

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

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Overview of Invited Talks and Sessions

(Lecture rooms: BH-N 128, BH-N 243, BH-N 333 and BH-N 334; Posters: A)

Invited Talks

DY 2.1	Mon	9:30–10:00	BH-N 243	Chemical warfare and survival strategies in bacterial range expansions — MARKUS F WEBER, GABRIELE POXLEITNER, ELKE HEBISCH, ERWIN FREY, •MADELEINE OPITZ
DY 9.1	Mon	15:00–15:30	BH-N 243	universal statistics of records in random sequences — •SATYA MAJUMDAR
DY 14.1	Tue	9:30–10:00	BH-N 243	Basins of Attraction for Chimera States — •ERIK ANDREAS MARTENS, MARK PANAGGIO, DANIEL ABRAMS
DY 14.2	Tue	10:00–10:30	BH-N 243	Hysteretic transitions and chaotic chimera states in networks of Kuramoto oscillators with inertia — •SIMONA OLMI
DY 14.3	Tue	10:30–11:00	BH-N 243	Transient amplitude chimeras: the impact of time delay and noise — •ANNA ZAKHAROVA, JULIEN SIEBERT, SARAH LOOS, ALEKSANDAR GJURCHINOVSKI, ECKEHARD SCHÖLL
DY 26.1	Wed	9:30–10:00	BH-N 243	Elusiveness of experimental evidence for directed percolation critical behavior — •HUGUES CHATÉ
DY 26.2	Wed	10:00–10:30	BH-N 243	Spatio-temporal dynamics in pipe flow and boundary layers — •BRUNO ECKHARDT
DY 27.1	Wed	9:30–10:00	BH-N 334	On the use and abuse of thermodynamic entropy — •PETER HÄNGGI, JOERN DUNKEL, STEFAN HILBERT
DY 32.1	Wed	15:00–15:30	BH-N 243	Turbulence and Instantons — TOBIAS GRAFKE, •RAINER GRAUER, TOBIAS SCHÄFER, STEPHAN SCHINDEL, ERIC VANDEN-EIJNDEN
DY 32.6	Wed	16:45–17:15	BH-N 243	Particle motion and irreversibility of turbulent flows — •ALAIN PUMIR, HAITAO XU, JENNIFER JUCHA, EBERHARD BODENSCHATZ
DY 41.1	Thu	9:30–10:00	BH-N 334	Ultrasoft particles under out-of-equilibrium conditions — •GERHARD KAHL
DY 42.1	Thu	9:30–10:00	BH-N 128	Time-delayed feedback control of self-organized structures in dissipative systems — •SVETLANA GUREVICH, FELIX TABBERT, ALEXANDER KRAFT
DY 50.1	Thu	15:00–15:30	BH-N 243	Branched Flows, Extreme Waves and the Random Focusing of Tsunami Waves — •RAGNAR FLEISCHMANN
DY 51.1	Thu	15:00–15:30	BH-N 334	Melting of soft disks: From liquid-hexatic coexistence to continuous transitions — •SEBASTIAN C. KAPFER, MANON MICHEL, WERNER KRAUTH
DY 65.1	Fri	9:30–10:00	BH-N 243	The "shear-gradient concentration coupling instability": non-uniform flow of sheared hard-sphere glasses. — •JAN K.G. DHONT
DY 65.2	Fri	10:00–10:30	BH-N 243	Active anisotropic fluids — •SRIRAM RAMASWAMY
DY 65.3	Fri	10:30–11:00	BH-N 243	Flow properties of anisotropic fluids — •SEBASTIAN HEIDENREICH, SABINE H. L. KLAPP, MARKUS BÄR
DY 65.4	Fri	11:00–11:30	BH-N 243	Concluding Remarks — •SIEGFRIED HESS
DY 66.1	Fri	9:30–10:00	BH-N 334	Demographic perspectives on the evolution of senescence — •ANNETTE BAUDISCH
DY 66.2	Fri	10:00–10:30	BH-N 334	Biological mechanisms of aging — •BJÖRN SCHUMACHER
DY 66.3	Fri	10:30–11:00	BH-N 334	Aging in out-of-equilibrium systems: an overview — •JEAN-PHILIPPE BOUCHAUD

DY 66.4 Fri 11:00–11:30 BH-N 334 **Aging in coarsening systems with non-algebraic growth laws** —
•MICHEL PLEIMLING

Invited talks of the joint symposium SYNPN

See SYNPN for the full program of the symposium.

SYNPN 1.1 Tue 9:30–10:00 H 0105 **Connectomics: The dense reconstruction of neuronal circuits** —
•MORITZ HELMSTÄDTER

SYNPN 1.2 Tue 10:00–10:30 H 0105 **Whole-brain imaging and analysis of network activity in behaving zebrafish** — •MISHA AHRENS

SYNPN 1.3 Tue 10:30–11:00 H 0105 **Circuit neurophysics: Theory and biophysics of information-flow through large-scale neuronal systems** — •FRED WOLF

SYNPN 1.4 Tue 11:15–11:45 H 0105 **Cognitive devices based on ion currents in oxide thin films** — •STUART PARKIN

SYNPN 1.5 Tue 11:45–12:15 H 0105 **Distributed neuro-physical interfaces: technology and "exciting" biophysics** — •SHY SHOHAM

Invited talks of the joint symposium SYPS

See SYPS for the full program of the symposium.

SYPS 1.1 Wed 9:30–10:00 H 0105 **Anticipating and avoiding tipping points** — •TIMOTHY M. LENTON

SYPS 1.2 Wed 10:00–10:30 H 0105 **Climate investment under uncertainty: the two degree target and the desire for dynamic consistency** — •HERMANN HELD, DELF NEUBERSCH

SYPS 1.3 Wed 10:30–11:00 H 0105 **What are the resources required to fulfil human needs?** — •JULIA STEINBERGER

SYPS 1.4 Wed 11:15–11:45 H 0105 **Design of Sustainable Supply Chains for Sustainable Cities** — •ANNA NAGURNEY

SYPS 1.5 Wed 11:45–12:15 H 0105 **Ecological econophysics for degrowth** — •SALVADOR PUEYO

Invited talks of the joint symposium SYHM

See SYHM for the full program of the symposium.

SYHM 1.1 Wed 15:00–15:30 H 0105 **Amplitude or Higgs Modes in Condensed Matter** — •CHANDRA VARMA

SYHM 1.2 Wed 15:30–16:00 H 0105 **Higgs Particles for Systems with U(1) Symmetry in Two Dimensions** — •LODE POLLET

SYHM 1.3 Wed 16:00–16:30 H 0105 **Massive Photons and the Anderson-Higgs Mechanism in Superconductors** — •DIRK VAN DER MAREL

SYHM 1.4 Wed 16:45–17:15 H 0105 **Amplitude Higgs Mode in 2H-NbSe₂ Superconductor** — •MARIE-AUDE MÉASSON, ROMAIN GRASSET, YANN GALLAIS, MAX CAZAYOUS, ALAIN SACUTO, PIERRE RODIÈRE, LAURENT CARIO

SYHM 1.5 Wed 17:15–17:45 H 0105 **The Higgs Mode in Disordered Superconductors Close to a Quantum Phase Transition** — •AVIAD FRYDMAN, DANIEL SHERMAN, UWE S. PRACHT, BORIS GORSHUNOV, MARTIN DRESSEL

Sessions

DY 1.1–1.3 Sun 16:00–18:30 H 0104 **Tutorial: From spin models to macroeconomics (joint tutorial SOE/ DY/ jDPG)**

DY 2.1–2.9 Mon 9:30–12:15 BH-N 243 **Statistical Physics in Biological Systems (joint session DY/ BP/ CPP)**

DY 3.1–3.9 Mon 9:30–12:00 BH-N 334 **Anomalous Diffusion (joint session DY/ CPP)**

DY 4.1–4.11 Mon 9:30–12:30 BH-N 128 **Granular Matter / Contact Dynamics Part I**

DY 5.1–5.12 Mon 9:30–12:45 C 130 **Colloids and Complex Liquids I (joint session CPP/ BP/ DY)**

DY 6.1–6.7 Mon 9:30–11:30 PC 203 **Crystallization, Nucleation and Self Assembly I (joint session CPP/ DY)**

DY 7.1–7.12	Mon	9:30–13:00	H 0104	Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/ DY)
DY 8.1–8.4	Mon	12:15–13:15	MA 001	Networks - From Topology to Dynamics Part I (joint session SOE/ DY / BP)
DY 9.1–9.13	Mon	15:00–18:45	BH-N 243	Brownian Motion and Transport (Joint session DY/ CPP/ TT)
DY 10.1–10.13	Mon	15:00–18:30	BH-N 334	Quantum Dynamics, Decoherence and Quantum Information (joint session DY/ TT)
DY 11.1–11.14	Mon	15:00–18:45	C 130	Colloids and Complex Liquids II (joint session CPP/ DY)
DY 12.1–12.6	Mon	15:30–17:00	BH-N 128	Granular Matter / Contact Dynamics Part II
DY 13.1–13.9	Mon	15:45–18:30	PC 203	Crystallization, Nucleation and Self Assembly II (joint session CPP/ DY)
DY 14.1–14.8	Tue	9:30–12:30	BH-N 243	Focus Session: Chimera states: symmetry-breaking in dynamical networks (joint session DY/ BP)
DY 15.1–15.11	Tue	9:30–12:30	BH-N 334	Statistical Physics - general
DY 16.1–16.11	Tue	9:30–12:30	BH-N 128	Microswimmers - Part I (joint session DY/ BP/ CPP)
DY 17.1–17.9	Tue	9:30–12:00	BH-N 333	Modeling and Data Analysis
DY 18.1–18.8	Tue	9:30–13:00	H 0104	Focus Session: Dynamics in Many-Body Systems: Equilibration and Localization (joint session TT/DY)
DY 19.1–19.10	Tue	9:30–12:15	A 053	Transport: Graphene (joint session TT/ CPP/ DS/ DY/ HL/ MA/ O)
DY 20.1–20.10	Tue	10:15–13:15	MA 001	Focus Session: Complex Contagion Phenomena (joint session SOE/ DY/ BP)
DY 21.1–21.8	Tue	14:00–16:00	H 3010	Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 3 (joint session TT/ DY)
DY 22.1–22.9	Tue	14:00–16:15	MA 001	Evolutionary Game Theory II (joint session SOE/ BP/ DY)
DY 23.1–23.7	Tue	14:30–16:15	BH-N 243	Reaction-Diffusion Systems
DY 24.1–24.6	Tue	14:30–16:00	BH-N 334	Quantum Chaos (joint session DY/ TT)
DY 25.1–25.5	Tue	15:00–16:15	BH-N 128	Nonlinear Stochastic Systems
DY 26.1–26.9	Wed	9:30–12:30	BH-N 243	Focus Session: Percolation and turbulent transition
DY 27.1–27.9	Wed	9:30–12:15	BH-N 334	Statistical Physics far from Thermal Equilibrium - Part I
DY 28.1–28.9	Wed	9:30–12:00	BH-N 128	Nonlinear Dynamics, Synchronization and Chaos - Part I
DY 29.1–29.12	Wed	9:30–13:15	H 1028	Statistical Physics of Biological Systems - Part II (joint session BP/DY/ CPP)
DY 30.1–30.5	Wed	9:30–12:15	H 0105	SYPS: Physics of Sustainability and Human-Nature Interactions (joint symposium SOE/ AKE/ BP/ DY/ jDPG)
DY 31.1–31.5	Wed	11:30–12:45	H 3005	Transport: Fluctuations and Noise (joint session TT/ CPP/ DY)
DY 32.1–32.12	Wed	15:00–18:45	BH-N 243	Focus Session: Statistics of fully developed turbulence
DY 33.1–33.12	Wed	15:00–18:15	BH-N 334	Critical Phenomena and Phase Transitions
DY 34.1–34.5	Wed	15:00–16:15	BH-N 128	Nonlinear Dynamics, Synchronization and Chaos - Part II
DY 35.1–35.7	Wed	15:00–16:45	BH-N 333	Complex Fluids and Soft Matter - Part I (joint session DY/ CPP / BP)
DY 36.1–36.5	Wed	15:00–17:45	H 0105	SYHM Higgs Modes in Condensed Matter and Quantum Gases
DY 37.1–37.5	Wed	15:00–16:30	A 151	Fluctuating Electricity Supply: Modelling of Generation, Backup and Storage (joint session AKE / DY / SOE)
DY 38.1–38.12	Wed	15:00–18:15	C 243	Wetting, Micro and Nanofluidics (joint session CPP/ DY)
DY 39.1–39.12	Wed	15:00–18:30	C 264	Flow-Induced Structures in Complex Fluids (joint session CPP/ DRG, Deutsche Rheologische Gesellschaft/ DY)
DY 40.1–40.6	Wed	16:45–18:30	MA 001	Physics of Sustainability and Human-Nature Interactions - Part I (joint session SOE/ DY/ jDPG/ BP/ AKE)
DY 41.1–41.7	Thu	9:30–11:45	BH-N 334	Complex Fluids and Soft Matter - Part II (joint session DY/ CPP / BP)
DY 42.1–42.5	Thu	9:30–11:00	BH-N 128	Delay and Feedback Dynamics
DY 43.1–43.12	Thu	9:30–12:45	BH-N 243	Energy Systems and Power Grid (joint session DY/ AK Energy /SOE)
DY 44.1–44.10	Thu	9:30–12:15	BH-N 333	Pattern Formation
DY 45.1–45.11	Thu	9:30–13:00	C 243	Focus: Disordered Systems, Glasses under Shear I (joint session CPP/ DY)

DY 46.1–46.9	Thu	9:30–12:00	C 264	Flow-Induced Structures in Complex Fluids - Part II (joint session CPP/ DRG, Deutsche Rheologische Gesellschaft/ DY)
DY 47.1–47.6	Thu	9:30–11:15	H 2053	Superconductivity: Higgs Modes in Condensed Matter and Quantum Gases (joint session TT/ DY/ MA/ O)
DY 48.1–48.5	Thu	12:00–13:15	MA 001	Networks: From Topology to Dynamics - Part II (joint session SOE/ DY/ BP)
DY 49.1–49.5	Thu	12:00–13:15	MA 001	Dynamics on and of Networks (joint session SOE/ DY / BP)
DY 50.1–50.7	Thu	15:00–17:00	BH-N 243	Extreme Events (joint session DY/ SOE)
DY 51.1–51.6	Thu	15:00–16:45	BH-N 334	Complex Fluids and Soft Matter - Part III (joint session DY/ CPP / BP)
DY 52.1–52.9	Thu	15:00–17:30	BH-N 128	Glasses and Glass transition (joint session DY/ DF/ CPP)
DY 53.1–53.5	Thu	15:30–17:00	C 243	Focus: Disordered Systems/Glasses under Shear (joint session CPP/ DY)
DY 54.1–54.7	Thu	15:45–18:00	PC 203	Microswimmers, Active Liquids - Part II (joint session CPP/ BP/ DY)
DY 55.1–55.6	Thu	16:00–18:00	Poster A	Poster - Quantum Systems
DY 56.1–56.23	Thu	16:00–18:00	Poster A	Poster - Statistical Physics
DY 57.1–57.16	Thu	16:00–18:00	Poster A	Poster - Diffusion
DY 58.1–58.14	Thu	16:00–18:00	Poster A	Poster - Fluids
DY 59.1–59.7	Thu	16:00–18:00	Poster A	Poster - networks
DY 60.1–60.9	Thu	16:00–18:00	Poster A	Poster - complex systems and data analysis
DY 61.1–61.4	Thu	16:00–18:00	Poster A	Poster - Glasses
DY 62.1–62.24	Thu	16:00–18:00	Poster A	Poster - Dynamics
DY 63.1–63.5	Thu	17:00–18:30	MA 001	Physics of Sustainability and Human-Nature Interactions II (joint session SOE/ DY/ jDPG/ BP)
DY 64	Thu	18:00–19:00	BH-N 334	Annual General Meeting of the Dynamics and Statistical Physics Division
DY 65.1–65.4	Fri	9:30–11:30	BH-N 243	Special Session in Honor of the 75th Birthday of Siegfried Hess: Non-equilibrium dynamics of anisotropic fluids
DY 66.1–66.6	Fri	9:30–12:00	BH-N 334	Focus Session: Aging in Physical and Biological Systems (joint session DY/ BP)
DY 67.1–67.12	Fri	9:30–12:45	BH-N 128	Networks: From Topology to Dynamics (joint session DY/ BP/SOE)
DY 68.1–68.7	Fri	9:30–11:15	C 243	Glasses and Glass Transition (joint session CPP/ DF/ DY)
DY 69.1–69.10	Fri	9:30–12:15	H 1058	Complex Fluids and Soft Matter (joint session BP/DY/ CPP)
DY 70.1–70.7	Fri	9:30–11:30	C 264	Microswimmers, Active Liquids - Part III (joint session CPP/ BP/ DY)

Annual General Meeting of the Dynamics and Statistical Physics Division

Donnerstag 18:00–19:00 BH-N 334

- Bericht
- Wahl
- Verschiedenes

DY 1: Tutorial: From spin models to macroeconomics (joint tutorial SOE/ DY/ jDPG)

Formulated as a minimal model of ferromagnets, the Lenz-Ising model received a recent renaissance serving as paradigmatic basis for the formulation and analysis of models of social and economic behaviour. Prominent examples are microscopic market and price formation models incorporating herding behaviour of the economic agents and leading to nonlinear and nonequilibrium macroeconomic dynamics. The Sznajd-Weron opinion formation model introduced spin models with outflow kinetics into quantitative social modeling. Finally, the macroscopic (replicator) equations of evolutionary game theory again can be based on microscopic (Glauber-like) reaction kinetics for discretized behavioral states, whereby the payoffs from the neighborhood resemble a local meanfield. This series of tutorial lectures shows that methods adapted from statistical physics can serve as concepts in quantitative social and economic theories and are worth the effort of bridging the disciplines, which includes properly connecting to economic frameworks. (Session compiled by Jens Christian Claussen.)

Time: Sunday 16:00–18:30

Location: H 0104

Tutorial DY 1.1 Sun 16:00 H 0104
Economics in a nutshell, for physicists — ●SYLVIE GEISENDORF — ESCP Europe Berlin

The talk explains why and how the economic mainstream, the theory of neoclassical economics, is based on the idea of Newtonian physics. It also discusses why a real Newtonism would probably have been a good idea and where economists deviate from it.

