments on the impact of different risk perception on the behavioral contagion dynamics in fish schools.

[1] Rosenthal, S.B., et al., PNAS 112, 15, 4690-4695 (2015)
[2] Dodds, P. & Watts, D.J., Phys Rev Lett, 92, 218701 (2004)

DY 76.12 Fri 12:45 MA 001

The effect of compatibility and heterogeneous adoptability in contagion processes — •Byungjoon Min and Maxi San Miguel — Instituto de Fisica Interdisciplinar y Sistemas Complejos (CSIC-UIB), Campus Universitat Illes Balears, E-07122 Palma de Mallorca, Spain

While competition and compatibility of multiple contagious entities and heterogeneous adoptability of agents are omnipresent in social contagions, so far these factors are overlooked in traditional models of contagion processes. Here, we study generalized contagion processes in two directions: i) unifying simple and complex contagions reflecting heterogeneous adoptability and ii) considering competition and compatibility among multiple transmittable entities. For a generalized contagion model unifying simple and complex contagion processes, we find a rich variety of phase transitions such as continuous and discontinuous phase transitions, criticality, tricriticality, and double transition. We also examine the role of dual users who possess multiple contagious technologies simultaneously, and find that the compatibility induced by the dual user facilitates spread of innovation and extinction of pre-existing technology.

DY 76.13 Fri 13:00 MA 001

Modeling of startling cascades and information transfer in fish — •Haider Klenz[1] and Pawel Romanczuk[1,2] — [1]Department of Biology, Humboldt-Universität zu Berlin, Berlin 10115, Germany — [2]Bernstein Center for Computational Neuroscience, Humboldt-

Universität zu Berlin, Berlin 10099, Germany

Animals come together in groups, e.g. school of bird or swarms of fish, in which information is processed collectively. Especially in situation where the collective is exposed to a threat, this information and the speed with which it propagates through the collective is of great importance to the individual.

This work focuses on shoals of *Poecilia Sulphuraria* and their reaction to danger. Through environmental dependencies the fish can only swim at the surface and therefore forms a 2D-system. When attacked by preying birds the fish dive down. This diving behavior then spreads through the swarm in a wave like fashion and is repeated for several minutes without further triggers.

We explored the mechanism behind wave spreading with agent-based modeling. We propose a stochastic contagion process and show that the speed of the wave depends on the underlying information network. Furthermore we study different possible explanations for repeated waves.

DY 77: Talk S. Herminghaus

Time: Friday 9:30–10:00 Location: BH-N 243

Invited Talk DY 77.1 Fri 9:30 BH-N 243

Mean field theory of ride sharing systems — •Stephan Herminghaus — MPI für Dynamik und Selbstorganisation, Am Fassberg 17, 37077 Göttingen

The dynamics of demand-driven ride sharing systems is considered in a mean-field approach. The relevant dimensionless quantities determining the performance and viability of such systems are identified. The framework for a class of route assignment algorithms is developed. In the presence of an already established dominant market participant with comparable service quality (like, e.g., the private car), the mutual interaction of the actors (i.e., the customers sharing rides) by virtue of the route assignment algorithm gives rise to a discontinuous transition between two strongly different modes of operation. One of them represents the typical (unfavorable) performance of current ride sharing systems, while the other represents a new mode of operation in which virtually all customers use ride sharing. We furthermore consider the impact of the spatial structure of the traffic environment. It is shown how the Riemann curvature of the traffic network can be determined in a simple way inspired by the Regge calculus, and how it can be implemented in the route optimization scheme.

DY 78: Talk M. Fuchs

Time: Friday 9:30–10:00 Location: BH-N 334

Invited Talk DY 78.1 Fri 9:30 BH-N 334

Emergence of long-ranged stress correlations at the liquid to glass transition — Manuel Maier[1], Annette Zippelius[2], and •Matthias Fuchs[1] — [1]FB Physik, Universität Konstanz, 78457 Konstanz — [2]Inst. Theo. Phys, Universität Göttingen, 37077 Göttingen

A theory for the non-local shear stress correlations in supercooled liquids is derived from first principles [1]. It captures the crossover from viscous to elastic dynamics at the liquid to glass transition and explains the emergence of long-ranged stress correlations in glass, as expected from classical continuum elasticity. The long-ranged stress correlations can be traced to the coupling of shear stress to transverse momentum, which is ignored in the classic Maxwell model. To rescue this widely used model, we suggest a generalization in terms of a single relaxation time for the fast degrees of freedom only. This generalized Maxwell model implies a divergent correlation length as well as dynamic critical scaling and correctly accounts for the far-field stress correlations. It can be rephrased in terms of generalized hydrodynamic equations, which naturally couple stress and momentum and furthermore allow to connect to fluidity and elasto-plastic models.

[1] M. Maier, A. Zippelius, and M. Fuchs, Phys. Rev. Lett. 119, 265701(2017)

DY 79: The Physics of Power-Grids – Fluctuations, Synchronization and Network Structures (joint session DY/SOE)

Time: Friday 10:00–12:15 Location: EB 107

DY 79.1 Fri 10:00 EB 107

Qualitative Stability and Synchronicity Analysis of Power Network Models in Port-Hamiltonian form — •Simona Olmi[1], Volker Mehrmann[2], Riccardo Morandini[2], and Eckehard Schöll[1] — [1]Institut fuer Theoretische Physik, Sekr. EW 7-1, TU Berlin, Hardenbergstr. 36, D-10623 Berlin — [2]Institut fuer Mathematik MA 4-5, TU Berlin, Str. des 17. Juni 136, D-10623 Berlin

In view of highly decentralized and diversified power generation concepts, in particular with renewable energies such as wind and solar power, the analysis and control of the stability and the synchronization of power networks is an important task that requires different levels of modeling detail for different tasks. A frequently used qualitative approach relies on simplified nonlinear network models like the Kuramoto model. Although based on basic physical principles, the usual formulation in form of a system of coupled ordinary differential equations is not always adequate. We present a new energy-based formulation of the Kuramoto model as port-Hamiltonian system of differential-algebraic equations. This leads to a very robust representation of the system with respect to disturbances, it encodes the underlying physics, such as the dissipation inequality or the deviation from synchronicity, directly in the structure of the equations, it explicitly displays all possible constraints and allows for robust We demonstrate the advantages of the modified modeling approach with analytic results and numerical experiments.

DY 79.2 Fri 10:15 EB 107

Influence of network topology in shaping the dynamics of power grid networks — •Halgurd Taher, Simona Olmi, and Eckehard Schöll — Institut fuer Theoretische Physik, Sekr. EW 7-1, TU Berlin, Hardenbergstr. 36, D-10623 Berlin

The increase of the inclusion of renewable energy sources into the power grid is rather a paradigm change for the entire European power grid, bringing new challenges for power grid operation. The reason behind this is the fact that the power output of renewable energy sources typically strongly fluctuates and, furthermore, the possible geographical locations for power plants based on renewable energies depend on geographical factors, thus including different forms of perturbations into the network. In this talk we investigate the role played by topology in shaping the dynamics of the German power grid and we present a new investigation method able to highlight the instabilities of the system. Based on the knowledge of the unstable nodes and directions suggested by the application of the Lyapunov vector, we are thus able to design a control method that enhances the synchronization and stabilizes the network, acting on small number of nodes/links. This minimal intervention suggests a procedure to control real grids that allows to save time, money and energy.

DY 79.3 Fri 10:30 EB 107

Influence of noise in shaping the dynamics of power grids —

•Liudmila Tumash, Simona Olmi, and Eckehard Schöll — Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, D-10623 Berlin

The aim of this work is to investigate complex dynamic networks which can model high-voltage power grids with renewable, fluctuating energy sources. For this purpose we use the Kuramoto model with inertia to model the network of power plants and consumers [1]. In particular, we analyze the synchronization transition of random Erdös-Renyi networks of N phase oscillators with inertia (rotators) whose natural frequencies are bimodally distributed. We also implement Gaussian white noise and investigate its role in shaping the dynamics.

[1] Filatrella, G., Nielsen, A. and Pedersen, N. Eur. Phys. J. B (2008) 61: 485.

DY 79.4 Fri 10:45 EB 107

Load Dependence of Power Outage Statistics — •Soumyajyoti Biswas[1] and Lucas Goehring[1,2] — [1]Max Planck Institute for Dynamics and Self-Organisation, Göttingen, Germany — [2]Nottingham Trent University, Nottingham, UK

The size distributions of power outages are shown to depend on the stress, or the proximity of the load of an electrical grid to complete breakdown. Using the data for the US and Canada between 2002-2017, we show that the outage statistics are dependent on the usage levels during different parts of the day. At higher load, not only are more failures likely, but the distribution of failure sizes shifts, to favor larger events. At a finer spatial scale, different regions within the US can be shown to respond differently in terms of the outage statistics to variations in the usage (load). The response, in turn, corresponds to the respective bias towards larger or smaller failures in those regions. We provide a simple model, using realistic grid topologies, which can nonetheless demonstrate such biases as a function of the applied load, as in the data. Given sufficient data, the method can be used to identify vulnerable regions in power grids prior to major blackouts.

15 min. break

DY 79.5 Fri 11:15 EB 107

Asymptotic Dynamical States in Networks of Kuramoto Oscillators with Inertia — •Anton Plietzsch — Potsdam-Institut für Klimafolgenforschung — Humboldt-Universität zu Berlin

The frequency dynamics of power grids can be modeled by networks of oscillators. I will show analytic and numerical results on the possible asymptotic states in the Kuramoto model with inertia. These states include states that can be understood as synchronized, partially synchronized, and distinct novel states that have no analytic explanation so far. I will show some analytic criteria for the stability and existence of solitary states of single desynchronized oscillators as well as partially synchronized clusters with distinct frequency on networks.

DY 79.6 Fri 11:30 EB 107

Modelling and Suppressing power output fluctuations of photovoltaic power plants — •Mehrnaz Anvari[1], Benjamin Werther[2], Gerald Lohmann[3], Matthias Waechter[3], Joachim Peinke[3], and Hans-Peter Beck[2] — [1]MPIPKS, Dresden, Germany — [2]TU Clausthal, Germany — [3]Institute of Physics and ForWind, Oldenburg, Germany

The use of solar photovoltaic (PV) power has recently increased in electric distribution grids. By the end of 2014, for example, PV power had already reached a total installed capacity of over 178 GW worldwide, which is expected to increase to between 396 and 540 GW by 2019. However, the stochastic properties of solar energy, such as intermittency can negatively affect power quality and cause grid instabilities, especially in microgrids. In this study, we use high resolution (i.e. 1 Hz) measured irradiance data in Hawaii (as an exemplary data) to study the stochastic behaviour of short-term PV fluctuations, and classify its states as cloudy, sunny and flickering. Our main aim is the construction of a simple dynamical equation (jump-diffusion stochastic equation) that governs the stochastic process of PV-fluctuations, so that the statistics of the modelled time series are identical to those of the measured ones. Using the obtained dynamical equation, we generate new synthetic data sets with varying jump rates. Finally, we implement a straightforward filtering method, i.e. a combination of an inverter and a battery storage system to show the applicability of our proposed stochastic method.

DY 79.7 Fri 11:45 EB 107

Power Grid Stability: Bounding the First Exit from the Basin — •Paul Schultz[1,2], Frank Hellmann[1], Kevin N. Webster[1], and Jürgen Kurths[1,2,3,4] — [1]Potsdam Institute for Climate Impact Research (PIK), Member of the Leibniz Association, P.O. Box 60 12 03, D-14412 Potsdam, Germany — [2]Department of Physics, Humboldt University of Berlin, Newtonstr. 15, 12489 Berlin, Germany — [3]Institute for Complex Systems and Mathematical Biology, University of Aberdeen, Aberdeen AB24 3UE, United Kingdom — [4]Department of Control Theory, Nizhny Novgorod State University, Gagarin Avenue 23, 606950 Nizhny Novgorod, Russia

We study the stability of deterministic systems given sequences of large, jump-like perturbations. Our main result is the derivation of a lower bound for the probability of the system to remain in the basin, given that perturbations are rare enough. To quantify rare enough, we define the notion of the independence time of such a system. This is the time after which a perturbed state has probably returned close to the attractor, meaning that subsequent perturbations can be considered separately. The effect of jump-like perturbations that occur at least the independence time apart is thus well described by a fixed probability to exit the basin at each jump, allowing us to obtain the bound. To determine the independence time, we introduce the novel concept of finite-time basin stability, which cor- responds to the probability that a perturbed trajectory returns to an attractor within a given time. The independence time can then be determined as the time scale at which the finite-time basin stability reaches its asymptotic value.