Although modern economists rarely refer to physics, economic theory is based on Newton's idea of universal gravity. Following Newton's discovery, physics became an exact science with rigorous mathematical descriptions. In physics, Newton marked the beginning of the era of rational mechanics. Society was fascinated by Newton's insights and economists based their theory on classical mechanics with the explicit aim to make economics a rational science as well. But instead of adopting Newton's laws of motion they employed the simplified principle of general maximization. Whereas the laws of motion name the forces acting in a system, optimization calculus only deduces the final outcome. Even in physics, the realization of global minima or maxima is only possible under specific conditions. In economics, where actions of bounded rational agents have to be considered, these conditions are even rarer. The talk argues that a real Newtonian approach could have moderated the current lack of contact with reality, economic theory displays, and could have facilitated the necessary transition to an evolutionary theory of the economy.

Tutorial DY 1.2 Sun 16:50 H 0104
Connecting microscopic behavioral economics to macroscopic financial market models — ●SEBASTIAN M. KRAUSE — Rudjer Boskovic Institute, Zagreb, Croatia

Time series of prices show the stylized facts of broadly distributed price jumps which occur clustered. This has serious implications for the accumulation of risk. Macroscopic price evolution models for estimating risk are commonly used. They extend the random walk by including auxiliary volatility variables to model time dependent volatility. On the other hand, agent based models that include behavioral insights are used to enlighten the mechanisms behind stylized facts. This could help to predict crashes and to improve market regulation.

After briefly illustrating this background, I discuss a way of interconnecting these two strands of research. Using an agent based model

with herding, I exemplify a general recipe for finding macroscopic models numerically: A macroscopic variable which might control volatility is identified; The stochastic process ruling this volatility variable is measured, using the numeric evolution of the microscopic model. This procedure is suitable for models with puzzling emergent behavior, as well as for complicated models with many parameters. The resulting macroscopic price evolution model can be much simpler, allowing for proceeding investigations. Therefore, the field of agent based modeling profits from a macroscopic description. Another advantage is the microfoundation of macroscopic financial market models which are so far pure phenomenological. The auxiliary volatility variable can inherit a clear behavioral meaning from the microscopic model.

Tutorial DY 1.3 Sun 17:40 H 0104
You are a young and aspiring physicist. Is working at the interface with economics a good idea? — ●TOBIAS GALLA — Theoretical Physics, School of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, UK

The terms econophysics and sociophysics describe research in which physicists apply their ideas and methods to problems in economics and the social sciences. What do you have to know about the field to find your own answer to the question in the title? Well, one way is to talk to as many 'older' physicists as possible who have worked in this area, and then to form your own opinion. In this tutorial I will give you my personal assessment of what physicists can contribute to the field of economics, and comment on why they cannot contribute as easily as it may seem. We will discuss the main achievements of physicists, for example the detection of non-Gaussian features and long-range correlations in financial data, theories of market impact, non-equilibrium ideas and bottom-up models of game theory, decision making and market microstructure. At the same time you will hear about the things physicists have not achieved (despite occasional claims to the contrary). I will then present some of our own work on chaotic dynamics in the learning of complicated games and discuss the potential consequences this has for agent-based market models, and the limitations of our work. In the final part of the tutorial I will comment on the potential hurdles young physicists moving into this area might want to be aware of, and I will highlight the potentials and benefits of working in this field.

DY 2: Statistical Physics in Biological Systems (joint session DY/ BP/ CPP)

Time: Monday 9:30–12:15

Location: BH-N 243

Invited Talk

DY 2.1 Mon 9:30 BH-N 243

Chemical warfare and survival strategies in bacterial range expansions — MARKUS F WEBER, GABRIELE POXLEITNER, ELKE HEBISCH, ERWIN FREY, and MADELEINE OPITZ — Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Munich, Germany

Spreading of species into uncolonized territory is a fundamental ecological process in the evolution and maintenance of biological diversity. Although interactions between species have experimentally been identified as major determinants of species coexistence in spatially extended populations, their role in spatially expanding populations is largely unknown. Here, we address the roles of resource and interference competition by genetically tuning a bacterial model system of three *Escherichia coli* strains: a toxin (colicin) producing strain, a sensitive strain, and a resistant strain. We show that maintenance of biodiversity is determined by three strongly interdependent ecological factors: the relative ratio of the competing strains, their growth rates and the strength of toxicity. Our mathematical analysis suggests, that despite general expectations, a non-hierarchical interaction network is not a necessary prerequisite for biological diversity. Moreover, we find that robust three-strain coexistence requires a balance between growth rates and a small enough toxicity range or, alternatively, a reduced initial ratio of the colicin-producing strain. We expect that the approach presented in this study will be useful to identify further mechanisms for the maintenance of biodiversity in microbial communities.

DY 2.2 Mon 10:00 BH-N 243

A New Dimension: The Influence of Two Dimensional Niche Space on Evolutionary Food Web Models — DANIEL RITTERSKAMP and BERND BLASIS — ICBM, University Oldenburg, Germany

Food webs encode feeding interactions of ecological communities, originating from an intricate interplay of evolutionary and ecological processes. This dynamic can be described by evolutionary food web models, in which feeding interactions between species are related to the relative distance of their adaptive traits (e.g., body size) on a niche axis. However, not much is known about evolutionary food web dynamics in space.

Here, we go beyond traditional approaches and develop an evolutionary food web model in a two dimensional niche space, where the additional niche axis might describe a spatial coordinate or an environmental variable. Using numerical simulations, we investigate population dynamics, evolutionary behaviour and the emerging community structure in space. The model is able to produce both static and dynamic food webs, depending on the width of the interaction kernel; whereas food web complexity is determined mainly by the interaction strength.

We observe rich dynamics including: spatio-temporal patterns, arms races, red queen dynamics, as well as sub-food webs moving in space. By sampling the spatial axis, local food webs are recovered, which can be related to empirical data. We conclude that the additional niche-dimension is essential to capture realistic patterns of spatially structured food webs.

DY 2.3 Mon 10:15 BH-N 243

Biodiversity and ecosystem functioning in evolving food webs — KORINNA T. ALLHOFF and BARBARA DROSSEL — TU Darmstadt, Germany

We analyze an evolutionary food web model where each species is characterized by three traits, namely its own body mass, its preferred prey body mass, and the width of its potential prey body mass spectrum. Population dynamics includes feeding and competition interactions and determines which species are viable and which ones go extinct. On a timescale much slower than population dynamics, new species emerge as modifications of existing species. The network structure emerges according to the interplay between population dynamics and evolutionary rules and shows an ongoing species turnover. The model thus gives insights into how the functional diversity changes during the initial network buildup as well as due to extinction avalanches. We investigate the relation between the functional diversity and five community level measures of ecosystem functioning. These are the metabolic loss of the predator community, the total biomasses of the basal and the predator community and the consumption rates on the

basal community and within the predator community.

DY 2.4 Mon 10:30 BH-N 243

Efficiency of cellular information processing — DAVID HARTICH, ANDRE C. BARATO, and UDO SEIFERT — II. Institut für Theoretische Physik, Stuttgart, Germany

We study theoretical models inspired by the *E. coli* sensory network, using the framework of stochastic thermodynamics for bipartite systems [1]. More precisely, we model the sensory system by an internal process measuring an external process, which is a ligand concentration jumping at random between two values. We show that the rate of conditional Shannon entropy reduction, characterizing the learning of the internal process about the external process, is bound by the thermodynamic entropy production [2]. This approach allows for the definition of an informational efficiency that can be used to study cellular information processing. We start with a simple model for which ATP must be consumed so that a protein inside the cell can learn about the external environment. A further discussion illustrates, *inter alia*, that a non-zero learning rate without dissipation inside the cell can only be obtained if the external process compensates for it.

[1] DH, ACB and US, J. Stat. Mech., P02016 (2014)

[2] ACB, DH and US, New J. Phys. **16**, 103024 (2014)

DY 2.5 Mon 10:45 BH-N 243

Tackling your free energy estimates with pyfeat — ANTONIA MEY, CHRISTOPH WEHMEYER, FABIAN PAUL, HAO WU, and FRANK NOÉ — Institut für Mathematik, FU Berlin

Understanding the equilibrium properties of physical systems is of general interest in many different areas of physics. In complex systems, equilibrium properties can often only be evaluated by means of numerical simulations, which are frequently plagued by rare event dynamics. One approach to circumvent rare event dynamics is to use enhanced sampling methods (e.g. replica exchange methods or umbrella sampling).

The range of established analysis methods to optimally estimate equilibrium properties from multi-ensemble simulations often requires an expert user for their implementation or even usage. Here, we introduce a new software package, the python free energy analysis toolkit – pyfeat, that facilitates the analysis of multi-ensemble simulation. Pyfeat provides an easy-to-use interface to well established methods such as WHAM or MBAR, as well as the recently introduced transition-based reweighting analysis methods (TRAM), which borrow ideas from Markov state models. The software’s straight forward usability makes comparing different estimation method applied to the same input data trivial.

Generally, any multi-ensemble simulation can be used for the analysis ranging from all-atom protein molecular dynamics simulations to simulations of condensed matter systems. Pyfeat is available for download at: <https://github.com/markovmodel/pyfeat>.

15 min. break

DY 2.6 Mon 11:15 BH-N 243

Lateral domain formation in membranes coupled to curvature — SINA SADEGHI, MARCUS MÜLLER, and RICHARD VINK — Institute of Theoretical Physics, Georg-August-Universität Göttingen, Göttingen, Germany

The lateral heterogeneity in the plasma membrane of eukaryotic cells is an important factor for regulating biological functions. As opposed to plasma membranes, model membranes (either artificially prepared membranes, or membranes extracted from living cells) typically phase separate. To address this paradox, we present computer simulations of a coarse-grained membrane model that undergoes macroscopic phase separation at low temperature. Considering a coupling between local composition and local curvature of the membrane, we show that the system exhibits composition fluctuations with a nontrivial length scale, resembling microemulsion. The latter is identified as a region where lipid rafts can form. We furthermore probe the nature of phase transition between the phase-separating regime and the mixed state. This transition is continuous and belongs to the two-dimensional Ising universality class for weak coupling to curvature, but becomes first-order for strong curvature-composition coupling.

DY 2.7 Mon 11:30 BH-N 243

DNA denaturation transition: environmental effects on scaling — ●CHRISTIAN VON FERBER¹ and YURIJ HOLOVATCH² — ¹Coventry University, UK — ²Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, UA

The Poland and Scheraga model for the DNA denaturation transition is reconsidered taking into account environmental effects. We apply field theoretical methods to discuss environmental effects on the nature of the transition. In particular we discuss variants of the transition that may occur due to particular properties of the environment. These are the presence of uncorrelated and power-law long-range correlated disorder which influences the transition as function of the power law exponent, the quality of the solution which may affect the self- and mutual interaction of both single and double strands and combination of these. All these have significant effects on the transition.

DY 2.8 Mon 11:45 BH-N 243

Variational approach to molecular dynamics — ●BETTINA KELLER — Freie Universität Berlin, Institut für Chemie und Biochemie, Takustraße 3, 14195 Berlin

The eigenvalues and eigenfunctions of the classical molecular dynamics propagator contain the essential information about the molecular thermodynamics and kinetics. A matrix representation of the propagator can be constructed by partitioning the conformational space into discrete states and estimating the state-to-state transition probabilities from molecular dynamics simulations, yielding a so-called Markov state model (MSM). The precision of an MSM depends sensitively on how well the discretization reproduces the shape of the dominant eigenfunctions. The difficulty to find a suitable discretization has limited the routine use of MSMs. Moreover, most discretizations are data-driven,

impairing the comparison between MSMs and the interpretation of the eigenvectors in terms of structural transitions.

Using a recently published variational approach, it is possible to construct a matrix representation of the propagator using an arbitrary basis set, allowing to use basis functions with gentle slopes. This reduces the discretization error. More importantly, the user can define basis sets which have a chemical meaning and can be used for entire classes of molecules, thereby allowing for direct comparison of the kinetic models. I will give an overview of the variational principle for the classical molecular dynamics propagator and propose a basis set for peptide dynamics which is based on the dominant eigenfunctions of individual amino acids

DY 2.9 Mon 12:00 BH-N 243

Simple association-dissociation-aging process: recursive solution — ●THOMAS NIEDERMAYER and REINHARD LIPOWSKY — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

The simple association-dissociation-aging process (SADAP) is characterized by the coupling of stochastic growth and shrinkage of one-dimensional structures to the random aging of the constituting subunits. Most prominently, SADAPs capture the essential features of the polymerization of actin filaments and microtubules. Previously employed mean field methods fail to describe the dynamics of SADAPs. We found an ansatz for the full master equation which allows us to study SADAPs analytically and derive a recursion relation for the steady state solution which enables the calculation of all emergent quantities with increasing accuracy. In particular, our method allows, for the first time, the precise calculation of the boundary between the growth and shrinkage regime, in excellent agreement with results from stochastic simulations.

DY 3: Anomalous Diffusion (joint session DY/ CPP)

Time: Monday 9:30–12:00

Location: BH-N 334

DY 3.1 Mon 9:30 BH-N 334

Anomalous diffusion in corrugated potentials with spatial correlations: faster than normal, and other surprises — ●IGOR GOYCHUK — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany

Normal diffusion in corrugated potentials with spatially uncorrelated Gaussian energy disorder famously explains the origin of non-Arrhenius $\exp[-\sigma^2/(k_B T)^2]$ temperature-dependence in disordered systems. We show [1] that unbiased diffusion remains asymptotically normal also in the presence of spatial correlations decaying to zero. However, due to a temporal lack of self-averaging transient subdiffusion emerges on mesoscale, and it can readily reach macroscale even for moderately strong disorder fluctuations of $\sigma \sim 4 - 5 k_B T$. Due to its nonergodic origin such subdiffusion exhibits a large scatter in single trajectory averages. However, at odds with intuition, it occurs essentially faster than one expects from the normal diffusion in the absence of correlations. We apply these results to diffusion of regulatory proteins on DNA molecules and predict that such diffusion should be anomalous, but much faster than earlier expected on a typical length of genes for a realistic energy disorder of several room $k_B T$, or merely $0.05 - 0.075$ eV.

[1] I. Goychuk and V. Kharchenko, Phys. Rev. Lett. **113**, 100601 (2014).

DY 3.2 Mon 9:45 BH-N 334

Path Probabilities of Continuous Time Random Walks — ●STEPHAN EULE — MPI fuer Dynamik und Selbstorganisation

Employing the path integral formulation of a broad class of anomalous diffusion processes, we derive exact relations for path probability densities of these processes. In particular, we obtain a closed analytical solution for the path probability distribution of a Continuous Time Random Walk (CTRW) process. This solution is given in terms of its waiting time distribution and short time propagator of the corresponding random walk as a solution of a Dyson equation. Applying our analytical solution we derive generalized Feynman-Kac formulae.

DY 3.3 Mon 10:00 BH-N 334

Nonergodicity in scaled Brownian motion — ●FELIX THIEL and

IGOR M. SOKOLOV — Institut für Physik der Humboldt Universität zu Berlin: Newtonstraße 15, 12489 Berlin, Deutschland

Scaled Brownian motion (sBm) is a random process described by a diffusion equation with explicitly time-dependent diffusion coefficient (Batchelor's equation), which is often used for fitting experimental data for subdiffusion of unclear genesis. We show that it describes the rescaled mean position of a cloud of independent continuous time random walkers. Like the latter, sBm is neither stationary nor ergodic. Unlike continuous time random walks, the nonergodicity of sBm is not accompanied by a strong difference between its different realizations: its heterogeneity ("ergodicity breaking") parameter tends to zero for long trajectories.

DY 3.4 Mon 10:15 BH-N 334

Understanding and Controlling Regime Switching in Molecular Diffusion — ●SARAH HALLERBERG¹ and ASTRID S. DE WIJN² — ¹Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — ²Department of Physics, Stockholm University

Diffusion can be strongly affected by ballistic flights (long jumps) as well as long-lived sticking trajectories (long sticks). Using statistical inference techniques in the spirit of Granger causality, we investigate the appearance of long jumps and sticks in molecular-dynamics simulations of diffusion in a prototype system, a benzene molecule on a graphite substrate. We find that specific fluctuations in certain, but not all, internal degrees of freedom of the molecule can be linked to either long jumps or sticks. Furthermore, by changing the prevalence of these predictors with an outside influence, the diffusion of the molecule can be controlled. The approach presented in this proof of concept study is very generic, and can be applied to larger and more complex molecules. Additionally, the predictor variables can be chosen in a general way so as to be accessible in experiments, making the method feasible for control of diffusion in applications. Our results also demonstrate that data-mining techniques can be used to investigate the phase-space structure of high-dimensional nonlinear dynamical systems.

Phys. Rev. E **90**, 062901, 2014

DY 3.5 Mon 10:30 BH-N 334

Optimisation of search efficiency by combination of Lévy flights and Brownian motion — ●VLADIMIR V. PALYULIN — Physics Department, Technical University of Munich, D-85747 Garching, Germany

Problems of target search occur in a wide range of applications ranging from animals looking for prey to diffusion control of molecular processes. For a long time the field was dominated before by a notion, that Lévy flights with a critical exponent $\alpha = 1$ are optimal. Recently we proved that this statement is not always correct, and often Brownian motion presents a better alternative [1]. In this new study we show that intermittent search, which consists of Lévy flights and Brownian motion presents even better alternative. In order to show that we computed an average of inverse rate of target location, which works as a good measure of search efficiency. Analytical and numerical results are obtained from fractional Fokker-Planck equation and supported by Monte-Carlo simulations.

[1] V.V. Palyulin, A.V. Chechkin and R. Metzler, Proc. Natl. Acad. Sci. USA, **111**, 2931 (2014).

15 min. break

DY 3.6 Mon 11:00 BH-N 334

Single-file diffusion in a quenched energy landscape — ●HENNING KRÜSEMANN¹ and RALF METZLER^{1,2} — ¹University of Potsdam, Potsdam, Germany — ²Tampere University of Technology, Tampere, Finland

The diffusion of hardcore interacting particles in a narrow (1D) channel is called single-file diffusion. Examples in physics can be found especially in biophysics, e.g. the transport of molecules through a narrow pore.

The dynamical properties in a single file differ strongly from those of freely diffusing particles and different types of subdiffusion can be observed.

In this talk we discuss the msd of single-file diffusion with different particle interactions in a quenched energy landscape. We present simulation results and approach the problem theoretically.

DY 3.7 Mon 11:15 BH-N 334

Dynamical consequences of oriented particles interacting with their fractal surrounding — ●JANETT PREHL¹, RENÉ HABER¹, HEIKO HERRMANN^{1,2}, and KARL HEINZ HOFFMANN¹ — ¹Institut für Physik, Technische Universität Chemnitz, Chemnitz, Deutschland — ²Centre for Nonlinear Studies, Tallinn University of Technology, Tallinn, Estland

In order to model diffusive particles in porous media, often random walks of point particles on fractals are utilized as model system. It exhibits subdiffusive behavior, where the anomalous diffusion exponent is smaller than one, and the corresponding random walk dimension is larger than two. This is due to the limited space available in fractal structures. Within this presentation we endow the particles with an orientation [1, 2] and analyze their dynamics on fractal structures. In particular, we focus on the dynamical consequences of the interactions

between the local surrounding fractal structure and the particle orientation, which are modeled using an appropriate move class. These interactions can lead to particles becoming temporarily or permanently stuck in parts of the structure. A surprising finding is that the random walk dimension is not affected by the orientation while the diffusion constant shows a variety of interesting and surprising features.

[1] R. Haber, J. Prehl, K. H. Hoffmann, and Heiko Herrmann, *J. Phys. A: Math. Theor.* **47** (2014) 155001

[2] R. Haber, J. Prehl, H. Herrmann, and K. H. Hoffmann, *Phys. Lett. A* **377** (2013) 2840–2845

DY 3.8 Mon 11:30 BH-N 334

Fractal grid comb model — ●TRIFCE SANDEV^{1,2}, ALEXANDER IOMIN^{2,3}, and HOLGER KANTZ² — ¹Radiation Safety Directorate, Partizanski odredi 143, P.O. Box 22, 1020 Skopje, Macedonia — ²Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — ³Department of Physics, Technion, Haifa 32000, Israel

A grid comb model is a generalization of the well known comb model, and it consists of N backbones. For $N=1$ the system reduces to the comb model where subdiffusion takes place with the transport exponent $1/2$. We present an exact analytical evaluation of the transport exponent of anomalous diffusion for finite and infinite number of backbones. We show that for an arbitrarily large but finite number of backbones the transport exponent does not change. Contrary to that, for an infinite number of backbones (fractal grid comb), the transport exponent depends on the fractal dimension of the backbone structure. Thus, the grid comb model, suggested here, establishes an exact relation between a complicated fractal geometry and the transport exponent. Such a product structure of backbones times comb is an idealization of more complex comb-like fractal networks, as they may appear e.g., in certain anisotropic porous media.

DY 3.9 Mon 11:45 BH-N 334

On diffusivity landscapes in soft matter — ●FELIX ROSEN-RUNGE¹ and DOMINIQUE J. BICOULT^{1,2} — ¹Institut Laue-Langevin, Grenoble, France — ²UMR 5525, CNRS and Université Grenoble 1, France

The concept of energy landscapes has been successfully and extensively applied for the understanding of a broad range of phenomena in complex soft matter systems, such as the glass transition and protein folding. However, many experimental accounts – e.g. single-particle tracking, scattering methods and diffusion MRI – access dynamical properties, and not the free energy landscape directly. Thus, it is important to understand and exploit the effects of diffusivity landscapes, i.e. an inhomogeneous diffusivity and viscosity. First, we discuss applicability, implications and limitations of the concept of diffusivity landscapes. Second, we provide analytical approximate solutions for the diffusion equation in dynamically heterogeneous environments. Third, the results can be connected to experiments on e.g. water diffusion in hydration shells, or tracer diffusion through membranes or porous structures.

DY 4: Granular Matter / Contact Dynamics Part I

Time: Monday 9:30–12:30

Location: BH-N 128

DY 4.1 Mon 9:30 BH-N 128

Vertically vibrated granular gas with van der Waals interactions — ●QIONG BAI, JAMES P. D. CLEWETT, STEPHAN HERMINGHAUS, and MARCO G. MAZZA — Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany

Although a lot of research has focused on granular matter, as a nonequilibrium system granular matter is still a field full of unexplored static and dynamic phenomena. An important system is granular gases with macroscopic van der Waals interactions, which play a critical role in the generation process of asteroids.

Here, we study with MD simulation a vertically vibrated, 3D granular gas with van der Waals interactions between grains. As the driving amplitude and filling fraction vary, the system shows three main regimes: homogeneous, solid-gas coexistence and clustered. Moreover, when the system is in a solid-gas coexistence state, we find crystalline clusters inside the solid plug and the cluster size dramatically changes with the driving amplitude and filling fraction.

DY 4.2 Mon 9:45 BH-N 128

Ordering of Granular Rod Monolayers Driven Far from Thermodynamic Equilibrium — THOMAS MÜLLER¹, DANIEL DE LAS HERAS², INGO REHBERG¹, and ●KAI HUANG¹ — ¹Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany — ²Theoretische Physik II, Universität Bayreuth, D-95440 Bayreuth, Germany

The orientational order of vertically agitated granular rod monolayers is investigated experimentally and compared with equilibrium Monte Carlo simulations and density functional theory. At sufficiently high density, short rods form a tetratic state and long rods form a uniaxial nematic state. The length-to-width ratio at which the order changes from tetratic to uniaxial is around 7.3 in both experiments and simulations. Such a comparison illustrates the universal aspects of the self-organization of rod-shaped particles across thermal and athermal systems.

DY 4.3 Mon 10:00 BH-N 128

About the adaptability of Edwards' theory to 2D granular assemblies — ●VOLKER BECKER and KLAUS KASSNER — Institut für theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Germany

A possible approach for the statistical description of granular assemblies is Edwards' assumption that all blocked states which occupy the same volume are equally probable (Edwards, *Physica A* 157,1989). Other authors claimed that a similar approach where all states with the same stress are assumed as equally probable are more suited for developing a granular statistical mechanics, and Blumenfeld et al. (PRL 238001, 2012) argued that only a combined volume-stress ensemble is an appropriate basis for granular statistics.

We performed computer simulations using two dimensional polygonal particles excited periodically by two different protocols, excitation by "pulses of negative gravity" and excitation by "rotating gravity". The first protocol shows a non-monotonous dependency $\phi(g)$ of the mean volume fraction on the pulse strengths.

We used the overlapping histogram method in order to test whether or not the volume is described by a Boltzman-like distribution and to calculate the inverse compactivity, up to an additive constant. We found that the mean volume is a unique function of the granular temperature, independently of the protocol and of the branch in $\phi(g)$. However, this is not case for the mean stress, which can be different for the same value of compactivity (or the mean volume).

DY 4.4 Mon 10:15 BH-N 128

Packing of spheres in a flat container and geometrical frustration — KIRSTEN HARTH and ●RALF STANNARIUS — Otto-von-Guericke-Universität Magdeburg

We study the packing of monodisperse spheres in a flat vertical box with cell gap slightly larger than the particle diameter. The particles form a nearly regular triangular lattice in the cell plane. The additional freedom of a displacement normal to the cell plane places them either at the front or rear cell plate, leading to a denser arrangement in the cell plane, but at the same time to frustrated states (two of three neighboring beads have to occupy the same cell wall). Analogies to order in antiferroelectric Ising spin systems on a triangular lattice and to colloidal assemblies in thin layers are evident. We analyse the packing statistics and compare them to Monte Carlo simulations. By tilting the container from the vertical, we can modify the relative occupation numbers of front and back sites, mimicking an external field similar to magnetic fields in spin systems. The experiment offers both insights in the influence of geometrical constraints on random packing, and a descriptive example of frustrated ordering.

DY 4.5 Mon 10:30 BH-N 128

The mechanism of pattern coarsening of granular mixtures in rotating drums — ●TILO FINGER¹, RALF STANNARIUS¹, and MATTHIAS SCHRÖTER² — ¹Otto-von-Guericke-Universität Magdeburg — ²MPI für Dynamik und Selbstorganisation Göttingen

Three fundamental segregation and pattern formation processes have been reported in granular mixtures in a rotating cylindrical drum: radial segregation, axial banding and coarsening of the band pattern. While for the first effect the mechanism is well understood and for the second effect several models have been proposed, the coarsening mechanism remained unexplained so far. We reveal the mechanism for the well-known unidirectional flow between neighboring bands in an axially segregated pattern. A process of microsegregation inside each band of small particles is reported, which was so far unrecognized. On the basis of our findings, the stability of individual bands can be easily controlled by minor alternations of their composition. We suggest viable hypotheses to explain the driving force behind the flow.

DY 4.6 Mon 10:45 BH-N 128

Mechanical stability of random packings of spherocylinders — ●PASCAL WIELAND and CLAUS HEUSSINGER — Georg-August-Universität Göttingen

We simulate random packings of soft, frictionless spherocylinders over a wide range of aspect ratios ($10 \leq \alpha \leq 80$) in the vicinity of the jamming point. In our studies we focus on the stability of these packings, especially the relation between average number of contacts $\langle Z \rangle$, aspect ratio α and volume fraction ϕ . Comparison of our results with previous works shows deviations and we try to extend the model used in previous works. The results are compared with experiments done using Spaghetinis.

15 min. break

DY 4.7 Mon 11:15 BH-N 128

Cooling of 3D Granular Gases: Microgravity Experiments — ●KIRSTEN HARTH, TORSTEN TRITTEL, SANDRA WEGNER, KATHRIN MAY, and RALF STANNARIUS — Institut für Experimentelle Physik, Otto von Guericke Universität Magdeburg

Granular gases represent one of the simplest systems for investigations of non-equilibrium statistical physics, yet they are still poorly understood. They represent ensembles of macroscopic grains interacting through inelastic collisions. The use of elongated grains facilitates the realization of 3D experiments beyond the Knudsen regime. We recently found non-gaussian velocity distributions and a violation of the equipartition of kinetic energy, i.e. rotational degrees of freedom are underexcited [1]. With a special preparation technique, we can study such systems during the short microgravity period offered by drop towers. We present the first experimental study based on 3D data, with focus on the initial period of granular cooling. Experiments were conducted at the ZARM drop tower in Bremen, with approx. 9.2 of microgravity. We analyze and compare velocity and density distributions as well as the decay of kinetic energy in different experimental realizations.

[1] K. Harth, U. Kornek, T. Trittel, U. Strachauer, S. Höme, K. Will, R. Stannarius, *Phys. Rev. Lett.* 110 144102 (2013)

DY 4.8 Mon 11:30 BH-N 128

Maxwell Construction for Nonequilibrium Steady-State Phase Separation in Granular Matter — ●JAMES CLEWETT — Max Planck Institute for Self Organisation, Bunsenstrasse, Goettingen 37077

Experiments and computer simulations are carried out to investigate phase separation in a granular gas under external vibration in a large sample cell. The densities of the dilute and the dense phase are found to follow a lever rule, suggesting an equation of state. We show that this equation of state, which exhibits a non-monotonic pressure-volume characteristic, $P(v)$, can be obtained from simulations of a small cell. A Maxwell construction is found to predict both the coexisting pressure and binodal densities remarkably well, despite the fact that $P(v)$ is not an isotherm. Although the system is far from equilibrium and energy conservation is strongly violated, we can derive this finding from an energy minimization argument of fluctuating currents.

DY 4.9 Mon 11:45 BH-N 128

Changing friction in ellipsoid packings — ●SIMON J.A. WEIS¹, FABIAN M. SCHALLER^{1,2}, GERD E. SCHRÖDER-TURK¹, and MATTHIAS SCHRÖTER² — ¹Theoretische Physik, FAU Erlangen, Germany — ²Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Friction is an important parameter for the stability of granular packings. We examine packings of ellipsoids- and spheres with different friction coefficients and aspect ratios. Interparticle friction is changed by grinding the particles in a rotating drum.

Various packings are prepared and structural properties like Voronoi cell shapes, mean and local contact numbers and packing fractions as well as angle distributions and -correlations are studied by means of Xray-tomography. Data for spheres is compared to numerical data from DEM simulations.

Additionally mechanical properties of packings are measured within a shear cell setup and correlated to the structural results to contribute to a better understanding of stability.

DY 4.10 Mon 12:00 BH-N 128

nonaffine deformation and mechanical response of dense granular materials — ●M REZA SHAEBANI¹ and JENS BOBERSKI² — ¹Department of Theoretical Physics, Saarland University, Saarbrücken, Germany — ²Department of Physics, University of Duisburg-Essen, Duisburg, Germany

The mechanical response of granular materials considerably differs from that of an ordinary elastic solid. Understanding the behavior, besides the scientific interest, has important practical applications. The emerging nonlinear relation between stress and strain can be attributed e.g. to the presence of disorder, nonlinearity of the contact force law, and Coulomb friction threshold. However, even in the absence of these elements in the nature of the interactions and the environment, the nonlinear elastic response may still exist because of the unilateral interactions in dry granular systems. Opening of a contact terminates

the local transmission of restoring or frictional forces, while formation of a contact provides new possibilities for it. We first show how taking the unilateral interparticle interactions into account would improve the analytical predictions for the mechanical response, and compare the results with simulations. We attribute the remaining discrepancy to the contribution of nonaffine motions during the deformation process, and discuss the possible ways to include these motions in the stochastic modeling of stress transmission in granular media. We also clarify how the evolution of the probability distributions of contact forces deviate from the affine assumption during isotropic compression or shear deformation processes.

DY 4.11 Mon 12:15 BH-N 128

DY 5: Colloids and Complex Liquids I (joint session CPP/ BP/ DY)

Time: Monday 9:30–12:45

Location: C 130

DY 5.1 Mon 9:30 C 130

Disclination lines at homogeneous and heterogeneous colloids immersed in a chiral liquid crystal — ●SERGEJ SCHLOTTHAUER¹, MICHAEL MELLE¹, CAROL K. HALL², ENRIQUE DIAZ-HERRERA³, and MARTIN SCHEON^{1,2} — ¹Technische Universität Berlin, Berlin, Germany — ²North Carolina State University, Raleigh (NC), USA — ³Universidad Autonoma Metropolitana-Iztapalapa, Iztapalapa, Mexico

We perform Monte Carlo simulations in the isothermal-isobaric ensemble to study defect topologies formed in a cholesteric liquid crystal due to the presence of a spherical colloidal particle. Topological defects arise because of the competition between anchoring at the colloidal surface and the local director. We consider homogeneous colloids with either local homeotropic or planar anchoring to validate our model by comparison with earlier lattice Boltzmann studies. The presence of a Janus colloid in a cholesteric host fluid reveals a rich variety of defect structures. Using the Frank free energy we analyze these defects quantitatively indicating a preferred orientation of the Janus colloid relative to the cholesteric helix.

DY 5.2 Mon 9:45 C 130

Anisometry versus anisotropy in systems of colloidal magnetic cubes — ●JOE DONALDSON¹ and SOFIA KANTOROVICH^{1,2} — ¹Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — ²Ural Federal University, Lenin av. 51, 620083, Ekaterinburg, Russia

Contemporary colloid science provides numerous ways of synthesising particles with non-spherical geometries. Indeed, a whole spectrum of shapes is now readily accessible, cubes being one such example. The directionally dependent interactions of these particles are key tools in the development of new soft materials. An additional internal anisotropy is introduced into the system when these particles are constructed from a magnetic medium. Consequently, the interplay between anisometry and anisotropy, and its influence on how magnetic particles self-assemble, can be studied. Two different magnetic orientations within the cube have been considered; the first is represented by a dipole aligned along the [001] crystallographic axis, and the second by a dipole aligned along the [111] axis. We have determined the ground state structure of isolated clusters for both systems and have shown for the [001] orientation a preference for a ground state dominated by chain formation. In contrast, clusters of [111] orientated particles tend to arrange in lattices within which dipoles form ring structures consisting of four dipoles. We shall discuss the consequences of these structural configurations on the bulk properties of such systems, including preliminary predictions of the magnetic properties of dilute suspensions.

DY 5.3 Mon 10:00 C 130

Active microrheology of a nematic Liquid crystal — ●TILLMANN STIEGER¹, ANDRÉS CÓRDOBA², MARCO G. MAZZA³, JUAN J. DE PABLO², and MARTIN SCHOEN¹ — ¹Technische Universität Berlin — ²University of Chicago — ³MPIDS Göttingen

The knowledge of rheological properties of soft matter is of great importance for a variety of applications such as lubricants or the reduction of friction. The rheology of materials becomes particularly relevant if systems are miniaturized to the nanometer length scale at

Heterogeneity of local mechanical properties in binary granular systems — ●SEBASTIAN PITIKARIS, PEIDONG YU, and MATTHIAS SPERL — DLR Institute of Materials Physics in Space, Cologne, Germany

We investigate the critical scaling behavior of the contact number above the critical packing fraction in binary mixtures. We use different particle concentrations and strongly varying size ratios to see whether there is an influence to the scaling exponent. The results can be compared to theoretical predictions.

From stress-birefringent images we can precisely identify rattlers and moreover reconstruct force distributions and thus compute the local shear modulus. The results can be compared to recent simulation work which predicts a heterogeneous shear modulus in disordered systems.

which physical properties of soft matter are altered significantly from their microscopic bulk properties. The focus of this work are nematic liquid crystals (LC) which are characterized by a high degree of orientational order along a specific direction. If now a colloid is immersed into such a nematic host phase properties of the later are effected greatly at the nanoscale. The colloid perturbs orientational order of the nematic LC in its vicinity. This causes defect topologies to arise. We present nonequilibrium molecular dynamics (MD) simulations of a homogenous colloid with either planar or perpendicular anchoring of LC molecules at the colloid's surface. This leads to well known defect topologies such as the Boojum defect or the Saturn ring. The colloid is moved periodically, comparable to a typical experimental setup where one uses optical tweezers. The phase shift and the magnitude of the measured force response is used to investigate viscoelastic properties of the LC host phase. Specifically, we are interested in calculating the dynamic modulus $G = G' + iG''$, where G' and G'' are storage and loss moduli. For both quantities we present analytic expressions that can be used to analyse our MD data.

DY 5.4 Mon 10:15 C 130

Characterizing Dissipation during the Crystallization Process — ●SVEN DOROSZ — 162a avenue de la faïencerie, L1511 Luxembourg

I present computational results on the compression of a hard sphere liquid into the solid phase in finite time.