DY 79.8 Fri 12:00 EB 107

Bridging from Kuramoto-like Networks to Real Power Grids: Lossy Grids, Voltage Regulation and Implementing Inverter Units — Katrin Schmietendorf[1], Joachim Peinke[1], and •Oliver Kamps[2] — [1]ForWind and Institute of Physics, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany — [2]Center for Nonlinear Science, Westfälische Wilhelms-Universität Münster, Münster, Germany

Kuramoto-like models of electric power grids give insights into power system dynamics on the short-term scale in terms of self-organized synchronization. From the applicational viewpoint, the most current issues in power system analysis concern grid decentralization and increasing feed-in fluctuations induced by renewables. In order to address these topics, certain complements to the basic Kuramoto approach have to be taken into account. We investigate three supplements, which are particularly relevant for the integration of renewable energy plants on the distribution grid level: (i) transferlosses due to non-zero line conductance on the low and medium voltage levels, (ii) local voltage regulation by means of a proportional controller, and (iii) different approaches on implementing inverter units into the Kuramoto-like framework. In this talk we present the implications of these model extensions on different aspects of system stability and power quality.

DY 80: Brownian Motion and Transport

Time: Friday 10:00–11:15 Location: BH-N 128

DY 80.1 Fri 10:00 BH-N 128

Analyzing Transport Properties of Nanoparticles in Magnetic Ratchets — •Daniel Kappe[1,2] and Andreas Hütten[1] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences, Germany

Magnetic nanoparticles have a broad range of possible applications, ranging from cancer treatment to drug delivery and diagnostics. When detecting biomolecules, nanoparticles are superior to micrometer sized particles, because their surface can only bind to a couple of molecules instead of a thousands. But directed, controlled transport is tricky, because of their high diffusivity. A magnetic ratchet utilizes this property and an asymmetric potential to drive the particles. We introduce a scheme to evaluate the transport efficiency of magnetic ratchets.

In order to calculate the efficiency of such setups, a Monte Carlo based numerical integration of the Langevin equation was implemented [1]. The algorithm considers viscous forces, Brownian motion and forces arising from magnetic field gradients, but no particle-particle interactions. Particles subject to a time and space dependent force field, governed by the setup in use. The efficiency of a setup is analyzed reviewing the mean displacement of all particles.

We aim to improve understanding of different setups and tune their parameters, like switching frequencies and external fields, to find and extend the range of particles working in a particular setup.

[1] D. Ermak, H. Buckholz, J. comp. Phys., 35, 169-182 (1980)

DY 80.2 Fri 10:15 BH-N 128

Quantum motion of ions in a molecular junction during current flow — •Lev Kantorovich — Physics, King's College London, London, WC2R 2LS

We consider a combined system of electrons and nuclei of a molecular junction. Initially the whole system is in thermal equilibrium at some temperature, no partitioning approximation is made. Then, a bias is applied causing a current to flow. Using path integrals and non-equilibrium Green*s Functions formalisms, an expression for the density matrix of ions (reduced with respect to electrons) is derived and hence the corresponding effective Liouville equation. It is assumed that atomic displacements with respect to average (and time dependent) atomic positions are small (the harmonisation approximation). Then a hierarchy of equations of motion for average ionic positions is obtained without any additional approximations. This work generalises the method of Ref. [Jing-Tao Lü et al, PRB 85, 245444 (2012)] in two main aspects: (i) going beyond the partitioned approximation and (ii) the stochastic equations of motion for quantum ions are rigorously derived.

DY 80.3 Fri 10:30 BH-N 128

Anomalies, Rare Events, and Brownian Motion — Jose M. Miotto[1], Simone Pigolotti[2], Aleksei V. Chechkin[3,4], and •Sandalo Roldan-Vargas[5] — [1]Leiden Institute of Advanced Computer Science, Leiden University, Netherlands — [2]Okinawa Institute for Science and Technology, Japan — [3]Institute for Physics and Astronomy, University of Potsdam, Germany — [4]Akhiezer Institute for Theoretical Physics, Kharkov, Ukraine — [5]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

In one of his celebrated 1905 papers, Albert Einstein proposed for the first time a statistical interpretation of Robert Brown innocent observation based on the corpuscular constitution of matter. His theory suggested that the long time motion of a Brownian particle is diffusive whereas the probability distribution of the particle displacements is Gaussian. For more than one hundred years these predictions were systematically validated in real systems and the coexistence between Diffusivity and Gaussianity became a paradigm. However, recent experiments on mesoscopic particle systems have claimed the existence of a time regime where diffusion is not accompanied by a purely Gaussian distribution of displacements. By molecular dynamics simulations of 2- and 3-D glass and gel forming-liquids we show the emergence of a non-Gaussian exponential tail in the probability distribution of particle displacements whose exponential rate is dimension dependent. We further show that the diffusive regime accompanying the non-Gaussian distribution of displacements is the result of a mixture of anomalous diffusivities.

DY 80.4 Fri 10:45 BH-N 128

Large deviation function for a driven underdamped particle in a periodic potential — •Lukas P. Fischer, Patrick Pietzonka, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Germany

Large deviation theory is a versatile tool that proved useful for establishing connections between current fluctuations and thermodynamic steady state properties, e.g. the thermodynamic uncertainty relation [1]. Previous studies, however, were limited to systems which are diffusive in all variables, i.e. overdamped Brownian motion or Markov jump processes. We extend the work to underdamped Brownian motion of a single, driven particle in a periodic potential [2]. To this end, we derive an explicit expression for the large deviation functional of the empirical phase space density, which replaces the level 2.5 functional used for overdamped dynamics. Using this approach, we obtain several bounds on the large deviation function of the particle current. We compare them to bounds for overdamped dynamics that have recently been derived. Furthermore, we assess the tightness of the bounds in a numerical case study for a cosine potential.

[1] A.C. Barato, U.S., Phys. Rev. Lett. **114**, 158101 (2015)
[2] L.P.F., P.P., U.S., submitted to Phys. Rev. E

DY 80.5 Fri 11:00 BH-N 128

Dynamic mode locking in a driven colloidal system — Michael Juniper[1], Urs Zimmermann[2], •Arthur Straube[3], Rut Besseling[4], Dirk Aarts[1], Hartmut Löwen[2], and Roel Dullens[1] — [1]Department of Chemistry, University of Oxford, UK — [2]Institute of Theoretical Physics, Heinrich-Heine-Universität Düsseldorf, Germany — [3]Freie Universität Berlin, Institute of Mathematics, Berlin, Germany — [4]InProcess-LSP, Oss, The Netherlands

We examine both experimentally and theoretically the microscopic dynamics underlying mode locking in a colloidal system [1,2]. We first look at a colloidal particle driven by a modulated force over a sinusoidal optical potential energy landscape. Coupling between the competing frequencies of the modulated drive and that of particle motion over the periodic landscape leads to synchronization of particle motion into discrete modes, manifesting as Shapiro steps in the average particle velocity. State diagrams from experiment, simulation, and theory agree well. Further, we use this approach to examine the enhancement of mode locking in a flexible chain of magnetically coupled particles, which we ascribe to breathing modes caused by mode-locked density waves. Finally, we demonstrate that an emergent density wave in a static colloidal chain mode locks as a quasi-particle, with microscopic dynamics analogous to those seen for a single particle.