I will discuss the properties of the resulting work distributions and in particular focus on the correlations between the dissipated heat during the process and the detected structures in the solid resp. melt.

DY 5.5 Mon 10:30 C 130

Colloidal Plastic Crystals of Hard Dumbbells under Shear — ●NILS HEPTNER^{1,2}, FANGFANG CHU^{1,2}, MATTHIAS BALLAUFF^{1,2}, and JOACHIM DZUBIELLA^{1,2} — ¹Helmholtz-Zentrum Berlin, Germany — ²Humboldt-Universität zu Berlin, Germany

We study the structural response of plastic crystals of colloidal dumbbells to an oscillatory shear field using Brownian Dynamics (BD) computer simulations. Under increasing shear strains, a discontinuous transition is found from a twinned-fcc like crystal to a partially oriented highly ordered sliding-layer state via a disordered intermediate state. In this novel partially oriented sliding-layer phase, sheared hard dumbbells exhibit a small but finite collective orientational order. We show that the orientations of only weakly anisotropic particles play a crucial role in non-equilibrium transitions. Our findings from simulations are compared to data obtained by rheo-SANS experiments and reveal the nature of a second rheological yielding event which has not been observed for crystalline suspensions of hard spheres.

DY 5.6 Mon 10:45 C 130

Experimental determination of structural and dynamical heterogeneities in a metastable colloidal fluid — SEBASTIAN GOLDE¹, MARKUS FRANKE², THOMAS PALBERG³, and ●HANS JOACHIM SCHÖPE⁴ — ¹Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — ²DB Systel GmbH, Weilburger Straße 22 B4.14, 60326 Frankfurt a. Main — ³Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — ⁴Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Metastable fluids exhibit heterogeneous dynamics as well as heterogeneous structure [1]. These dynamical and structural heterogeneities play an important role in the understanding of the glass transition and crystallization. Simulations suggest that these heterogeneities in dynamics and structure are linked, but the direct experimental proof is still lacking [2]. Using space- and time-resolved dynamic light scattering and time-resolved multi angle static light scattering [3], we study the dynamics and structure in a model system of colloidal hard spheres during crystallization and vitrification. For the first time, direct correlation between the temporal evolution of the dynamical heterogeneities and the structural heterogeneities was obtained from an analysis of the subensemble resolved particle dynamics and the evolution of the static structure factor.

[1] L. Berthier and G. Biroli, *Rev.s of Mod. Phys.*, 83, (2011),[2] T. Kawasaki and H. Tanaka, *JPCM*, 22 (2010),[3] M. Franke, S. Golde and H.J. Schöpe, *Soft Matter* 10, 5380 (2014)

15 min. break

DY 5.7 Mon 11:15 C 130

Dense Colloidal Suspensions in Microfluidic Flow — ●PHILIPP KANEHL and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Dense colloidal suspensions in a pressure driven flow accumulate in the center of the microchannel. Bidisperse mixtures partially demix depending on their densities [1]. In very dense colloidal systems, one observes oscillations in the colloidal flow velocity which is attributed to transient jamming. The oscillations ultimately become irregular when density is further increased [2].

To develop a theoretical understanding of all these effects, we simulate hard spheres under pressure-driven flow in two and three dimensions using the mesoscale simulation technique of multi-particle collision dynamics which is an efficient solver of the Navier-Stokes equation and includes thermal motion.

In our simulations, we reproduce the experimental observations that a monodisperse suspension enriches the channel center and a binary mixture segregates into its two species. Comparison with our analytical model suggests that Brownian motion is crucial for demixing and that the non-diagonal elements of the collective diffusion tensor determines, which species enriches the center. Qualitative differences between 2 and 3 dimensions are found.

Finally, we present first results on monodisperse suspensions near close packing to understand flow oscillations and transient jamming.

[1] D. Semwogererea and E. R. Weeks, *Phys. Fluids*, 20, (2008).

[2] A. I. Campbell and M. D. Haw, *Soft Matter* 6, (2010).

DY 5.8 Mon 11:30 C 130

Rheological study of anisometric pigment particle suspensions — ●YONG GENG, ALEXEY EREMIN, and RALF STANNARIUS — Otto-von-Guericke-Universität Magdeburg, FNW/IEP/ANP, Postfach 4120, 39016 Magdeburg, Germany

Rheological properties of colloidal suspensions formed by nanometer size rod-shaped pigment particles dispersed in a non-polar solvent are studied. Experiments have shown that these suspensions possess unusual properties such as liquid crystalline behaviour at high dispersant concentration, field-induced phase separation at low and intermediate concentrations, switching in electric fields, and a reversible response to the adsorbing light affecting current transients in sandwich cells.1 By doping with small amounts of ferrofluid these pigment dispersions can form a basis for magneto-responsive materials. A strong magneto-optical effect has been confirmed. In our studies, we demonstrate a strong shear-induced birefringence and shear thinning behaviour in pure dispersions. We also discuss the effects of magnetic fields on the rheological properties of the pigment/ferrofluid mixtures. This helped to get a deeper insight into the properties of these suspensions and understand the mechanisms of the structural changes under external field such as electric, magnetic and flow.

1. Eremin, Alexey, et al., *Adv. Funct. Materials* 21.3 (2011): 556-564.

DY 5.9 Mon 11:45 C 130

Structure analysis of stable and metastable hard sphere fluids by confocal microscopy — ACHIM LEDERER¹ and ●HANS JOACHIM

SCHÖPE² — ¹Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — ²Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

The structural properties of the metastable melt play a key role in the understanding of the glass transition and crystal nucleation. Using laser scanning confocal microscopy we study the structure of stable and metastable colloidal hard sphere fluids. The used system was characterized with extreme care to allow a meaningful comparison with theory and simulation. While the Percus-Yevick (PY) approximation works quite perfectly for stable fluids at moderate volume fractions, it starts to fail for volume fractions larger than 0.45 approaching the freezing transition at 0.494. Strong deviation can be observed in metastable fluids: In the pair correlation function $g(r)$ the experimental data display a significant higher principal peak and a different shape in the higher order peaks than the PY-approximation. In the static structure factor $S(q)$ the data display a split in the second structure factor maximum suggesting a local short range crystalline like order. An analysis on the particle level reveals the existence of clusters with higher bond orientation order ($\langle q_6(i)q_6^*(j) \rangle$), although the overall hexagonal order of the ensemble does not increase.

DY 5.10 Mon 12:00 C 130

Effects of shear and walls on the diffusion of colloids in microchannels — ●SOMNATH GHOSH, FRIEDER MUGELE, and MICHEL DUITTS — Physics of Complex Fluids group, MESA+ institute, University of Twente PO Box 217, 7500 AE Enschede, The Netherlands

Colloidal suspensions flowing through micro-channels were studied for the effects of both shear flow and the proximity of walls on the particles* self-diffusion. Use of hydrostatic pressure to pump micron-sized silica spheres dispersed in water-glycerol through poly (dimethylsiloxane) channels with a cross section of 30x24 micron, allowed variation of the Péclet number ($Pé$) from 0.01 to 50. To obtain diffusion coefficients, image-time series from a Confocal Scanning Laser Microscope were analysed with a method that, after finding the particle trajectories, subtracts the instantaneous convective displacements and subsequently measures the slopes of the Mean Squared Displacement in the flow (x) and shear (y) directions. The thus obtained D_x and D_y , which should be equal to the free diffusion coefficient (regardless of shear) in the dilute limit, both increase strongly with Péclet number (for $Pé > 10$) in a concentrated suspension. This effect of shear-induced collisions is counteracted by the contribution of walls, which cause a strong local reduction in D_x and D_y .

DY 5.11 Mon 12:15 C 130

Transport of active particles in low-porosity structures — FRANK WIRNER¹, CHRISTIAN SCHOLZ¹, and ●CLEMENS BECHINGER^{1,2} — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Transport of active bacteria in porous media is of importance in many different fields, ranging from bioremediation, groundwater contamination and enhanced oil recovery to blood perfusion inside the body. We study the motion of active particles in artificially created porous media by a semi-experimental approach. In porous media with low porosities the presence of stagnant parts can lead to a temporary trapping of active particles in such regions, which can vastly increase their retention times. We compare the distributions of retention times and the transport properties of active and purely Brownian particles.

DY 5.12 Mon 12:30 C 130

Isobutyric acid and water mixture confined in a silica nanopore — ●MICHAEL HARRACH and BARBARA DROSSEL — Institut für Festkörperphysik, TU Darmstadt, Darmstadt, Germany

We analyze the phase behaviour of water and isobutyric acid mixtures of differing weight percentages, in a silica nanopore of roughly 4 nm diameter and a corresponding smooth-walled confinement based on the average potential as given by the pore. While experimental studies have been interpreted as showing evidence for a phase separation of water and isobutyric acid with the water situated at the pore wall we observe the converse, with the water rich part of the mixture preferring the pore center. The comparison of the smooth and rough pore allows us to further determine the importance of potential hydrogen bond sites and their influence on the static and dynamic characteristics of the mixture.

DY 6: Crystallization, Nucleation and Self Assembly I (joint session CPP/ DY)

Time: Monday 9:30–11:30

Location: PC 203

DY 6.1 Mon 9:30 PC 203

Wang-Landau type Monte Carlo study of crystallization in melts of short semi-flexible polymers — ●TIMUR SHAKIROV and WOLFGANG PAUL — University of Halle, Halle, Germany

Phase transitions in polymer melts have been under intensive experimental as well as theoretical investigation during the last years. Wang-Landau type Monte Carlo simulations were successfully applied to investigate of single polymer chains, but they weren't used for simulations of dense polymer systems. We present results of Wang-Landau simulations of melts of short semi-flexible polymers. The estimated density of state functions cover more than 5000 orders of magnitude and describe thermodynamical properties at the full energy range of the system. An analysis of the density of states shows that our model system undergoes a first-order phase-transition upon increasing the chain stiffness at fixed density. The investigation of chain properties demonstrates crystallization of the model system into a rotator-like phase. Because inter-molecular interactions have a purely repulsive nature, the phase transition is driven by maximization of the system entropy. Ordering perpendicular to the director is governed by the effective thickness of the chains and this part of the ordering process is similar to the transition into a hexatic phase of 2d hard-disks systems. Due to the equal size of all beads and the purely repulsive inter-chain interaction the chains remain mobile along the nematic director. So that in contrast to the real rotator-phase systems (for instance stiff n-alkane chains) our system demonstrates only a weak tendency to produce lamellar positional ordering.

DY 6.2 Mon 9:45 PC 203

Double-Crystalline Diblock Copolymer Nanostructures by Crystal Thickening — ●ROBERT SCHULZE, TOBIAS N. BÜTTNER, and KLAUS D. JANDT — Chair of Materials Science (CMS), Otto-Schott-Institute for Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany

Semi-crystalline diblock copolymers (DBCP) can form defined nanostructures by crystal thickening. In double-crystalline DBCP, both blocks can crystallize and, thus, be used for crystal thickening, which was not investigated, so far.

Here, the hypothesis was tested, that an increase of the lamellar period can be achieved by controlled crystal thickening of both blocks of a linear poly(ethylene)-block-poly(ethylene oxide) DBCP.

In the bulk, we found annealing induced crystal thickening for both blocks using differential scanning calorimetry. Initially crystallized bulk samples were characterized by X-ray scattering and featured a lamellar long-period that corresponded to the extended chain length of the copolymer. Similarly crystallized thin films were characterized by atomic force microscopy and the lamellar long-period was found to be one-half of the extended chain length. Annealing these thin films at elevated temperatures caused crystal thickening and an increase of the lamellar long-period.

The controlled crystal thickening of double-crystalline DBCP can be used to fabricate tailorable nanopatterns which are interesting for applications requiring surface structures with different sizes, as e.g., in photonics or the biomedical field.

Invited Talk

DY 6.3 Mon 10:00 PC 203

Direct observation of prefreezing at the interface melt-solid in polymer crystallization — ANN-KRISTIN LÖHMANN, THOMAS HENZE, and ●THOMAS THURN-ALBRECHT — Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany

The microscopic ordering process that a liquid undergoes during crystallization is often initiated at an interface to a solid. This observation is classically explained by the assumption of a reduced barrier for crystal nucleation at the interface. However, an interface can also induce crystallization by prefreezing, i.e., the formation of a crystalline layer that is already stable above the bulk melting temperature. We present an atomic force microscopy (AFM)-based in situ observation of a prefreezing process at the interface of a polymeric model system and a crystalline solid, namely polyethylene on graphite. Explicitly, we show the existence of an interfacial ordered layer that forms well above the bulk melting temperature with thickness that increases on approaching melt-solid coexistence. Below the melting temperature, the ordered layer initiates crystal growth into the bulk, leading to an

oriented, homogeneous semicrystalline structure.

DY 6.4 Mon 10:30 PC 203

Experimental test of Tammann's nuclei development approach in crystallization of macromolecules — ●EVGENY ZHURAVLEV¹, JÜRGEN W.P. SCHMELZER¹, and ALEXANDER S. ABYZOV² — ¹University of Rostock, Rostock, Germany — ²Kharkov Institute of Physics and Technology, Kharkov, Ukraine

A first attempt to probe the size distribution of homogeneously formed nuclei in polymers was realized employing Tammann's two-stage crystal nuclei development method and fast scanning calorimetry. A transfer heating rate of 500,000 K/s prevents nuclei growth on heating in poly(ϵ -caprolactone). The employed temperature profile was adapted from Tammann's two-stage crystal nuclei development method implying formation of nuclei at large undercooling (low temperatures) and following their isothermal growth at higher temperatures. Fast scanning calorimetry allowed us to reach the deep supercooling of the melt at 100,000 K/s avoiding heterogeneous and homogeneous nuclei formation and growth. Then crystal nuclei were allowed to form isothermally at the temperature corresponding to the maximum of the steady-state nucleation rate for homogeneous nucleation (210 K for PCL, $T_g = 209$ K), where both the effect of heterogeneous nucleation and the growth rate are low. The presence of these crystal nuclei and its effect on crystallization was probed by heating the sample to higher temperatures and observation of the overall crystallization process, determining the crystallization half-time. A theoretical explanation of the observations was developed.

DY 6.5 Mon 10:45 PC 203

Morphological development of poly(butadiene)-block-poly(ethylene oxide) during annealing — ●TOBIAS N. BÜTTNER¹, STEFAN HÖLZER², ROBERT SCHULZE¹, and KLAUS D. JANDT¹ — ¹Chair of Materials Science (CMS), Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany — ²Laboratory of Organic Chemistry and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany

Nanostructures of semi-crystalline diblock copolymers (DBCP) can be tuned by controlled crystal thickening, whereby the knowledge of the mechanisms and kinetics is relevant for possible applications.

In the present study we tested the hypothesis that the morphological development of a poly(butadiene)-block-poly(ethylene oxide) depends on the kinetics of crystal thickening during annealing and can be described by combining time- and temperature-dependent X-ray scattering (SAXS) and differential scanning calorimetry (DSC).

Depending on the annealing temperature, three effects predominated: crystal thickening, thermal fractionation and complete melting. We investigated the absolute long period growth due to crystal thickening by SAXS measurements. In addition, DSC based crystal thickness distributions were used to explain the running processes during annealing. The combination of both methods enables the precise tailoring of DBCP nanostructures without changing the degree of polymerization.

Nanostructures with defined dimensions are interesting for nanotemplating applications, e.g. the biomedical field.

DY 6.6 Mon 11:00 PC 203

Crystallization of binary colloidal mixtures with polymer-induced attraction — ●NICOLE SCHAERTL^{1,2}, THOMAS PALBERG³, and ECKHARD BARTSCH^{1,2} — ¹Institut für Physikalische Chemie, Universität Freiburg, Deutschland — ²Institut für Makromolekulare Chemie, Universität Freiburg, Deutschland — ³Institut für Physik, Universität Mainz, Deutschland

Polystyrene (PS) microgel colloids serve as model system for hard spheres (HS). Binary mixtures of dispersed small (S) and large (L) PS particles with diameter ratios of S to L close to a value of $\Gamma = 0.8$ have been widely used to investigate glass formation as well as re-entrant melting introduced by short-ranged depletion attraction. Previously, we have shown that depletion attractions not only enhance particle mobility, leading to a melting of the glass, but also enforce crystallization of a colloidal eutectic which is kinetically suppressed in the corresponding HS system [1]. Here we show that a subtle change of the system parameters to slightly larger Γ leads to a completely different enforced

crystallization scenario. Using static light scattering to investigate structure and kinetics including crystal size growth and packing, we observe hexagonal superlattices instead of single-component crystals. Our findings can be rationalized by the occurrence of stable binary crystals LS2, so-called Laves phases, in agreement with computer simulations by Hynninen et al. [2].

[1] Kozina et al., *Soft Matter* **10**, 9523 (2014) [2] Hynninen et al., *J. Chem. Phys.* **131**, 064902 (2009)

DY 6.7 Mon 11:15 PC 203

Frühe Belege zur Kettenfaltung in Lamellen bei massivem HDPE — •HEINZ PREUSS — 31785 Hameln

Mit dem Oberflächenabriss von aus der Schmelze bei langsamer Ab-

kühlung erstarrten massiven Proben aus Niederdruckpolyethylen (HDPE) gelang die mechanische Trennung der Lamellen längs ihrer Grenzflächen (H.H.W.Preuß, *physica status solidi* Vol. 3, 1963 S. K209 ff.). Dies belegt sowohl, dass die in elektronenmikroskopischen Oberflächenbildern sichtbaren Terrassenstufen tatsächlich die Ränder von Lamellen sind, die sich als relativ selbständige Struktureinheiten in das Probeninnere fortsetzen, als auch die schwächere Bindung der Lamellen aneinander. Zugleich erfährt das Modell der Kettenfaltung (z. B. A. Keller, *Kolloid * Zeitschrift*, 165 (1959), s. 15) eine Bestätigung. Mit dessen Hilfe lässt sich erklären, dass die Molekülketten, welche senkrecht zu den Lamellengrenzflächen orientiert sind, sich in den Lamellen kristallografisch geordnet in den Lamellen unterbringen lassen, obwohl deren Dicke D (8 bis 15 nm) deutlich kleiner ist als die Kettenlänge L .

DY 7: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/ DY)

Time: Monday 9:30–13:00

Location: H 0104

Topical Talk

DY 7.1 Mon 9:30 H 0104

Entanglement in the Many-Body Localized Phase and Transition — •JENS H. BARDARSON — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The study of entanglement, both in eigenstates and its evolution after quenches, has been instrumental in advancing our understanding of many-body localized phases—the interacting analogs of the Anderson insulator. In this talk I will discuss in detail three observations related to the entanglement properties of many-body localized systems: (i) A global quench within the many-body localized phase gives rise to a slowly (logarithmically) increasing entanglement entropy. This is due to interaction induced dephasing that is absent in the Anderson insulator and therefore serves as a unique signature of the many-body localized phase. (ii) A local quench from an eigenstate leads to an extensive increase in the entanglement entropy only at the many-body localization transition itself. And (iii) at the many-body localization transition the distribution of entanglement entropies becomes extensively broad, while it vanishes both in the extended metallic phase and in the localized phases. The width of the entanglement distribution, like the long time limit of the local quench, is therefore a useful diagnostic for a many-body localization transition. I explicitly demonstrate how all these features are observed in microscopic spin chain models of many-body localization, and, in particular, discuss how they can be used to detect a many-body mobility edge.

[1] JHB, Pollmann, and Moore, *PRL* **109**, 017202 (2012).

[2] Kjall, JHB, and Pollmann, *PRL* **113**, 107204 (2014).

DY 7.2 Mon 10:00 H 0104

Dynamics of competing orders in YBCO triggered by ultrafast light pulses — •JUNICHI OKAMOTO, ROBERT HÖPPNER, BEILEI ZHU, and LUDWIG MATHEY — Institute for Laser Physics, University of Hamburg, Hamburg, Germany

In the emerging field of optically driven strongly correlated systems, laser-excited high- T_c cuprates are one of the most fascinating topics. In equilibrium, the underdoped region of high- T_c cuprates exhibit various competing orders, e.g., stripes, density-waves and superconductivity. In this talk, we will explore the possibility of optically controlling such competing orders. In particular, we will focus on the underdoped region of YBCO, where d -wave superconductivity and charge-density waves coexist. We will present preliminary results of numerical simulations of optically driven competing orders in the material.

DY 7.3 Mon 10:15 H 0104

Ultrafast dynamics in CeTe₃ near the pressure-induced charge-density-wave transition — JONAS TAUCH¹, HANJO SCHÄFER^{1,2}, MANUEL OBERGFELL¹, JURE DEMSAR^{1,2,3}, PAULA GIRALDO⁴, IAN R. FISHER⁴, and •ALEXEJ PASHKIN^{1,5} — ¹Department of Physics and Center for Applied Photonics, University of Konstanz, Germany — ²Institute of Physics, Ilmenau University of Technology, Germany — ³Institute of Physics, Johannes Gutenberg-University Mainz, Germany — ⁴Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University, USA — ⁵Helmholtz-Zentrum Dresden-Rossendorf, Germany

Femtosecond pump-probe spectroscopy is an efficient tool for studying

ultrafast dynamics in strongly correlated electronic systems, in particular, compounds with a charge-density-wave (CDW) order. Application of external pressure often leads to a suppression of a CDW state due to an impairment of the Fermi surface nesting.

We combine time-resolved optical spectroscopy and diamond anvil cell technology to study electron and lattice dynamics in tri-telluride compound CeTe₃. Around pressures of 4 GPa we observe a gradual vanishing of the relaxation process related to the recombination of the photoexcited quasiparticles. The coherent oscillations of the phonon modes coupled to the CDW order parameter demonstrate even more dramatic suppression with increasing pressure. These observations clearly indicate a transition into the metallic state of CeTe₃ induced by the external pressure.

DY 7.4 Mon 10:30 H 0104

Mechanism of Ultrafast Relaxation of a Photo-Carrier in Antiferromagnetic Spin Background — •LEV VIDMAR — University of Munich, Germany

Understanding of relaxation dynamics in correlated condensed-matter systems is vital for identification of dominant couplings in pump-probe experiments, as well as for designing setups where ordered phases are manipulated using external fields. In many cases, phonons represent an important relaxation channel, however, in two-dimensional systems with antiferromagnetic correlations, this relaxation channel may not be the dominant one [1]. By applying state-of-the-art numerical simulations of the t-J model [2] we show that the relaxation due to coupling to antiferromagnetic spin excitations can be very fast [3]. We show that the key relaxation mechanism at very short times corresponds to the creation of high-energy antiferromagnetic excitations in the close proximity of the photo-excited holes. Such a mechanism enables an energy transfer of more than 1 eV on a 10 femtosecond time scale.

[1] L. Vidmar, J. Bonca, T. Tohyama, and S. Maekawa, *Phys. Rev. Lett.* **107**, 246404 (2011).

[2] M. Mierzejewski, L. Vidmar, J. Bonca, and P. Prelovsek, *Phys. Rev. Lett.* **106**, 196401 (2011).

[3] D. Golez, J. Bonca, M. Mierzejewski, and L. Vidmar, *Phys. Rev. B* **89**, 165118 (2014).

DY 7.5 Mon 10:45 H 0104

Pattern formation in non-equilibrium correlated electronic systems — •PEDRO RIBEIRO¹, ANDREY ANTIPOV², and ALEXEY RUBTSOV¹ — ¹Russian Quantum Center, Business-center "Ural", Novaya street 100A, Skolkovo village, Odintsovo district, Moscow area, 143025 Russia — ²Department of Physics University of Michigan, Randall Laboratory, 450 Church Street, Ann Arbor, MI 48109-1040

Strong non-equilibrium conditions eventually drive a system away from its linear response regime, deeply affecting the properties of the underlying equilibrium phase. A well known example is the Rayleigh-Bernard convection arising for classical fluids that develop convection rolls of a specific wave-length. We report on recent results regarding effects of large bias voltages applied across a half-filled Hubbard chain. At equilibrium this system shows a charge gap and strong antiferromagnetic correlations. We show that out of equilibrium the wave-vector maximizing the spin-susceptibility shifts from its equilibrium antiferromagnetic value $q = \pi$ as a function of the applied voltage

and temperature. We describe a rich set of phases induced by the interplay between electron-electron interactions and non-equilibrium conditions. Some of phases found are examples of non-equilibrium-induced spacial pattern formation. We comment on the properties and stability of these phases. Finally we argue that, although no symmetry breaking arises in the 1D system, these results suggest that a spatially modulated charge gap may be observed experimentally by STM in engineered atomic chains and nano-wires.

DY 7.6 Mon 11:00 H 0104

Time-dependent Gutzwiller wave function for the Hubbard model in nonequilibrium — ●MARCUS KOLLAR¹ and CHRISTIAN GRAMSCH^{1,2} — ¹Theoretische Physik III, Universität Augsburg — ²I. Institut für Theoretische Physik, Universität Hamburg

In previous studies the time-dependent Gutzwiller wave function (GWF) has been applied to the fermionic Hubbard model in nonequilibrium [1], using the Gutzwiller approximation which is known to become exact in the limit of infinite lattice dimension. As an alternative, we employ the variational formalism for the GWF which applies in arbitrary dimensions, recovering the dynamics obtained in Ref. [1]. We present results for the one-dimensional Hubbard model, for which exact evaluations of the GWF are available. In particular we find that the GWF captures the transient momentum distribution on short timescales [2].

- [1] M. Schiró and M. Fabrizio, Phys. Rev. Lett. **105**, 076401 (2010).
[2] S. A. Hamerla and G. S. Uhrig, Phys. Rev. B **87**, 064304 (2013).

15 min. break.

DY 7.7 Mon 11:30 H 0104

Nonequilibrium dynamics of screening in the extended Hubbard model — ●DENIS GOLEŽ and PHILIPP WERNER — University of Fribourg

We will present a study of the non-equilibrium dynamics in the extended Hubbard model on the square lattice using time-dependent extended dynamical mean-field theory. The short-time effect of the dynamical screening due to the photo-doping is the reduction of the effective static interaction. On the same time scale the fully screened interaction is transformed from the single to double mode structure due to photo-doped charge carriers. At longer times the dynamical screening enhance the relaxation dynamics.

DY 7.8 Mon 11:45 H 0104

Continuous monitoring of a quantum many-body system — ●THOMAS KIENDL¹, VINAY RAMASESH², SHAY HACOEN-GOURGY², IRFAN SIDDIQI², and FLORIAN MARQUARDT¹ — ¹Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen, Germany — ²QNL, University of California, Berkeley

At the heart of quantum mechanics lies the fact that a measurement causes back-action on the system itself. A prominent example is the quantum Zeno effect. Observing a system continuously with a large measurement strength freezes the system's dynamics. We explore how such phenomena transfer to a quantum many-body system, employing a chain of qubits as an experimentally relevant example. Using the concept of weak, continuous measurements we investigate new timescales caused by continuous monitoring of the chain. In this context, we present new results on relaxation dynamics and thermalization for both integrable and non-integrable Hamiltonians.

DY 7.9 Mon 12:00 H 0104

Influence of quadrupolar interactions in the anisotropic central spin model — ●JOHANNES HACKMANN and FRITHJOF B. ANDERS — Technische Universität Dortmund, Lehrstuhl für theoretische Physik II, 44221 Dortmund, Germany

We have investigated spin noise in an ensemble of semiconductor quantum dots (QDs). A single electron (or hole) doped QD is described by the anisotropic central spin model. Additionally, the quadrupole

moments of the nuclei couple to strain induced electric fields in the QD. We investigated the influence of these quadrupolar couplings on the central spin dynamics, that are calculated via the correlation functions $\langle S^z(t)S^z \rangle$ and $\langle S^z(\omega)S^z \rangle$. We demonstrate that our results are in good agreement with recent experiments and show that quadrupolar interactions have a large impact on measurements on hole doped QDs, while they almost are negligible for the case of electron doped QDs.

DY 7.10 Mon 12:15 H 0104

The generic fixed point model for pseudo-spin-1/2 quantum dots in nonequilibrium: Spin-valve systems with compensating spin polarizations — STEFAN GÖTTEL^{1,2}, FRANK REININGHAUS^{1,2}, and ●HERBERT SCHOELLER^{1,2} — ¹Institute for Theory of Statistical Physics, RWTH Aachen — ²JARA-Fundamentals of Future Information Technology

We study a pseudo-spin-1/2 quantum dot in the cotunneling regime close to the particle-hole symmetric point. For a generic tunneling matrix we find a generic fixed point with interesting nonequilibrium properties, characterized by effective reservoirs with compensating spin orientation vectors weighted by the polarizations and the tunneling rates. At large bias voltage we study the magnetic field dependence of the dot magnetization and the current. The fixed point can be clearly identified by analysing the magnetization of the dot. We characterize in detail the universal properties for the case of two reservoirs.

DY 7.11 Mon 12:30 H 0104

First order dynamical phase transitions — ●ELENA CANOVI¹, PHILIPP WERNER², and MARTIN ECKSTEIN¹ — ¹Max Planck Research Department for Structural Dynamics, University of Hamburg (CFEL), Building 99, Luruper Chaussee 149, 22761 Hamburg, Germany — ²Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland

Recently, dynamical phase transitions have been identified based on the non-analytic behavior of the Loschmidt echo in the thermodynamic limit [1]. By introducing conditional probability amplitudes, we show how dynamical phase transitions can be further classified, both mathematically, and potentially in experiment. This leads to the definition of first-order dynamical phase transitions. Furthermore, we develop a generalized Keldysh formalism which allows to use nonequilibrium dynamical mean-field theory to study the Loschmidt echo and dynamical phase transitions in high-dimensional, non-integrable models. We find dynamical phase transitions of first order in the Falicov-Kimball model and in the Hubbard model.

- [1] Heyl et al., Phys. Rev. Lett. **110**, 135704 (2013).

DY 7.12 Mon 12:45 H 0104

Holography of the toric code — ●JOHANNES OBERREUTER and STEFAN KEHREIN — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

Dynamics of quantum-many-body systems at weak coupling can be effectively described by quasi-particles. At strong coupling, the quasi-particle picture breaks down. Instead of resorting to numerics one can use a duality, which relates strongly coupled (conformal) field theories to classical, weakly coupled (Einstein) gravity in one dimension higher, the so-called gauge/gravity duality or AdS/CFT-correspondence. The correlation functions of the field theory can then in principle be computed from a calculation in classical gravity. The correspondence, however, in general only applies to conformal field theories and it is difficult to describe systems of interest in condensed matter theory. The observation of similarities in calculating the entanglement entropy in AdS/CFT and in MERA, a particular tensor network of a quantum state, has led to the conjecture that MERA might be a discrete version of the gauge-gravity duality. It is in principle possible to represent any quantum state in MERA. We investigate this idea in the toric code, where the representation is known exactly [1] and comment on the non-generic behaviour of this model including its dynamics.

- [1] M. Aguado, G. Vidal, Phys. Rev. Lett. **100**, 070404 (2008).

DY 8: Networks - From Topology to Dynamics Part I (joint session SOE/ DY / BP)

Time: Monday 12:15–13:15

Location: MA 001

DY 8.1 Mon 12:15 MA 001

How mutational networks shape evolutionary processes — ●HENNING SIEMEN, BENJAMIN MAIER, and DIRK BROCKMANN — Robert Koch-Institut, Berlin

Dynamic processes on complex networks have attracted a lot of attention in the past. The majority of the studies focus on understanding how topological network features shape dynamics. Several interesting results have been obtained in the context of epidemics and contagion phenomena recently, for instance the absence of epidemic thresholds in scale free networks, or the context of synchronization phenomena where certain network topologies can sustain chimera states. However, evolutionary processes on networks received comparatively little attention. It is largely unresolved how network topologies influence mutation and selection dynamics. Here, we investigate a network system of genetic strains in which each node represents a strain and links represent possible mutational pathways. We compare generic network topologies ranging from ordinary lattices and Erdos-Renyi networks to small world and scale free networks. We find that network topologies can have a substantial impact on equilibrium strain distributions. We show that locally clustered networks such as small world and lattice topologies tend to generate local maxima composed of communities with high fitness. Furthermore, we find that scale free topologies as opposed to ER networks are more likely to exhibit a lower error threshold.

DY 8.2 Mon 12:30 MA 001

Possible Origin of Stagnation and Variability of Earth's Biodiversity — ●JAN NAGLER¹, THEO GEISEL², and FRANK STOLLMEIER² — ¹ETH Zurich — ²MPI DS, Göttingen

The magnitude and variability of Earth's biodiversity have puzzled scientists ever since paleontologic fossil databases became available. We identify and study a model of interdependent species where both endogenous and exogenous impacts determine the nonstationary extinction dynamics. The framework provides an explanation for the qualitative difference of marine and continental biodiversity growth. In particular, the stagnation of marine biodiversity may result from a global transition from an imbalanced to a balanced state of the species dependency network. The predictions of our framework are in agreement with paleontologic databases.

[1] Stollmeier, Geisel, Nagler, Phys. Rev. Lett. 112, 228101 (2014)

DY 8.3 Mon 12:45 MA 001

Excitable dynamics and cellular automata dynamics on loop-free networks — ●ANNE-WIEBKE HARDER^{1,2} and JENS CHRISTIAN CLAUSSEN^{2,1} — ¹Institut für Neuro- und Bioinformatik, Universität zu Lübeck — ²Computational Systems Biology Lab, Jacobs University Bremen

Spreading dynamics on graphs or networks have attracted considerable attention in the context of pattern formation and infection dynamics [1]. Here we investigate patterns generated by excitable dynamics [2] comprised by the states of susceptible - excitable - recovered, as well as cellular automata dynamics started from a localized seed on lattices and loop-free graphs [3]. The latter type of dynamics exhibits interesting characteristics as $1/f$ type spectra [4] and relates to new integer sequences [5]. Finally we investigate cellular-automata (CA) like limiting cases of the SER dynamics.

[1] C. Kamp PLoS Comput Biol 6 e1000984 (2010)

[2] M. Müller-Linow, C. Marr, M.-T. Hütt, Phys. Rev. E 74 026112 (2006)

[3] J.C. Claussen, J. Math. Phys. 49 062701 (2009)

[4] J. Nagler and J.C. Claussen Phys. Rev. E 71 067103 (2005)

[5] J.C. Claussen, in: Online Encyclopedia of Integer Sequences, entries <http://oeis.org/A138276> and <http://oeis.org/A138277> (2008)

DY 8.4 Mon 13:00 MA 001

Noise in Coevolving Networks — ●MARINA DIAKONOVA, VICTOR EGUILUZ, and MAXI SAN MIGUEL — Instituto de Física Interdisciplinar y Sistemas Complejos IFISC (CSIC-UIB), E07122 Palma de Mallorca, Spain

Coupling dynamics of the states of the nodes of a network to the dynamics of the network topology leads to generic absorbing and fragmentation transitions. The coevolving voter model is a typical system that exhibits such transitions at some critical rewiring. We study the robustness of these transitions under two distinct ways of introducing noise. Noise affecting all the nodes destroys the absorbing-fragmentation transition, giving rise in finite-size systems to two additional regimes: bimodal magnetisation and dynamic fragmentation. Noise Targeting a fraction of nodes preserves the transitions but introduces shattered fragmentation with its characteristic fraction of isolated nodes and one or two giant components. Both the lack of absorbing state for homogenous noise and the shift in the absorbing transition to higher rewiring for targeted noise are supported by analytical approximations.

DY 9: Brownian Motion and Transport (Joint session DY/ CPP/ TT)

Time: Monday 15:00–18:45

Location: BH-N 243

Invited Talk

DY 9.1 Mon 15:00 BH-N 243

universal statistics of records in random sequences — ●SATYA MAJUMDAR — cnrs, lptms, universite paris-sud, orsay, france

Records are rather common in everyday life: we are always talking of record rainfall, record temperature, records in sports and stock prices etc. When the random sequence consists of independent random variables, the record statistics is well known. In this talk, I'll discuss the record statistics in a strongly correlated random walk sequence and show that they are universal, i.e., independent of the noise (jump) distribution. Several applications and extensions will be discussed—such as the effect of a constant drift and the effect of measurement errors.