[1] M. Juniper, A. Straube, R. Besseling, D. Aarts, R. Dullens, Nat. Commun. 6, 7187 (2015)
[2] M. Juniper, U. Zimmermann, A. Straube, R. Besseling, D. Aarts, H. Löwen, R. Dullens, New J. Phys. 19, 013010 (2017)

DY 81: Nonlinear Dynamics, Synchronization, Chaos II

Time: Friday 10:00–12:30 Location: BH-N 243

DY 81.1 Fri 10:00 BH-N 243

Phase coherence and intermittency of a turbulent field based on a system of coupled oscillators — •José-Agustín Arguedas-Leiva and Michael Wilczek — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland

Intermittency, i.e. a non-self-similar scale dependence of fluctuations, is a hallmark of fully developed turbulence. In turbulent flows, velocity fluctuations display Gaussian large-scale statistics with a transition to non-Gaussian statistics on smaller scales. For a Gaussian random field, the Fourier modes are statistically independent. Conversely, it can been shown that Fourier modes with random phases produce approximately Gaussian real-space statistics under quite general conditions. Non-Gaussianity and phase coherence are therefore intimately related. This motivates our study of intermittency in a turbulent flow as a scale-dependent coherence phenomenon of the Fourier phases. To better understand the relation between real-space intermittency and spectral-space coherence, a simple coupled oscillator model is proposed, which is reminiscent of the spectral-space formulation of the Navier-Stokes equations, in which sets of three phases are coupled in so-called triads. By studying this model we show that the three-oscillator probability density functions (PDFs) can be completely identified in terms of triad PDFs. Furthermore, a convenient parametrization allows for quantitative description of each triad's PDF using only one parameter. Using this parameter, we can isolate each triad's contribution to the real-space statistics, thereby establishing a relation between phase coherence phenomena and real-space intermittency.

DY 81.2 Fri 10:15 BH-N 243

Memristive Devices in a Chua Circuit: Comprizing Memory and deterministic Chaos — •Tom Birkoben[1], Mirko Hansen[1], Martin Ziegler[1], Karlheinz Ochs[2], Enver Solan[2], and Hermann Kohlstedt[1] — [1]Chair of Nanoelectronics, Faculty for Electrical Engineering and Information Technology, Kiel University, Germany — [2]Chair of Digital Communication Systems, Department of Electrical Engineering and Information Science, Ruhr University Bochum, Germany

Chua's circuit consists at least of one non-linear electronic device, a locally active resistor and three energy-storage elements. The circuit attracts considerable interest because it allows the study of a variety of chaos related phenomena, such as double scroll attractors and bifurcation diagrams. Here we present experimental results of a Chua circuit compromising real memristive double barrier $Nb/Al/Al_2O_3/Nb_xO_y/Au$ junctions. The devices are forming free and the I-V curves are characterized by an analog switching mechanism with a typical R_{off}/R_{on} ratio of about 100 at 0.7 V. Besides inserting a single memristive device in parallel to Chua's diode, the diode was replaced by two anti-parallel connected memristive devices. In this way, multiple scroll attractors were obtained. The dynamics of the system were characterized by chaotic oscillations interrupted by minute long time intervals in which the oscillations were suppressed. The results will be discussed in the framework of time series measurements and compared to simulations in LTSpice.

DY 81.3 Fri 10:30 BH-N 243

Control of multistability of driven nonlinear oscillators by two-frequency forcing — •Ferenc Hegedus[1], Werner Lauterborn[2], Ulrich Parlitz[3], and Robert Mettin[2] — [1]Department of Hydrodynamic Systems, Budapest University of Technology and Economics, Budapest, Hungary — [2]Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany — [3]Research Group Biomedical Physics, Max Planck Institute for Dynamics and Self-Organization and Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Göttingen, Germany

One of the main challenges of applied nonlinear science is the non-feedback control of multistability, that is, how to force a system to settle down onto a pre-selected attractor. In the present study, a novel approach for solving this control task is presented for sinusoidally driven nonlinear oscillators, which is suitable to target attractors directly (only with limited constraints). The method is based on the observation, that, for example, a period-2 attractor can be continuously transformed into a period-3 orbit (and vice versa) by applying a second, sinusoidal component to the driving (with suitable tuning of the excitation amplitudes). The pair of commensurate frequencies used for dual-frequency driving has to be properly chosen according to the periods of the transformed orbits.

DY 81.4 Fri 10:45 BH-N 243

Dynamics in ensembles of excitable units with global repulsive coupling — •Michael Zaks — Humboldt Universität zu Berlin, Institut für Physik

We consider ensembles build from excitable elements. In contrast to oscillators, isolated excitable units feature no oscillatory dynamics but stay at rest. Excitability means that for finite-size disturbances relaxation to the equilibrium is preceded by a large-scale excursion in the phase space. Description of this property, shared e.g. by many cortical cells, can be reduced to dynamics on the circle: the so-called "active rotator". Attractive coupling draws together an ensemble of excitable elements: stability of the equilibrium is enhanced. In contrast, repulsive coupling (an example is delivered by inhibitory neurons), weakens stability. Under sufficiently strong repulsion the equilibrium gets destabilized, and the large-scale oscillations commence: the formerly quiescent system acquires dynamics that completely owes to the interactions. For an ensemble of identical active rotators with global repulsive coupling the onset of oscillations occurs via the global event: the transcritical heteroclinic bifurcation. The number of unstable states of equilibrium, involved in the bifurcation, exponentially grows with the size of the ensemble. This transition gives rise to a large amount of stable periodic motions; moreover, if the coupling to the global field is restricted to the first Fourier harmonics of the rotator phase, the Strogatz-Watanabe phenomenon takes place, and the attracting periodic states fill high-dimensional continua. We discuss collective oscillations both for small ensemble of excitable units and in the thermodynamical limit.