DY 9.2 Mon 15:30 BH-N 243

Three-dimensional Brownian motion of 3D-shaped particles — ●FELIX HÖFLING — Max Planck Institute for Intelligent Systems, Stuttgart, and Institute for Theoretical Physics IV, Universität Stuttgart, Germany

The three-dimensional (3D) Brownian motion of colloidal particles of general 3D-shape is considered in the overdamped limit. First for an ellipsoidal particle, the Smoluchowski equation for the joint distribution of position and orientation is solved exactly through an expansion in moments. The non-Gaussian parameter is shown to simultaneously quantify the anisotropic positional diffusion and the orientational diffu-

sion. The results are applied further to the interpretation of scattering experiments (e.g., dynamic light scattering) on suspensions of active (self-propelled) and passive nanoparticles.

Second, a screw-like shape, paradigmatic for chiral particles, is studied which gives rise to a strong hydrodynamic coupling between rotation and translation. Coupled Langevin equations for the six degrees of freedom are used to calculate auto- and cross-correlation functions of first and second order exactly. A suitable displacement-orientation correlation is shown to display a maximum at intermediate times, from which the strength of the rotation-translation coupling can be inferred. Finally, the above findings are generalised for a hydrodynamic friction matrix of general form, which encodes an arbitrary particle shape. The analytical results are supported by numerical simulations of the corresponding stochastic equations.

DY 9.3 Mon 15:45 BH-N 243

Velocity fluctuations of Brownian particle in inhomogeneous media and driven by colored noise as a source of $1/f$ fluctuations — ●RYTIS KAZAKEVICIUS and JULIUS RUSECKAS — Institute of Theoretical Physics and Astronomy, Vilnius University, A. Gostauto 12, LT-01108 Vilnius, Lithuania

Nonlinear stochastic differential equations generating signals with $1/f$ spectrum in a broad range of frequencies have been used so far to

describe socio-economical systems [1]. We have derived such equation from Langevin equations that describe the motion of a Brownian particle in an inhomogeneous environment. The inhomogeneous environment can be a result of a linear potential affecting the Brownian particle together with the steady state heat transfer due to the difference of temperatures at the ends of the medium. The correlation of collisions between the Brownian particle and the surrounding molecules can lead to the situation where the finite correlation time becomes important, thus we have investigated the effect of colored noise in our model. Existence of colored noise leads to the additional restriction of the diffusion and exponential cut-off of the distribution of particle positions. Narrower power law part in the distribution of the particle positions results in the narrower range of frequencies where the spectrum has power law behavior.

[1] V. Gontis, J. Ruseckas and A. Kononovicius, *Physica A*, 389 100 (2010).

DY 9.4 Mon 16:00 BH-N 243

Hydrodynamically enforced entropic trapping of Brownian particles — ●STEFFEN MARTENS¹, ARTHUR STRAUBE², GERHARD SCHMID³, LUTZ SCHIMANSKY-GEIER², and PETER HÄNGGI³ — ¹Technische Universität Berlin, Berlin, Germany — ²Humboldt-Universität zu Berlin, Berlin, Germany — ³Universität Augsburg, Augsburg, Germany

In small systems spatial confinement causes entropic forces that in turn implies spectacular consequences for the control for mass and charge transport. Therefore, recent efforts in theory triggered activities which allow for an approximate description that involves a reduction of dimensionality. Up to present days, the focus was on the role of conservative forces and its interplay with confinement. Within the presented work, we overcome this limitation and succeeded in considering also "magnetic field" like, so termed non-conservative forces that derive from a vector potential [S. Martens et al., *Phys. Rev. Lett.* **110**, 010601 (2013)]. A relevant application is the fluid flow across microfluidic structures where a solute of Brownian particles is subject to both, an external bias and a pressure-driven flow. Then a new phenomenon emerges; namely, the intriguing finding of identically vanishing average particle flow which is accompanied by a colossal suppression of diffusion [S. Martens et al., arXiv:1407.5673]. This entropy-induced phenomenon, which we termed *hydrodynamically enforced entropic trapping*, offers the unique opportunity to separate particles of the same size in a tunable manner [S. Martens et al., *Eur. Phys. J. ST* **222**, 2453-2463 (2013)].

DY 9.5 Mon 16:15 BH-N 243

On the Applicability of the Caldeira-Leggett Model to Condensed Phase Vibrational Spectroscopy — ●FABIAN GOTTWALD, SERGEI IVANOV, and OLIVER KÜHN — Institut für Physik University of Rostock, Rostock, Germany

Formulating a rigorous system-bath partitioning approach remains an open issue. In this context the famous Caldeira-Leggett (CL) model that enables quantum and classical treatment on equal footing has enjoyed popularity. Although this model is by any means useful as a theoretical tool, its validity for describing anharmonic dynamics of real systems is often taken for granted. We investigate the applicability of the model by comparing the spectra resulting from the Generalized Langevin dynamics that is based on the CL model, with their counterparts from explicit classical molecular dynamics. It is shown that the model is not able to describe real systems unless the system part of the potential is effectively harmonic. We demonstrate that it is this anharmonicity, that is at the core of all deficiencies of the model and also point out the mathematical origin of its breakdown.

15 min. break

DY 9.6 Mon 16:45 BH-N 243

Dynamics of stochastic resistive switching — ●PAUL RADTKE¹, ARTHUR STRAUBE¹, ANDREW HAZEL², and LUTZ SCHIMANSKY-GEIER¹ — ¹Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — ²School of Mathematics, University of Manchester, Manchester, UK

Classes of dielectrics such as TiO_2 alter their resistance under the influence of an electric field or a current flowing through the system, an effect called resistive switching (RS). Thereby the resistance depends also on the past states of the system, it has a memory.

We will show how a particular one-dimensional lattice model for a

bipolar device. In it, oxygen vacancies hop in between consecutive sites and thereby alter local resistances. Their dynamics governed by a Master equation with jumping rates modulated by an external electric field. We discuss the system properties and show that dynamics of the vacancies can be formulated in terms of a Burgers like equation. With its help the underlying motion of the oxygen vacancies is interpreted as nonlinear traveling waves.

DY 9.7 Mon 17:00 BH-N 243

Simulation of colloidal particles in channel geometries — ●ULLRICH SIEMS and PETER NIELABA — University of Konstanz, Germany

This talk will present the results of Brownian Dynamics Simulations of colloidal particles in external fields confined in channels. Colloidal particles are well suited model-systems for a variety of problems on different length scales, ranging from gravitational collapses over the description of pedestrians to models for atomic sized problems. In such systems confinement into channels can have a great influence on the diffusion and transport properties.

DY 9.8 Mon 17:15 BH-N 243

Nonlinear Microrheological response to a step force — ●THOMAS FRANOSCH — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Innsbruck, Austria

In a microrheological experiment the thermal or forced motion of a colloidal particle is monitored to obtain information on mechanical properties of the surroundings. While the linear response is well-characterized in terms of the fluctuation-dissipation theorem, few exact results are available for strong driving.

Here we consider the time-dependent velocity of a colloidal particle immersed in a dilute suspension of hard spheres in response to switching on a finite constant force. The dimensionless number quantifying the strength of the driving is the Péclet number $Pe = F\sigma/k_B T$. We present an analytical solution exact to first order in the packing fraction. In particular, we show that at *finite times* the response is an analytic function of the Péclet number, but displays singular behavior for infinite times. Our solution technique extends the stationary state calculation [1] to the time-dependent case. The non-commutativity of the limits $Pe \rightarrow 0$ and time $t \rightarrow \infty$ is traced back to the long-time tail in the velocity-autocorrelation function due to repeated encounters with the same colloid. The scenario is strongly reminiscent of a driven particle in a lattice Lorentz model with frozen obstacles [2], and corroborates that linear response becomes qualitatively wrong at long times for arbitrarily small driving.

[1] T.M Squires and J.F. Brady, *Phys. Fluids* 17, 073101 (2005)

[2] S. Leitmann, T. Franosch, *Phys. Rev. Lett.* 111, 190603 (2013)

DY 9.9 Mon 17:30 BH-N 243

Enhancement of mobility in a feedback controlled 1D colloidal system with repulsive interactions — ●ROBERT GERNERT and SABINE H. L. KLAPP — Institut für theoretische Physik, Technische Universität Berlin

Feedback control schemes are a promising way to design static and dynamic properties of colloidal suspensions [1]. In the collective transport of colloids through 1D tilted washboard potentials clusters of attractive particles are known to overcome the hindering influence of the potential barriers [2]. Here we consider a corresponding system with repulsive interactions. To enhance the mobility we propose a feedback control scheme and demonstrate its function theoretically. The control is modelled by a symmetrically confining potential, like an optical tweezer, and it is always centered around the mean particle position. For the theoretical demonstration we use Dynamical Density Functional Theory (DDFT) with ultra-soft as well as hard-core particle interactions. For either type of interaction the influence of the hindering washboard potential can be suppressed completely – corresponding to an enhancement of the mobility by several orders of magnitude. Further, in the regime of moderate amplification velocity oscillations are induced.

[1] B. Qian, D. Montiel, A. Bregull, F. Cichos, and H. Yang, *Chem. Sci.* 4, 1420 (2013)

[2] M. Evstigneev, S. von Gehlen, and P. Reimann, *PRE* 79, 011116 (2009)

DY 9.10 Mon 17:45 BH-N 243

Surface interactions of active Janus particles on a hexagonal close-packed colloidal crystal surface — ●UDIT CHOUDHURY¹, JOHN G. GIBBS^{1,2}, and PEER FISCHER^{1,3} — ¹Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany

— ²Dept. of Physics & Astronomy, Northern Arizona University, Flagstaff, AZ 86011, USA — ³Institute for Physical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Autonomous, self-driven colloidal particles are being given greater attention in recent years due to the interesting dynamics associated with out-of-equilibrium systems. Although particle-particle interactions of active colloids, e.g. self-assembly and clustering, are beginning to be regularly studied, particle-surface interactions are less well investigated. Herein, we empirically study the surface interactions of spherical Janus-particles half-coated with Pt in the presence of hydrogen peroxide. The surface consists of close-packed 2D monolayer of hard spheres (beads). This non-planar surface thus corresponds to a periodic potential akin to a fcc (111) lattice face. In this way, the system is an analogue of surface diffusion of adatoms that possess kinetic energy. We find that as the concentration of hydrogen peroxide is increased, the effective translational diffusion also increases which is comparable to enhanced diffusion of adatoms on surfaces at higher temperatures. Rotational diffusion dictates fluctuations in the orientation of the driven bead that lead to jumps from one potential well to its nearest neighbor.

DY 9.11 Mon 18:00 BH-N 243

Charged transfer in a dynamical Landau-Zener Model: Application in QCA — ●ALEJANDRO SANTANA-BONILLA¹, MIRNA KRAMAR¹, RAFAEL GUTIERREZ^{1,2}, and GIOVANNI CUNIBERTI^{1,2} — ¹Technische Universität Dresden Faculty of Mechanical Science and Engineering Institute for Materials Sciences — ²Max Bergmann Center of Biomaterials

The development of molecular based quantum cellular automata (mQCA) would open the possibility to low-dissipation information processing. One key parameter in the mQCA paradigm is the stability of intra-molecular charge transfer, which guarantees the association of $*1*$ and $*0*$ to two different charge configurations in the mQCA building cell. Specifically, a given charge configuration needs to be stable against thermal fluctuations. Also important is how the mQCA charge state reacts to an external driver with a given time-dependence. In this study we present a theoretical study based on the solution of the time-dependent Schrödinger equation to describe intra-molecular charge transfer in an effective model of an mQCA cell under the action of a time-dependent driver field and including thermal fluctuations. The model is parametrized via first-principle calculations in a toy molecular system able to catch the minimal requirements of a mQCA cell

DY 9.12 Mon 18:15 BH-N 243

Calibration free 3D tracking of confined nanoparticles in a

tunable nanofluidic slit — ●STEFAN FRINGES, MICHAEL SKAUG, HEIKO WOLF, URS T. DÜRIG, and ARMIN W. KNOLL — IBM Research, 8803 Rüschlikon, Switzerland

We investigate the behavior of nanoparticles in a nanofluidic slit with tunable confinement and spatial and temporal resolution of 10nm and 2ms, respectively. The high speed detection of the particles' X, Y and Z coordinates allows us to obtain the spatiotemporal probability distribution of individual particles and thus to study their confining potential-landscape both in lateral and vertical direction. To obtain the 3D trajectory of a nanometer-sized particle we use interferometric scattering detection (iSCAT). The method exploits the interference between the scattered wave from the particles and the highly reflective reference surface for a precise localization in vertical direction [1]. Evaluating the particle contrast for varying slit distances enables us to measure the scattering phase, amplitude, and consequently the z-position of individual particles without prior calibration of the particle contrast [2]. Precise knowledge of the nanoparticles' paths and surrounding potentials allows us to study confinement effects on Brownian motion and charge regulation at the participating interfaces. It further enables us to precisely trap and immobilize nanoparticles at a specific location on the substrate.

[1] P. Kukura et al., Nature Methods 6, 923-927 (2009).

[2] N. Mojarad et al., Optics Express 21, 8, 9377-9389 (2013).

DY 9.13 Mon 18:30 BH-N 243

Towards single molecule trapping and manipulation with dynamic temperature gradients — MARCO BRAUN, ANDREAS BREGULLA, and ●FRANK CICHOS — Molecular Nanophotonics Group, Universität Leipzig, Linnéstraße 5, 04103 Leipzig

Single nano-objects in solution are driven by Brownian motion which is fueled by thermal energy. These Brownian fluctuations increase in strength with increasing temperature. Therefore, it is at first glance counter intuitive to confine Brownian fluctuations with the help of elevated temperatures. In thermal nonequilibrium, however, temperature gradients induce thermo-phoretic and thermo-osmotic drifts which provide the means for single particle manipulation in solution. Here we describe experiments which use optically heated metal nanostructures to create dynamical temperature profiles in solution. These temperature profiles induce well defined thermo-phoretic drift fields and act as effective potentials for objects suspended in liquid. Combined with optical feedback mechanisms, such effective potentials can be shaped to store and manipulate single or even multiple objects in a small observation volume. The developed thermophoretic trapping system therefore paves the way for extended single molecule studies in solution or even well-controlled bi- or multi molecular interaction studies.

DY 10: Quantum Dynamics, Decoherence and Quantum Information (joint session DY/ TT)

Time: Monday 15:00–18:30

Location: BH-N 334

DY 10.1 Mon 15:00 BH-N 334

Cooling a Magnetic Nanoisland by Spin-Polarized Currents — ●PETER NALBACH¹, JOCHEN BRÜGGEMANN¹, STEPHAN WEISS², and MICHAEL THORWART¹ — ¹I. Institut für Theoretische Physik, Universität Hamburg, Germany — ²Theoretische Physik, Universität Duisburg-Essen and CENIDE, Germany

We investigate cooling of a vibrational mode of a magnetic quantum dot by a spin-polarized tunnelling charge current exploiting the magneto-mechanical coupling. The spin-polarized current polarizes the magnetic nano-island, thereby lowering its magnetic energy. At the same time, Ohmic heating increases the vibrational energy. A small magneto-mechanical coupling then permits us to remove energy from the vibrational motion and cooling is possible. We find a reduction of the vibrational energy below 50% of its equilibrium value. The lowest vibration temperature is achieved for a weak electron-vibration coupling and a comparable magneto-mechanical coupling. The cooling rate increases at first with the magneto-mechanical coupling and then saturates.

see: Phys. Rev. Lett. 113, 076602 (2014).

DY 10.2 Mon 15:15 BH-N 334

Dissipative Landau-Zener transitions with longitudinal and transversal noise — ●SAMANEH JAVANBAKHT, PETER NALBACH,

and MICHAEL THORWART — I. Institut für Theoretische Physik Universität Hamburg Jungiusstraße 9, 20355 Hamburg

We have studied the Landau-Zener transition probability in a dissipative environment exhibiting both, longitudinal as well as transversal, noise. We employed the numerically exact quasi-adiabatic path integral as well as the approximate nonequilibrium Bloch equations. We find that transversal noise influences the Landau-Zener probability much stronger than longitudinal noise at equal temperature and system-bath coupling. Furthermore we reveal that transversal noise renormalizes the tunnel coupling independent of temperature. Finally, we observe that longitudinal and transversal noise cannot be treated independently but are correlated. This results in an unexpected dependence on the relative sign of the transversal and the longitudinal system-bath coupling.

DY 10.3 Mon 15:30 BH-N 334

Landau-Zener transitions in a bosonic bipartite quantum system — ●KATHARINA KOPPER, RALF BLATTMANN, and PETER HÄNGGI — Universität Augsburg, D-86135 Augsburg

We study a bipartite quantum system consisting of two coupled optical micro-cavities as an analogue of the bosonic Landau-Zener setup. To account for dissipative effects we employ a Markovian master equation to describe the open system dynamics.

Within this framework we regard the time evolution of the system and its dependency on the characteristic parameters and discuss our findings.

DY 10.4 Mon 15:45 BH-N 334

Verification for quantum emulation in thermal equilibrium — ●IRIS SCHWENK, MICHAEL MARTHALER, and GERD SCHÖN — Institut für Theoretische Festkörperphysik - KIT, Karlsruhe

A quantum emulator is an experimental setup that mimics an interesting physical system of some relevance for physics or applications. In order to explore the reliability of a quantum emulator we analyse a system-bath setting in thermal equilibrium. Therefore we compute the reduced density matrix of the system analytically. Applying a diagrammatic approach we get a determining equation for the reduced density matrix. Using this equation we discuss restrictions of the scalability of a quantum emulator and possibilities to avoid them.

DY 10.5 Mon 16:00 BH-N 334

Fully pulse-controlled gate operations on qubit chains with always on coupling — HOLGER FRYDRYCH¹, ●MICHAEL MARTHALER², and GERNOT ALBER¹ — ¹Institut für Angewandte Physik, Technische Universität Darmstadt, D-64289 Darmstadt — ²Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

We investigate a linear chain of qubits with strong, always-on nearest-neighbour couplings. Always-on coupling is simple to realize, but it raises the question of how to decouple the qubits. One possibility would be strong detuning, but the energy splitting of many qubits can only be changed slowly or the energy is fixed by tuning to a symmetry point which reduces decoherence. We propose a selective dynamical decoupling scheme, which is capable of dynamically suppressing any coupling in the chain as needed, by applying certain sequences of local pulses to individual qubits. We demonstrate how this pulse control can be used to implement single-qubit rotations and an entangling two-qubit gate between any neighbouring qubits in the chain. We find that high fidelities can be achieved as long as the number of permanently coupled qubits is not too large. As a specific example we discuss the concrete parameters needed to implement our proposal with superconducting flux qubits.

DY 10.6 Mon 16:15 BH-N 334

Entanglement content of non-equilibrium steady states — ●ZOLTÁN ZIMBORÁS¹ and VIKTOR EISLER² — ¹University College London, UK — ²Eötvös University, Budapest, Hungary

We study the nonequilibrium steady state of a chain of harmonic oscillators and a chain of free fermions, resulting from an initial state where the two sides of the system are prepared at different temperatures. The steady state is constructed explicitly and the logarithmic negativity and mutual information is calculated between two adjacent segments of the chain. We find that, for the fermion chain the mutual information diverges logarithmically, while for the harmonic chain the steady-state negativity follows an area law and is a sum of contributions pertaining to left- and right-moving excitations emitted from the two reservoirs. As a particular case, we also discuss a local quench where both sides of the chain are initialized in their respective ground states.

[1] V. Eisler, Z. Zimborás, Phys. Rev. A 89, 032321 (2014)

[2] V. Eisler, Z. Zimborás, arXiv:1406.5474

DY 10.7 Mon 16:30 BH-N 334

Numerical Complexity in Non-Markovian Quantum Dynamics — ●MICHAEL WIEDMANN and JÜRGEN T. STOCKBURGER — Institute for Complex Quantum Systems, Ulm University, Albert-Einstein-Allee 11, D-89069 Ulm

Decoherence phenomena beyond perturbation theory are commonplace in condensed-matter physics, biophysics and strongly driven systems. The stochastic Liouville-von Neumann equation (SLN) [1] builds an exact, time-local and non-perturbative framework to tackle non-Markovian open system dynamics in these cases. In this technique the propagation of individual samples is non-unitary, the norm of quantum states is not preserved. Any resource-conscious numerical implementation faces the problem of deteriorating signal-to-noise ratios and increasing numbers of required trajectories. We present a propagation scheme that offers significant advances in sample statistics' efficiency with emphasis on strong dephasing. Apart from transient dynamics we consider system correlation functions of steady states in equilibrium

and non-equilibrium settings.

[1] J. T. Stockburger and H. Grabert, PRL 88, 170407 (2002)

15 min. break

DY 10.8 Mon 17:00 BH-N 334

Universal short-time response and formation of correlations after quantum quenches — ●KLAUS MORAWETZ — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP), Avenida Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The short-time evolution of two distinct systems, the pump and probe experiments with semiconductor and the sudden quench of cold atoms in an optical lattice, is found to be described by the same universal response function. This analytic formula at short time scales is derived from the quantum kinetic theory approach observing that correlations need time to be formed. The influence of finite trapping potential is derived and discussed as well as Singwi-Sjölander local field corrections. The quantum kinetic equation allows to understand how two-particle correlations are formed and the screening and collective modes are build up.

K. Morawetz, Phys. Rev. B 90 (2014) 075303:

K. Morawetz, P. Lipavský, M. Schreiber, Phys. Rev. B 72 (2005) 233203:

K. Morawetz, Phys. Rev. E 66 (2002) 022103:

K. Morawetz, M. Bonitz, V. G. Morozov, G. Röpke, D. Kremp, Phys. Rev. E 63 (2001) 20102:

K. Morawetz, V. Spicka, P. Lipavský: Phys. Lett. A 246 (1998) 311:

DY 10.9 Mon 17:15 BH-N 334

Computing the Markovian dynamics of periodically driven systems — ●DANIEL PAGEL, ANDREAS ALVERMANN, and HOLGER FEHSKE — Institut für Physik, Ernst-Moritz-Arndt-Universität, 17487 Greifswald, Germany

The dissipative dynamics of a quantum system that is weakly coupled to an environment can be studied with Markovian master equations. Solution of the master equation requires the choice of a computational basis. In this work we describe how exact diagonalization and the Floquet approach can be combined in a solution strategy for the master equation that is applicable also for periodically driven systems. For the example of strongly coupled quantum bits, where the usually employed quantum optical master equation has to be replaced by the master equation in the coupled eigenbasis, we compute the dissipative dynamics of initially entangled states and study the properties of the asymptotic state using correlation functions.

DY 10.10 Mon 17:30 BH-N 334

Non-equilibrium quantum dynamics of Gaussian states in open harmonic chains — ●THOMAS MOTZ, JÜRGEN T. STOCKBURGER, and JOACHIM ANKERHOLD — Institute for complex quantum systems, Ulm University, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

Strong driving in open quantum systems can reveal counterintuitive effects such as the dynamical creation of negative entropy changes [1] and entanglement between two Gaussian modes in a common reservoir [2]. The effect that dissipation and strong driving in combination can lead to specific quantum characteristics like entanglement and offers much potential for quantum information processing and the studies of mesoscopic thermodynamics. A rich tool to study dynamic effects in open systems proved to be the stochastic Liouville-von Neumann equation [3]. We avoid the stochastic sampling in our approach where the dynamics of the covariance matrix in a few-body system is directly described by a deterministic equation of motion. We apply this approach to a bipartite asymmetric system where entanglement generation and its sensitivity to the asymmetry is studied. Since the memory requirements for Gaussian states grow only quadratically with system size, our approach is also targeted at more complex settings like multiple coupled modes in a common or several separated reservoirs. Our equations of motion allow optimal control theory to be applied with ease.

[1] R. Schmidt et al., PRL 107, 130404 (2011).

[2] R. Schmidt et al., PRA 88, 052321 (2013).

[3] J. T. Stockburger and H. Grabert, PRL 88, 170407 (2002).

DY 10.11 Mon 17:45 BH-N 334

Markovianity and Consistency in closed spin lattices —

•DANIEL SCHMIDTKE and JOCHEN GEMMER — Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany

Dynamics of closed quantum systems may be mapped onto stochastic processes in case they are in accordance with conditions regarding Markovianity and Consistency. These conditions can be derived from the path measures of the Consistent Histories approach by introducing a decoherence functional and conditional transfer-probabilities. Depending on the so called memory range one distinguishes one-step, two-step, ... etc. Markovianity. To demonstrate that these conditions are indeed fulfilled in some closed quantum systems an detailed numerical investigation of spin lattices has been done by directly quantifying the negligible Non-Markovianity and negligible Non-Consistency. Though Markovianity and Consistency show very similar dependencies on, e.g., the time steps between measurements or coupling strengths within the spin system, there are no analytical proofs regarding this correlation.

DY 10.12 Mon 18:00 BH-N 334

Dynamics of the dissipative Dicke Model for a large number of atoms — •CHRISTOS BOKAS, BJÖRN KUBALA, and JOACHIM ANKERHOLD — Institute for Complex Quantum Systems, Ulm University, Ulm, Germany

The Dicke Hamiltonian is used to model the coupling of a cloud of atoms to a harmonic oscillator mode. In the thermodynamic limit, a phase transition occurs when increasing the coupling strength, shifting the system from a 'normal' to a 'superradiant' state, which exhibits strong correlations between the two subsystems.

Dynamics *close to this equilibrium state* is described by the well-

known Holstein-Primakov approach [1] in terms of two effective Hamiltonians containing two coupled harmonic degrees of freedom.

We aim to describe the *full coherent and dissipative dynamics* by deriving a mapping to a single effective potential valid for a large number of atoms. Starting from a highly excited atomic state, oscillations of excitations between atoms and cavity and the eventual decay to equilibrium can, hence, be studied within this approach.

[1] C. Emary and T. Brandes, Phys. Rev. E **67**, 066203 (2003).

DY 10.13 Mon 18:15 BH-N 334

Dynamics of the dissipative Dicke model: superradiance of cold atoms via a superconducting cavity — SEBASTIAN FUCHS^{1,2}, •BJÖRN KUBALA¹, MILES BLENCOWE³, and JOACHIM ANKERHOLD¹ — ¹Institute for Complex Quantum Systems, Ulm University, Ulm, Germany — ²Northwestern University, Evanston IL, USA — ³Dartmouth College, Hanover NH, USA

Superradiance is associated with two physical effects: Firstly, the cooperative emission of radiation of a large number of excited atoms into free space in a quick, strong 'superradiant burst'. Secondly, for sufficiently strong coupling of many atoms to an electromagnetic cavity mode, modeled with the Dicke Hamiltonian, a 'superradiant phase' is found, which shows macroscopic photon occupation and atomic excitation.

The two facets of superradiance can be combined in studying the dissipative dynamics of an initially excited state of the atoms towards equilibrium. We identify and characterize the analogue of the free-space burst in this scenario, and discuss how signatures of normal or superradiant phase are observable for a mesoscopic number of atoms.

DY 11: Colloids and Complex Liquids II (joint session CPP/ DY)

Time: Monday 15:00–18:45

Location: C 130

DY 11.1 Mon 15:00 C 130

TIRM at liquid/liquid interfaces — •KILIAN DIETRICH — University of Stuttgart, Germany

Total Internal Reflection Microscopy (TIRM) is a well-established method for the direct measurement of interaction potentials between a spherical colloidal particle and a solid wall. It is based on the tracking of the particle's vertical motion from which interaction forces with the interface can be inferred with a resolution down to 10fN. In contrast to previous measurements, which were performed at solid/liquid interfaces, here we demonstrate that TIRM can be applied also to liquid/liquid interfaces. These are of special interest not only due to their frequent appearance but they also exhibit an exceptional smoothness. In our study, we present a novel inverted TIRM apparatus which is capable to measure the motion of a colloidal probe particle in water close to an oil-water interface. First measurements indicate the counterplay of electrostatic interactions and van-der-Waals forces for interfaces treated with different ionic and non-ionic surfactants. In each case surface charge densities of particle and interface could be determined. The detailed knowledge of interactions can provide valuable information for the stability of emulsions and dispersions.

DY 11.2 Mon 15:15 C 130

Short Ranged Repulsive Energy in Oscillatory Structural Forces — •SEBASTIAN SCHÖN and REGINE VON KLITZING — Technische Universität Berlin Strasse des 17. Juni 124 D-10623 Berlin

Oscillatory structural forces are a genuine feature observed for simple and complex fluids in the vicinity of smooth wall. The origin of these forces is related to the characteristic quality of molecules or nanoparticles to form well-ordered layers in the vicinity of a confining wall. These forces can be described by the following function as proposed by Israelachvili: $f(x) = -A \cdot e^{-(x/\xi)} \cdot \cos(2\pi(x-\Delta x)/\lambda)$, with f the force as a function of x , the separation. The Amplitude A describes the strength of the particle interaction, the decay length ξ is a measure of how fast the order decays and the wavelength λ is directly related to the inter-particle distance. Structural oscillation forces are long ranged compared to the common DLVO forces and can be used in a variety of applications e.g. oil removal or separation of bidisperse particle suspensions. For both it is important to know the strength of the oscillatory forces at very small separations. An additional repulsive term is introduced to describe deviations observed between experimental data and the common fit function, this allows accurate fitting of experi-

mental data down to very small separations and removes systematic deviations in A , λ and ξ depending on the starting point of the fit. The short ranged repulsive energy described by the new term is investigated at different particle concentrations, measurement speed and under the addition of NaOH, HCl and NaCl at different concentrations.

DY 11.3 Mon 15:30 C 130

Complex nanoparticle arrangements via wrinkle-assisted self-assembly — •CHRISTOPH HANSKE, MORITZ TEBBE, CHRISTIAN KUTTNER, MUNISH CHANANA, TOBIAS KÖNIG, and ANDREAS FERY — Physical Chemistry II, University of Bayreuth, 95447, Germany

Template-assisted assembly enables the arrangement of colloidal particles into well-defined structures that often demonstrate special optical, biological, or catalytic functionality due to the hierarchical internal organization. A major bottleneck so far is the limited scalability of lithographic template fabrication. As an alternative strategy, we utilize wrinkled elastomer substrates exhibiting periodicities on the micron or submicron scale. The topographic features of such templates allow the arrangement of hydrophilic nanoparticles into regular, close-packed chains, which can further be transferred site-selectively onto flat substrates by wetting controlled printing. This versatile method is applicable for polymeric, inorganic and metallic particles with spherical as well as anisotropic shapes. We discuss the influence of interfacial properties originating from the employed particle and substrate coatings and demonstrate the formation of complex structures on chemically patterned substrates.[1] Further, the realization of macroscopic, gold nanoparticle assemblies is shown.[2, 3] Due to small interparticle distances of few nanometers, strong plasmonic coupling is achieved, which grants access to surfaces with tailored optical properties.

[1] C. Hanske et al., Langmuir, 2012, 28, 16745-16750. [2] C. Hanske et al., Nano Letters, 2014, DOI:10.1021/nl502776s. [3] M. Tebbe et al., submitted.

DY 11.4 Mon 15:45 C 130

Linking intermolecular interactions, microstructure, and macroscopic rheology in protein suspensions — •ALESSIO ZACCONE¹, MIRIAM SIEBENBÜRGER², HENNING WINTER³, FRANK SCHREIBER⁴, and MATTHIAS BALLAUFF² — ¹Physics-Department, Technische Universität München — ²Helmholtz-Zentrum Berlin für Materialien und Energie — ³University of Massachusetts Amherst — ⁴Applied Physics, University of Tübingen

We propose a microscopic framework based on nonequilibrium statistical mechanics to connect the microscopic level of colloidal biopolymer self-assembly with the macroscopic rheology of protein gelation. The method is based on the master kinetic equations for the time evolution of the self-assembled cluster size distribution, from which the relaxation time spectrum during the gelation process can be extracted. The relaxation spectrum is a simple stretched-exponential, with a stretching exponent related to the mass fractal dimension of the self-assembling clusters. In the case of thermoreversible gelation, for weak interparticle attractions, the attraction energy is finite and plays the role of the control parameter driving a nonequilibrium phase transition into a nonequilibrium steady-state (the gel). Our theory is in good agreement with experimental data of different systems published by other authors, for which no theory was available. Further, it allows us to interpret new experimental data on the gelation of BSA which provides a benchmark system to connect the level of coarse-grained protein interactions with the macroscopic oscillatory rheology of the protein suspension.

DY 11.5 Mon 16:00 C 130

Molecular versus macroscopic perspective on the phase separation mechanisms of thermo-responsive solutions — ●MARTINE PHILIPP¹, RALITSA ALEKSANDROVA², ULRICH MÜLLER², JAN K. KRÜGER², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — ²Université du Luxembourg, LPM, Luxembourg, Luxembourg

The phase separation of thermo-responsive solutions is known to strongly affect the volume expansion behaviour and the elastic properties, being directly coupled to the macroscopic order parameter [1-3]. On the molecular scale, massive changes in H-bond and hydrophobic interactions, and in structure govern the demixing process. However, the relationship between the molecular and macroscopic order parameters is poorly understood for such complex segregating solutions. We contribute to the clarification of this problem by first following the diffusion behaviour of the hydration water across the phase transition of model aqueous poly(N-isopropylacrylamide) solutions using quasi-elastic neutron scattering [2]. By probing the molecular bond polarisabilities, we adopt an alternative, highly revealing perspective on the changes in molecular interactions and in structure happening within dilute to concentrated phase-separating solutions [1, 3]. [1] M. Philipp, et al., *Soft Matter* 10, 7297-7305 (2014), [2] M. Philipp, et al., *J. Phys. Chem. B* 118, 4253-4260 (2014), [3] R. Aleksandrova, et al., *Langmuir* 30, 11792-11801 (2014)

DY 11.6 Mon 16:15 C 130

Cononsolvency in P(S-*b*-NIPAM) diblock copolymers - a time-resolved SANS study of the aggregation process — KONSTANTINOS KYRIAKOS¹, MARTINE PHILIPP¹, JOSEPH ADELSBERGER¹, SEBASTIAN JAKSCH¹, ANATOLY V. BEREZKIN¹, DERSY M. LUGO², WALTER RICHTERING², ISABELLE GRILLO³, ANNA MIASNIKOVA⁴, ANDRÉ LASCHEWSKY⁴, PETER MÜLLER-BUSCHBAUM¹, and ●CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²RWTH Aachen University, Institut für Physikalische Chemie — ³Institut Laue-Langevin, Grenoble, France — ⁴Universität Potsdam, Institut für Chemie, Potsdam-Golm

In mixtures of water and methanol, the thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) exhibits the cononsolvency effect, i.e. an enhanced tendency for phase separation at certain solvent compositions. We investigate the effect of adding methanol to (i) micellar solutions of polystyrene-*b*-poly(N-isopropylacrylamide) (PS-*b*-PNIPAM) diblock copolymers and (ii) PNIPAM homopolymers in D₂O using a stopped-flow instrument. The structural changes on mesoscopic length scales were followed by time-resolved small-angle neutron scattering (TR-SANS) with a time resolution of 0.1 s. In both systems, the pathway of the aggregation depends on the content of deuterated methanol; however, it is fundamentally different for homopolymer and diblock copolymer solutions. We propose a logarithmic coalescence model based on an energy barrier which is proportional to the aggregate radius.

1. Kyriakos et al., *Macromolecules* 47, 6867 (2014)

DY 11.7 Mon 16:30 C 130

Cation-activated attractive patches to control protein interactions — ●FELIX ROOSEN-RUNGE¹, FAJUN ZHANG², FRANK SCHREIBER², and ROLAND ROTH³ — ¹Institut Laue-Langevin, Grenoble, France — ²Institut für Angewandte Physik, Universität Tübingen

— ³Institut für Theoretische Physik, Universität Tübingen

We present evidence for an explicit ion-activated mechanism to cause a patchy attraction between proteins [1]. Experimentally, ion bridges of multivalent cations between protein molecules have been observed in protein crystals [2]. Modeling this mechanism via particles with ion-activated attractive patches, a broad variety of experimental results for protein solutions with multivalent cation is explained and understood very naturally, including charge reversal, reentrant condensation, metastable liquid-liquid phase separation, cluster formation and different pathways of crystallization [1,3]. The good agreement between theory and experiments indicates that protein-cation solutions represent a natural model system for patchy particles. The mechanism of ion-activated patches can be embedded seamlessly into theory and simulations of charged soft matter, and promises rational design of phase behavior and crystallization pathways in protein solutions based on the statistical physics of patchy particles.