15 min. break

DY 81.5 Fri 11:15 BH-N 243

Mechanism of underdrive pacing for low-energy defibrillation — •Pavel Buran, Markus Bär, and Thomas Niedermayer — 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 more gently than a single high-energy pulse. During this low-energy antifibrillation pacing (LEAP), only tissue near sufficiently large conduction heterogeneities, such as large coronary arteries, is activated. Theoretical approaches to understand LEAP have often focussed on unpinning and removal of a small number of stable spirals and suggest LEAP protocols using overdrive or underdrive pacing or combinations of it. In this talk, we demonstrate that for typical cellular models, which exhibit stable pinned spirals, the process of unpinning and drift of spirals does not appear during successful LEAP. We present an alternative mechanism of underdrive pacing, which explains both the termination of stable spirals and spatiotemporal chaos.

DY 81.6 Fri 11:30 BH-N 243

Normal and anomalous diffusion in soft Lorentz gases — •Rainer Klages[1], Sol Selene Gil Gallegos[1], Janne Solanpää[2], Mikka Sarvilahti[2], and Esa Räsänen[2] — [1]Queen Mary University of London, School of Mathematical Sciences — [2]Laboratory of Physics, Tampere University of Technology

Motivated by electronic transport in artificial graphene, we study the diffusion of point particles in a soft periodic Lorentz gas modeled by repulsive Fermi potentials on a triangular lattice. We find that the diffusion coefficient is a highly irregular function of the minimal distance between adjacent scatterers as a control parameter. Parameter regions of normal diffusion alternate with regions exhibiting superdiffusion. The latter are due to islands of periodic orbits in phase space whose origin and structure we explore in detail. The coarse functional form of the parameter-dependent diffusion coefficient is well reproduced by simple random walk models [1].

[1] R.Klages, S.S.G.Gallegos, J.Solanpää, M.Sarvilahti, E.Räsänen, submitted

DY 81.7 Fri 11:45 BH-N 243

Dependency of musical instrument forced oscillations on viscoelastic internal damping — •Rolf Bader — Institute of Systematic Musicology, University of Hamburg, Germany

A viscoelastic model for the internal damping of musical instruments is implemented within a Finite-Difference Time Domain (FDTD) method. Internal damping of wood, leather, neylon, mylar, glue or varnish strongly change the timbre of musical instruments and the precise spectrum of this damping contributes strongly to the individual instrument character. The model assumes a complex, frequency-dependent and linear stiffness in the frequency domain, which is analytically transferred into the time-domain using a Laplace transform. The resulting mass-weighted restoring force integral of the respective membrane or plate differential equation is solved using a circular buffer accumulation method for each spatial node on the geometry, which is effective, as the model is implemented on a massive parallel Graphics Processing Unit (GPU). The model is able to reproduce arbitrarily shaped internal damping frequency responses with sharp bandwidth and fast response. Due to the time-delay feedback loop of viscoelastic damping additional sidebands appear around damped partials which are caused by amplitude oscillations. The piano soundboard driven by a string is forced to vibrate with the strings frequencies as it is higher in dimensionality as well as damped stronger. The forced oscillation patterns are strongly depending on the amount of internal damping.

DY 81.8 Fri 12:00 BH-N 243

The Nature of Microtiming Deviations in Musical Performances — Mathias Sogorski[1,2], •Theo Geisel[1,2], and Viola Priesemann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]Bernstein Center for Computational Neuroscience, Göttingen

Musical rhythms performed by humans typically show temporal fluctuations. While they have been characterized in simple rhythmic tasks in laboratory settings, it is an open question what is the nature of temporal fluctuations, when several musicians perform music jointly in all its natural complexity. To study such fluctuations in over 100 original jazz and rock/pop recordings played with and without metronome we developed a semi-automated workflow allowing the extraction of cymbal beat onsets with millisecond precision.

Analyzing the inter-beat interval (IBI) time series revealed evidence for two long-range correlated processes characterized by power laws in the IBI power spectral densities. One process dominates on short timescales (t<8 beats) and reflects microtiming variability in the generation of single beats. The other dominates on longer timescales and reflects slow tempo variations. Whereas the latter did not show differences between musical genres (jazz vs. rock/pop), the process on short timescales showed higher variability for jazz recordings, indicating that jazz makes stronger use of microtiming fluctuations within a measure than rock/pop. Our results elucidate principles of rhythmic performance and can inspire algorithms for artificial music generation.

DY 81.9 Fri 12:15 BH-N 243

Measuring the information dimension in chaotic scattering — •Domenico Lippolis — Institute for Applied Systems Analysis, Jiangsu University, Zhenjiang, China

Measuring the fractal dimension of a non-attracting chaotic set embedded in the phase space of an open system is, in general, a challenging task to fulfill. While the existing box-counting techniques are designed for numerical estimations, they are largely impractical for an actual experiment. In the present contribution, the information dimension of a two-dimensional chaotic saddle is alternatively estimated by means of a numerical simulation of a scattering experiment, measuring the response of a cross section to perturbations (uncertainty function), which is, in principle, realizable in the laboratory. In addition, a theoretical argument relating the estimated uncertainty dimension to the conventional information dimension is provided. Generalization to partially absorbing systems such as optical or microwave cavities is also discussed.

DY 82: Glasses and Glass Transition (joint session DY/CPP)

Time: Friday 10:00–12:45 Location: BH-N 334

DY 82.1 Fri 10:00 BH-N 334

Can the glass transition occur in non-equilibrium? — •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Recently, there have been great advances in the simulation of equilibrated hard sphere systems up to high densities that can even exceed the athermal jamming packing fraction (see, e.g., [1]). As a consequence, several researchers claim that all previous simulations were obsolete and that it even was not allowed to do further studies of non-equilibrium systems.

In my contribution I want to motivate that by limiting the research to systems in equilibrium one misses important and interesting phenomena that exist in non-equilibrium systems, e.g., ageing, avoidance of crystallization, history-dependence, as well as many other properties of the dynamical glass transition and of glasses. I argue that dynamical glasses obtained by rapid quenches can be significantly different from ideal, structural glasses that might occur in equilibrated systems.

[1] A. Ninarello, L. Berthier, and D. Coslovich, Phys. Rev. X 7, 021039 (2017).

DY 82.2 Fri 10:15 BH-N 334

Nonlinear response theory: simple stochastic models — •Gregor Diezemann — Institut für Physikalische Chemie, Universität Mainz

The effect of large electric fields on the relaxation of supercooled liquids and also other systems like ionic liquids and crystals has been studied intensively during the last decade. Due to the formal lack of an analogue to the well known fluctuation dissipation theorem valid for linear response, one essentially relies on model calculations in the nonlinear case. There are a number of different models that have been used to compute the nonlinear response of glassforming systems, such as the so-called box model, the model of isotropic dipole reorientations or the dipole flips in an asymmetric double well potential (ADWP). I will discuss the results of model calculations of the nonlinear response for simple stochastic models for the dynamics. In particular, I will consider the ADWP model which is known to exhibit a peak in the modulus of the third-order response in a narrow temperature range around some characteristic temperature. Interestingly, in fifth order one observes peaks in the modulus around two characteristic temperatures. These peaks are related to the vanishing of the nonlinear static susceptibility in the respective order. The results will be discussed in the light of recent experimental observations.

DY 82.3 Fri 10:30 BH-N 334

Lokaler Debye-Prozess? Einblicke in 1-Propanol mit Hilfe der Triplett-Solvatationsdynamik — •Daniel Koestel[1], Peter Weigl[2], Thomas Blochowicz[2] und Thomas Walther[1] — [1]TU Darmstadt, Institut für Angewandte Physik — [2]TU Darmstadt, Institut für Festkörperphysik

Mit Hilfe der Triplett-Solvatationsdynamik (TSD) ist es möglich das Relaxationsverhalten unterkühlter Flüssigkeiten und auch in geometrisch eingeschränkten Systemen lokal zu untersuchen [1]. Dabei wird ein Farbstoff in geringer Konzentration in der Probe gelöst und mittels eines UV-Laserpulses in einen langlebigen Triplett-Zustand angeregt. Durch die Relaxation der den Farbstoff umgebenden Moleküle kommt es zu einer Rotverschiebung des vom Farbstoff emittierten Spektrums. Diese zeitabhängige Stokes-Verschiebung kann zur Bestimmung des lokalen Relaxationsverhaltens der Solvationshülle genutzt werden [1]. Wasserstoffbrückenbildende Flüssigkeiten sind von besonderem Interesse, da diese auch in biologischen Systemen eine zentrale Rolle einnehmen. Besonders Monohydroxy Alkohole weisen dabei in der dielektrischen Spektroskopie den prominenten Debye-Prozess auf [2], dessen mikroskopischer Ursprung nach wie vor Gegenstand kontroverser Diskussion ist und meist der Relaxation einer transienten, supermolekularen Kettenstruktur zugeschrieben wird, die sich aufgrund von Wasserstoffbrücken ausbildet [3]. Dabei gehen wir der Frage nach, ob und wie diese Kettendynamik von einer lokalen Sonde detektiert wird.

[1] R. Richert. J. Chem. Phys. 113 (2000) [2] J. Gabriel et al. J. Phys. Chem. B 121 (2014) [3] R. Böhmer et al. Phys. Rep. 545 (2014)

DY 82.4 Fri 10:45 BH-N 334

Analytical solution of the spin model on the Bethe lattice — •Koray Önder[1,2], Till Kranz[1,2], and Matthias Sperl[1,2] — [1]Institut für Theoretische Physik, Uni Köln — [2]Institut für Materialphysik im Weltraum, DLR Köln

The cooperative facilitation scenario (CFS) on the Bethe lattice shows similarities in the correlation functions with the mode coupling theory (MCT). The first studies by fitting some critical exponents on the CFS are in good agreement with the MCT predictions [1].

The fact that the CFS on the Bethe lattice yields a bifurcation scenario can be used to describe the asymptotic dynamics of the system. As a result we obtain analyticaly exact predictions for the critical exponents and the master function.

[1] M. Sellitto, Phys. Rev. Lett. **115**, 225701 (2015)

DY 82.5 Fri 11:00 BH-N 334

Structure and dynamics of water-like models — •Robin Horstmann and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

Among glass-forming liquids tetrahedral network formers like water have a special position. Their vast amount of anomalies make the transfer of models like density scaling difficult. We thus use molecular dynamics simulations to examine a family of water-like molecules produced by systematically varying the partial charges of the SPC/E and TIP4P2005 water models [1]. The geometry of the molecules remains unchanged but the inter-molecular interactions of the models vary strongly. We show that the resulting dynamics spread over a wide temperature range with the glass transition temperature T_g and the high temperature activation energy E_∞ both changing by a factor of five. Models of the glass transition are tested using observables from these studies on water-like models in the bulk and from concomitant work on these systems in confimenent which allows us to determine structural and dynamical length scales. Common behavior of the models can be found using a recently proposed empirical function that splits the activation free energy into a constant value E_∞ and an exponentially growing contribution $E_c(T)$ [2]. A common ratio of E_∞/T_g is found. Modification of the partial charges also changes the phase diagram preparing the ground for studies of water's two supercooled phases.

[1] Horstmann, R., and M. Vogel. J Chem Phys **147**, 034505 (2017)
[2] Schmidtke, B. et al., Phys. Rev. E **86**, 041507 (2012)

DY 82.6 Fri 11:15 BH-N 334

Secondary Relaxation Dynamics Observed by Photon-Correlation-Spectroscopy — •Till Böhmer, Jan Gabriel, Andreas Helbling, Florian Pabst, and Thomas Blochowicz — TU Darmstadt, Institut für Festkörperphysik, Germany

Secondary relaxation processes in simple molecular glass formers have been a long-standing topic in research of supercooled liquids and amorphous solids. In particular understanding the mechanism behind Johari-Goldstein-β-relaxation is considered to be important, because it originates from the dynamic of the entire molecule and is expected to be a universal feature of the glass-transition.

To obtain a new perspective, photon-correlation-spectroscopy (PCS) was utilized to examine reorientational dynamics in various monohydroxy alcohols. After improvements regarding the experimental setup secondary relaxation processes were successfully resolved in PCS. By comparing the results of light scattering experiments with those of broadband dielectric spectroscopy, focusing on the differences in amplitude and shape of the respective processes, insight on the mechanism behind the JG-β-relaxation can be gained.

15 min. break

DY 82.7 Fri 11:45 BH-N 334

Emergent Many-body Interactions and Inapplicability of Hard Sphere Jamming Theory — •Yoav G. Pollack[1], Murari Singh[1], Giorgio Parisi[2], Corrado Rainone[1], and Itamar Procaccia[1] — [1]Weizmann Institute of Science, Israel — [2]Sapienza Universit di Roma, Italy

The mechanism of jamming in soft matter was recently argued to be dimensionally independent by studying the scaling exponents predicted within an infinite-Dimensional mean-field hard-sphere theory. The predicted critical exponents were found to match surprisingly well the numerical measurements in finite-D including 2D and 3D. Such a match seemingly suggests that the infinite-D theory is applicable to realistic systems. Our current work addresses the puzzle of this lack of strong D dependence usually observed in critical phenomena.

We study the jamming transition using *effective* inter-particle forces. In thermal materials where nevertheless the mean positions are well defined on a given time-scale, these effective forces are what keeps the particles "in place". We observe emergent effective many-body forces, and quantify the non-binary contributions Vs. proximity to jamming. For hard spheres the effective forces are binary *precisely* at jamming, similarly to the infinite-D limit and propose that this explains the match of theory and measurements. We further conclude that the predictions of infinite-D hard spheres should not be inapplicable to more realistic particles which are never absolutely hard[1].

[1]G. Parisi, Y.G. Pollack, I. Procaccia, C. Rainone and M. Singh, Submitted for publication, arXiv:1709.01607.

DY 82.8 Fri 12:00 BH-N 334

Controlled crystallization of luminescent lithium borate glasses — •A. Charlotte Rimbach[1], Juliane Schuppich[1], Bernd Ahrens[1,2], Franziska Steudel[2], and Stefan Schweizer[1,2] — [1]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

Lanthanide-doped borate glasses are promising candidates as frequency-converter for LED applications. The borate glass system provides high transparency in the visible spectral range, good lanthanide ion solubility and high mechanical stability. The lanthanide ions terbium (Tb^{3+}) and europium (Eu^{3+}) show a bright luminescence therein with quantum efficiency values of approx. 60 % (486 nm excitation) and 90 % (396 nm excitation), respectively. However, since the absorption coefficient of the lanthanide ions is low, only a small amount of the excitation light is absorbed resulting in a poor conversion efficiency. To increase the optical absorption by prolonging the optical pathway through multiple scattering within the glass, the as-made luminescent borate glasses are processed to glass ceramics. The focus of this work is on the analysis of the crystallization process by means of differential scanning calorimetry (DSC), in situ x-ray diffraction (XRD) as well as optical spectroscopy and quantum efficiency (QE) measurements.

DY 82.9 Fri 12:15 BH-N 334

Glassy dynamics as reflected in its inter- and intra-molecular interactions — •Friedrich Kremer, Wilhelm Kossack, and Markus Anton — Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

The inter- and intra-molecular interactions of low molecular weight and polymeric glass-forming model systems are studied by Broadband Dielectric (BDS) - and Fourier-Transform Infrared (FTIR) - Spectroscopy. Analyzing the temperature dependencies of specific IR absorption bands, reflecting the intramolecular potentials of dedicated molecular moieties, enables one to unravel on an intramolecular scale the process of glass formation and to compare it with the dielectrically determined primarily intermolecular dynamics. Molecular systems to be studied are typical glassformers as glycerol, propyleneglycol, polypropyleneglycol, propylenecarbonate and polypropylencarbonate. By that a wealth of novel information is obtained proving that the different molecular moieties of a glass former show often strongly different characteristic, temperature dependencies. This demonstrates the fundamental importance of intra-molecular dynamics giving refined insights into the underlying interactions beyond coarse-grained models treating the glassformer as rigid body.

DY 82.10 Fri 12:30 BH-N 334

Site energy distributions in ion conducting glasses — •Martin Schäfer and Karl-Michael Weitzel — Philipps-Universität Marburg, Marburg, Germany

In a crystalline sample of an ion-conducting material all ions exhibit the same surrounding and thus the same site energy. In an ion-conducting glass ions exhibit different local surroundings. Thus, a distribution of site energies will apply. So far all information on such site energy distributions appears to either come from theory or indirect experiments. This site energy distribution is evidently crucial for all transport processes involving the transport of considerable fractions of mobile ions, e.g. in battery materials. Consequently, direct information on this energy distribution best comes from an experiment, where all ions of a certain kind are almost completely depleted, e.g. by a foreign ion.

By reanalysis of previously published concentration depletion profiles within the foreign ion bombardment induced ion transport [1] we are now able to derive the complete site energy distribution of sodium ions in a calcium-sodium-phosphate glass. The occupied part of the site energy distribution spans a width of about 0.28 eV FWHM [2].

[1]*L. Rossrucker, P.V. Menezes, J. Zakel, M. Schäfer, B. Roling and K.-M. Weitzel, Zeitschrift für Physikalische Chemie, 226, 341-353, (2012).
[2]*M. Schäfer, K.-M. Weitzel, to be submitted

DY 83: Pattern Formation II

Time: Friday 10:00–12:15 Location: BH-N 333

DY 83.1 Fri 10:00 BH-N 333

Fast propagation regions of a specific geometry can cause reentry in excitable media — •Vladimir Zykov, Alexei Krekhov, and Eberhard Bodenschatz — Max Plank Institute for Dynamics and Self-Organization, Goettingen, Germany

Many theoretical and experimental studies indicate that a propagation block represents an important factor in spiral wave initiation in excitable media. The analytical and numerical results we obtained for a generic two-component reaction-diffusion system demonstrate quantitative conditions for the propagation block in a one-dimensional and a two-dimensional medium due to a sharp spatial increase of the medium's excitability or the coupling strength above a certain critical value. Here we prove that this critical value strongly depends on the medium parameters and the geometry of the inhomogeneity. For an exemplary two-dimensional medium we show how the propagation block can be used to initiate spiral waves by a specific choice of the size and shape of the medium's inhomogeneity.

DY 83.2 Fri 10:15 BH-N 333

Wave propagation in spatially modulated domains — •Steffen Martens, Alexander Ziepke, and Harald Engel — Technische Universität Berlin, Institut für Theoretische Physik, 10623 Berlin, Germany

Propagation of traveling wave patterns plays in crucial role in various technological and biophysical processes such as catalysis, CO_2 sequestration, chemical computing, neural information processing, and self-organized pattern formation in cells. Often, the medium supporting wave propagation exhibits an irregular shape and/or is limited in size, leading to complex wave phenomena.

Recently [S. Martens et al., PRE **91**, 022902; JCP **145**, 094108], we have provided a first systematic treatment by applying asymptotic perturbation analysis leading to an approximate description that involves a reduction of dimensionality; the 3D RD equation with spatially dependent no-flux boundary conditions on the reactants reduces to a 1D reaction-diffusion-advection equation. Numerical simulations demonstrate that our analytical results predict properly the nonlinear dependence of the propagation velocity on the ratio of the period of the cross-section's spatial modulation to the intrinsic width of the wave solution. As a main feature, we observe finite intervals of propagation failure of waves induced by the tube's modulation.

Proofing the assumptions made in our analytic approach, we perform experiments on the propagation of traveling pulses in the Belousov-Zhabotinsky reaction through sinusoidal modulated channels being milled into acryl glas.

DY 83.3 Fri 10:30 BH-N 333

Front propagation in agitated wet granular matter — Andreas Zippelius and •Kai Huang — Experimentalphysik V, University of Bayreuth, 95440 Bayreuth, Germany

Abstract: From sand dunes to Faraday heaping, granular materials (i.e. large agglomeration of macroscopic particles) are rich pattern forming systems. When the particles are partially wet (e.g. wet sand on the beach), a different pattern forming scenario arises due to cohesion: Kink-wave fronts were found to be the dominating pattern [1]. Here, we focus on the formation of density-wave fronts in an oscillated wet granular layer undergoing a gas-liquid-like transition [2]. The threshold of the instability is governed by the amplitude of the vertical vibrations. Fronts, which are curved into a spiral shape, propagate coherently along the circular rim of the container with leading edges. They are stable beyond a critical distance from the container center. Based on the measurement of the critical distance and the rotation frequency, we propose a model for the pattern formation by considering the competition between the time scale for the collapse of cohesive particles and that of the energy injection resisting this process.

[1] Butzhammer, L., Völkel, S., Rehberg, I. & Huang, K. *Phys. Rev. E* 92, 012202 (2015).
[2] Zippelius, A. & Huang, K. *Sci. Rep.* 7, 3613 (2017)

DY 83.4 Fri 10:45 BH-N 333

Structuring of the epithelial tissue — •Jakov Lovrić[1], Michael A. Klatt[2], Sara Kaliman[3], Gerd E. Schröder-Turk[4,5], and Ana-Sunčana Smith[3] — [1]Division of Physical Chemistry, Ruđer Bošković Institute, Zagreb, Croatia — [2]Karlsruhe Institute of Technology (KIT), Institute of Stochastics, Karlsruhe, Germany — [3]PULS Group, Institut für Teoretische Physik and EAM Cluster of Exellence, FAU Erlangen-Nürnberg, Erlangen, Germany — [4]Institut für Teoretische Physik, FAU Erlangen-Nürnberg, Erlangen, Germany — [5]Murdoch University, School of Engineering and IT, Murdoch, Australia

Structural properties of space tessellations are important to understand various problems in many fields of science and industry. One of the existing questions is how to tessellate space with the maximized centrality of the cells, usually known as Quantizer problem. Here we study stable solutions of Quantizer problem by applying Lloyd's algorithm on various disordered random point processes. We find that Lloyd's algorithm converges to a universal amorphous structure with a long-range order. Furthermore, we investigate the role of cell centrality in the epithelium tissue. First, we find that the tissue can be represented by the tessellation based on the nuclear shape of constituting cells. In the following, we explore the interplay between finite size effects and the Lloyd minimisation and find that during the epithelial tissue development, centrality as a concept may play a role and is tightly controlled by the activity of the cell.

15min. break

DY 83.5 Fri 11:15 BH-N 333

Influence of additive noise on spatially one- and two-dimensional localized structures in the Kuramoto-Sivashinsky-Verhulst equation — •Christoph Kabelitz and Stefan Jakob Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

In the past years, spatially localized structures in physical systems and mathematical models became popular [1, 2]. While mathematical models are usually deterministic, experiments suffers from noise. We present an analysis concerning the Kuramoto-Sivashinsky-Verhulst equation with additive noise. The model equation is representative for stochastic partial differential equations whose deterministic versions have stable localized structures as solutions. In both, the spatially one- and the spatially two-dimensional case, the localized structures become unstable due to noise. We will show that the average time till a structural change occurs depends primarily on the strength of noise and the distance to the pinning border of the localized structures in the equation's deterministic variant in parameter space.

[1] E. Knobloch, Annu. Rev. Cond. Matter Phys., 6, 325 (2015).
[2] D. J. B. Lloyd et al., SIAM J. on Appl. Dyn. Sys., 7, 1049 (2008).

DY 83.6 Fri 11:30 BH-N 333

Nikolaevskiy turbulence: Development and test of amplitude equations — •Steffen Richters-Finger and Stefan Jakob Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Germany

The Nikolaevskiy equation, originally introduced as a model for seismic waves [1], also appears in many different contexts ranging from instabilities of fronts over electroconvection to reaction-diffusion-systems and serves as a paradigmatic minimal model for the appearance of soft-mode turbulence in most parameter ranges. The known set of

amplitude equations describing the chaotic dynamics close to the instability were originally derived by Matthews and Cox [2]. Using Lyapunov exponents, we present an alternative approach for identifying additional scales and test a practical method for the measurement of the qualitative deviation between the full system and its amplitude model.

[1] V. Nikolaevskii, Lecture Notes in Engineering **39**, 210 (1989). [2] P. C. Matthews and S. M. Cox, Phys. Rev. E **62**, R1473 (2000).

DY 83.7 Fri 11:45 BH-N 333

DNS of the Navier-Stokes equations — •Sebastian Richter and Michael Bestehorn — Department of Theoretical Physics, BTU, 03044, Cottbus, Germany

We present a numerical method for free-surface problems of the Navier-Stokes equations under external excitation. The evolution of a two-dimensional fluid layer on a vibrating substrate is considered. Based on the nonlinear transformation $z = h(x,t) \cdot \tilde{z}$ of the vertical coordinate, we derive an algorithm that pares the required interpolations down to the minimum. The results of our simulations show good agreement with the lubrication-approximation-based model investigated in [1] and [2].

[1] M. Bestehorn, "Laterally extended thin liquid films with inertia under external vibrations", Phys. Fluids 25, 114106 (2013)
[2] S. Richter and M. Bestehorn, "Thin-Film Faraday patterns in three dimensions", Eur. Phys. J. Special Topics 226, 1253-1261

DY 83.8 Fri 12:00 BH-N 333

A Tower of Scales in Ensemble Modeling: Order, Disorder, Fusion — Antonina N. Fedorova and •Michael G. Zeitlin — Russia, 199178, St.Petersburg, V.O. Bolshoj pr., 61, IPME RAS, Mathematical Methods in Mechanics Group

A fast and efficient numerical-analytical approach is proposed for the description of complex behaviour in non-equilibrium ensembles both in the BBGKY framework and in a number of its (Vlasov-Poisson/Maxwell-like) reductions. We construct a multiscale representation for the hierarchy of partition functions by means of the variational approach and multiresolution decomposition. Modeling shows the creation of various internal structures from fundamental localized (eigen)modes. These patterns determine the behaviour of ensembles. The Waveleton, localized (meta) stable long-living pattern with minimal entropy and zero measure, is proposed as a possible model for the energy confinement state (the fusion state) in plasma.