[1] F. Roosen-Runge, F. Zhang et al. *Sci. Rep.* 4 (2014) 7016

[2] F. Zhang, A. Sauter et al. *J. Appl. Cryst.* 44 (2011) 755

[3] F. Zhang, R. Roth et al. *Soft Matter* 8 (2012) 1313

DY 11.8 Mon 16:45 C 130

Buckling of paramagnetic chains in soft gel — ●SHILIN HUANG and GÜNTER K. AUERNHAMMER — Max Planck Institute for Polymer Research, Mainz, Germany

We study the magneto-elastic coupling behavior of paramagnetic chains in a soft polymer gel. To this end, the laser scanning confocal microscope is used to observe the morphology of the paramagnetic chains as well as the deformation field in the polymer gel. The paramagnetic chains in a soft polymer gel show rich morphologies under an oblique magnetic field. Depending on the chain length, the chains rotate, bend and buckle. In a perpendicular magnetic field, longer chains form wavy structure with higher number of buckles. A higher magnetic field strength and a lower modulus of gel matrix lead to higher amplitude of the buckling. The deformation field around a deformed magnetic chain confirms that the polymer network is strongly coupled with the paramagnetic chain. A theoretical model is developed to describe the buckling of the chain.

15 min. break

DY 11.9 Mon 17:15 C 130

Environmentally compatible microemulsion at solid surfaces: Wetting behavior and extraction properties — ●SALOMÉ VARGAS RUIZ¹, CHRISTOPH SCHULREICH², RAMASIA SREICH², MARTIN JUNG³, REGINE VON KLIZING¹, THOMAS HELLWEG², and STEFAN WELLERT¹ — ¹Stranski Laboratory, TU Berlin, Str. d. 17 Juni 124, 10623 Berlin, Germany — ²Physical Chemistry III, University Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany. — ³Armed Forces Scientific Institute for NBC Protection, Humboldtstraße 1, 29633 Munster, Germany.

Microemulsions based on sugar surfactants and food grade oil are potential decontamination media for the remediation of sorptive surfaces exposed to highly toxic compounds (e.g. nerve agents, pesticides). The main advantage of microemulsions relies on their capability to degrade the solubilized toxic compound by means of active ingredients hosted in the water phase. Although microemulsions have good performance on the detoxification process, the overall efficiency of the decontamination process is also determined by their ability to wet the treated surfaces and to extract the contaminants. In this study, we examined firstly the wettability and penetration properties of microemulsion formulated with sugar surfactant SL55 and methyl oleate oil, and secondly we evaluated their ability to extract lipophilic contaminants via spectroscopic and chromatographic techniques. Here, the formulated microemulsions can wet and penetrate hydrophobic and hydrophilic sorptive surfaces and their extraction properties are greatly influenced by their structure and oil content.

DY 11.10 Mon 17:30 C 130

Supramolecular structure of pure and mixed monohydroxy alcohols — ●THOMAS BÜNING¹, CHRISTIAN STERNEMANN¹, SEBASTIAN PETER BIERWIRTH¹, CATALIN GAINARU¹, JENNIFER BOLLE¹, MICHAEL PAULUS¹, CHRISTOPH J. SAHLE², ROLAND BÖHMER¹, and METIN TOLAN¹ — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany — ²European Synchrotron Radiation Facility (ESRF), F-38000 Grenoble, France

Hydrogen bonds are essential for the structure and dynamics of alco-

hols, aqueous solutions, and water. Due to their low tendency of crystallization and large variability in molecular configuration, monohydroxy alcohols (MAs) are often studied as model systems for hydrogen-bonded fluids in general [1]. MAs are supposed to form supramolecular structures such as chains and rings via hydrogen bonding in the liquid phase. Based on their small dielectric absorption, ringlike arrangements were suggested for neat MAs with a sterically hindered polar hydroxyl group [1], e.g., for 4-methyl-3-heptanol and 2-hexyl-1-decanol. Mixtures of these MAs show a significantly enhanced dielectric absorption which hints at a change of supramolecular topology [2]. We present combined X-ray diffraction and X-ray Raman measurements of MA mixtures. Here, the first X-ray diffraction peak and the shape of the oxygen K-edge, respectively, are sensitive to the local arrangement of MAs. The results are interpreted with respect to a transformation from ringlike to chainlike structures upon mixing. [1] R. Böhmer et al. Phys. Reports 545 125-195 (2014) and references therein; [2] S. P. Bierwirth, et al. Phys. Rev. E 90, 052807 (2014).

DY 11.11 Mon 17:45 C 130

The role of the cation and polarization on lithium ion coordination in ionic liquids — ●VOLKER LESCH¹, ZHE LI², DMITRY BEDROV², and ANDREAS HEUER¹ — ¹Westfälische Wilhelms-Universität Münster — ²University of Utah

MD-simulations are a powerful tool to investigate microscopic processes in complex systems as ionic liquids. The interactions between the cation and the anion are only weak but in the case of adding lithium to an ionic liquid the anions strongly interact with this small lithium ion. The role of the cation on this interaction was never investigated.

Here, we compare the cations 1-ethyl-3-methylimidazolium with N-methyl-N-propylpyrrolidinium and as counterion bis-(trifluoromethanesulfonyl)-imide was used. Both cations differ in size and viscosity but on the microscopic scale only a comparison for pure ionic liquids is published. We performed MD-simulations for the two ionic liquids doped with lithium salts at different temperatures and different oxygen polarizations. The change of the TFSI oxygen polarization was necessary due to new DFT calculations that predicts the Li⁺ - Ntf₂ binding energy more accurate. We observed a dramatic influence of the polarization on structural properties while the dynamics are only slightly affected. The comparison of the cations shows only small differences for the lithium ion coordination.

DY 11.12 Mon 18:00 C 130

A systematic study of the influence of trivalent metal ions on phase behaviour in protein solutions — ●OLGA MATSARSKAIA¹, MICHAL BRAUN¹, ANDREA SAUTER¹, MARCELL WOLF¹, ROLAND ROTH², FAJUN ZHANG¹, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — ²Institut für Theoretische Physik, Universität Tübingen

Thermodynamic phenomena such as reentrant condensation (RC) and liquid-liquid phase separation (LLPS) are involved in various protein-related processes, e.g. protein condensation diseases and protein crystallisation. We could show that these transitions are inducible in protein solutions using various trivalent cations [1], [2]. In this work, the influence of cation size on such phase behaviour in bovine serum albumin (BSA) was studied systematically in the presence of salts with increasing cation sizes (YbCl₃, YCl₃, GdCl₃, CeCl₃ and LaCl₃). The results reveal that charge inversion, the prerequisite of RC and LLPS in these systems, is found independent of cation size. Interestingly, however, salt concentration ranges in which macroscopic LLPS is observed decrease with increasing cations: while Yb³⁺ leads to the largest LLPS area, Ce³⁺ features the smallest one. La³⁺, the largest cation stud-

ied, induces RC, but does not lead to LLPS at all. The findings thus indicate that the size of cations present in the environment of a protein influences the strength of protein-cation interactions and therefore plays an important role in phase transitions of the protein.

[1] Zhang et al (2008). Phys. Rev. Lett., 101(14), 148101; [2] Zhang et al (2012). Soft Matter, 8, 1313-1316.

DY 11.13 Mon 18:15 C 130

New relaxation process for water in electric fields — ●ZORAN MILIČEVIĆ¹, DAVID M. SMITH^{2,3}, and ANA-SUNČANA SMITH^{1,3} — ¹Institut für Theoretische Physik and Cluster of Excellence: Engineering of Advanced Materials, FAU Erlangen-Nürnberg, Erlangen, Germany — ²Computer Chemie Centrum, FAU Erlangen-Nürnberg, Erlangen, Germany — ³Ruder Bošković Institute, Zagreb, Croatia

Despite a heavily increasing number of electrochemical applications, theoretical and experimental studies of solvent shear properties in the presence of electric fields are almost non-existent. Here we study the shear viscosity of water by performing extensive MD simulations using the GROMACS software package as a function of the electric field strength which breaks the otherwise isotropic nature of the solvent. The shear viscosity is related to the autocorrelation function (ACF) of the off-diagonal elements of the pressure tensor by the Green-Kubo relation. The value of the shear viscosity is determined from the plateau value of the time integral of the ACF or, alternatively, by exploiting the Kohlrausch fit curve of the ACF using a uniform 2-step (fast plus slow) relaxation function. Apart from the fact that the two approaches show an excellent agreement, we find that the field decreases the component of the shear viscosity perpendicular to itself and increases the components which are parallel. Importantly, the field induces an additional slow relaxation process (decoupled from the fast relaxation) only in the parallel direction, increasing by about tenfold the total relaxation time with respect to the perpendicular direction. Furthermore, the overall water shear viscosity increases slightly with the field strength.

DY 11.14 Mon 18:30 C 130

Excess entropy scaling for the segmental and global dynamics of polyethylene melts — ●EVANGELOS VOYIATZIS, MICHAEL BÖHM, and FLORIAN MÜLLER-PLATHE — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Center of Smart Interfaces, Technische Universität Darmstadt, Alarich-Weiss-Strasse 4, D-64287 Darmstadt, Germany

The range of validity of the Rosenfeld and Dzugutov excess entropy scaling laws is analyzed for linear polyethylene chains. We consider two segmental dynamical quantities, the bond and the torsional relaxation times, and two global ones, the chain diffusion coefficient and the viscosity. The excess entropy is approximated by either a series expansion of the entropy in terms of the pair correlation function or by an equation of state for polymers. For all temperatures and chain lengths considered, the two excess entropy estimates are linearly correlated. The scaled segmental relaxation times fall into a non-linear master curve. For a fixed chain length, the reduced diffusion coefficient and viscosity scale linearly with the excess entropy. An empirical reduction to a chain length independent master curve is accessible for both quantities. The Dzugutov scheme predicts an increased value of the scaled diffusion coefficient with increasing chain length which contrasts physical expectations. The origin of this trend can be traced back to the density dependence of the scaling factors. In connection with diffusion coefficients and viscosities, the Rosenfeld scaling appears to be of higher quality than the Dzugutov. An empirical excess entropy scaling is also proposed which leads to a chain length-independent correlation.

DY 12: Granular Matter / Contact Dynamics Part II

Time: Monday 15:30–17:00

Location: BH-N 128

DY 12.1 Mon 15:30 BH-N 128

Dissipation in quasistatically sheared wet and dry sand under confinement — ●MARYAM PAKPOUR¹, JORGE E. FISCINA^{1,2}, ABDOULAYE FALL³, NICOLAS VANDEWALLE¹, CHRISTIAN WAGNER², and DANIEL BONN^{4,5} — ¹GRASP, Physics Department B5, University of Liège, B-4000 Liège, Belgium — ²Experimental Physics, Saarland University, Saarbrücken Germany — ³Laboratoire Navier (UMR CNRS 8205), Université Paris Est, Champs-sur-Marne, France — ⁴Van der waals-Zeeman Institute, University of Amsterdam, Amsterdam, the Netherlands — ⁵Laboratoire de Physique Statistique de l'ENS, 75231 Paris Cedex 05, France

We investigated the stress-strain behavior of granular materials with and without small amounts of liquid near the jamming transition under steady and oscillatory shear. Partially saturated sand has a much higher yield stress and should therefore have a much higher apparent viscosity for slow flows. For this reason, it is commonly believed that dry sand should deform more easily and wet sand shows a larger resistance to flow, i.e., more viscous than dry sand. In this study, using a new technique to quasistatically push the sand through a tube with an enforced parabolic (Poiseuille-like) profile, we minimize the effect of avalanches and shear localization. We observe that the resistance against deformation of the wet (partially saturated) sand is much smaller than that of the dry sand, and that the latter dissipates more energy under flow. This is also observed in large-amplitude oscillatory shear measurements using a rotational rheometer, showing that the effect is robust and holds for different types of flow.

DY 12.2 Mon 15:45 BH-N 128

DWS measurements on fluidized granular media — ●PHILIP BORN, STEFFEN REINHOLD, and MATTHIAS SPERL — DLR Institute of Materials Physics in Space, Cologne, Germany

Diffusing wave spectroscopy (DWS) measurements indicate glass-like dynamics in dense, fluidized granular media close to jamming. This suggests fundamental similarities among the jamming transition in granular media and the glass transition in other fluid systems. However, the glass-like dynamics appear as a localization of the mean-squared displacement of the particles on length scales of a few 10 nm. Such length scales are not present in measurements using complementary techniques. In order to confirm the present results, we perform DWS measurements in microgravity, which promises isotropic agitation. Additionally, we tailor particle interactions to test the influence of long-ranges and short-ranged interactions. The results indicate that DWS measurements have to be evaluated with care, as omnipresent particle interactions prevent pure hard-sphere behavior, and incoherent intensity fluctuations put in question the localization interpretation of the intensity fluctuations.

DY 12.3 Mon 16:00 BH-N 128

Flow and clogging of anisometric granular matter in a hopper — ●SANDRA WEGNER¹, TAMÁS BÖRZSÖNYI², BALÁZS SZABÓ², and RALF STANNARIUS¹ — ¹Otto-von-Guericke-University, Magdeburg, Germany — ²Department of Complex Fluids, Wigner RCP SZFI, Budapest, Hungary

Granular matter is processed and stored in many branches of industry. This storage is often done in silos or hoppers. When the granular material is flowing out of a hopper, jamming is a frequent problem. We address this phenomenon by means of a three-dimensional experimental investigation of the jammed state in cylindrical and conical hoppers. We detect the jamming of differently shaped particles with X-ray computed tomography. With the complete three-dimensional information of grain positions and orientations, packing fractions and orientational ordering of the systems can be calculated and compared. We find differences for grains of different shapes and surface properties.

DY 12.4 Mon 16:15 BH-N 128

The Mach number determines the onset of clustering in a dissipative gas — ●MATHIAS HUMMEL, JAMES CLEWETT, STEPHAN HERMINGHAUS, and MARCO G. MAZZA — Max Planck Institut für Dynamik und Selbstorganisation

We perform direct numerical simulations of granular hydrodynamics to study the clustering of a dissipative gas for constant coefficients of restitution in three dimensions. We demonstrate that clustering appears when the ratio between local bulk velocity and local thermal velocity, that is the Mach number, reaches a threshold value $\mathcal{M}_t \approx 10^{-3}$, independently of the coefficient of restitution. We also find that the local Mach numbers, and not the coefficient of restitution, determine the evolution of the clusters.

DY 12.5 Mon 16:30 BH-N 128

Stability of Dune Fields — ●SVEN AUSCHRA, MARC LÄMMEL, and KLAUS KROY — University of Leipzig, Institute for Theoretical Physics

Arid regions on Earth and Mars are often covered with vast assemblies of crescent-shaped sand dunes, so-called barchans. The observation that single barchans either shrink or grow indefinitely if fed by a constant homogeneous influx of sand [1], makes the existence and stability of such barchan fields a conundrum [2].

We investigate the steady-state configuration of consecutive barchan dunes interacting by wind-driven sand transport. Based on well-established equations for isolated dunes [1,3] we derive a coarse-grained description of the dominant pair interactions within a field. Sand supplied from the horns of windward dunes to its downwind neighbor initiates a complex response of its shape and mass. Based on a dimensionally reduced description justified by a closeby shape attractor, a fixed point equation for the mass balance of the fed dune is derived and analyzed for stable solutions. We provide evidence that this process is a good candidate for explaining the stabilization of barchan dunes in the field.

[1] Fischer, E., Cates, M. E., Kroy, K., 2008. Dynamic scaling of desert dunes. *Phys. Rev. E* 77, 031302.

[2] Duran, O. *et al.*, 2011. Size distribution and structure of barchan dune fields. *Nonlin. Processes Geophys.* 69, 455-467.

[3] Kroy, K., Sauermann, G., Herrmann, H. J., 2002. Minimal Model for Sand Dunes. *Phys. Rev. Lett.* 88, 5.

DY 12.6 Mon 16:45 BH-N 128

Aeolian sand sorting and megaripple formation — ●MARC LÄMMEL, ANNE MEI WALD, and KLAUS KROY — Institut für Theoretische Physik, Universität Leipzig, Germany

Turbulent flows drive sand along riverbeds or blow it across beaches and deserts. This seemingly chaotic process creates a whole hierarchy of structures ranging from ripple patterns over dunes to vast wavy sand seas. Moreover, by the very same process, grains are constantly being sorted, because smaller grains advance faster while their heavier companions trail behind. Starting from the grain-scale physics, we model the sorting dynamics by erosion and show how it creates the characteristic bimodal grain size distribution that is a prerequisite for the formation of so-called megaripples [1]. Due to the separation into small and big grains, these structures have a lot in common with their bigger relatives, aeolian sand dunes, whose physics is much better understood. This enables us to adapt a well established dune model [2] to predict formation, morphology, and dynamics of the megaripples. Preliminary tests against field data strongly support our approach, which, moreover, provides a roadmap for future systematic field and laboratory measurements.

[1] Qian, G. *et al.*, *Sedimentology* 59, 1888 (2012)

[2] Kroy, K. *et al.*, *Phys. Rev. Lett.* 88, 054301 (2002)

DY 13: Crystallization, Nucleation and Self Assembly II (joint session CPP/ DY)

Time: Monday 15:45–18:30

Location: PC 203

DY 13.1 Mon 15:45 PC 203

Estimation of crystal nucleation barriers from Monte Carlo simulations — ●ANTONIA STATT^{1,2}, PETER VIRNAU², and KURT BINDER² — ¹Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 9, 55128 Mainz, Germany — ²Graduate School of Excellence Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany

A fluid in equilibrium in a finite volume V with particle number N at a density exceeding the onset density of freezing may exhibit phase coexistence between a crystalline nucleus and surrounding fluid. Using a method suitable for the estimation of the chemical potential of dense fluids we obtain the excess free energy due to the surface of the crystalline nucleus. There is neither a need to precisely locate the interface nor to compute the (anisotropic) interfacial tension [1]. As a test case, a soft version of the Asakura-Oosawa model [2] for colloid polymer-mixtures is treated. While our analysis is appropriate for crystal nuclei of arbitrary shape, we find the nucleation barrier to be compatible with a spherical shape, and consistent with classical nucleation theory.

[1] A. Statt, P. Virnau and K. Binder, PRL 2014 (in press)

[2] M. Dijkstra, R. van Roij and R. Evans, Phys. Rev. E 59, 5744-5771, 1999

DY 13.2 Mon 16:00 PC 203

Nano-Dewetting in Colloidal Crystal Drying — ●MULDA MULDARISNUR and FRANK MARLOW — MPI für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany

The drying of colloidal crystals is connected with a continuous shrinkage process [1]. However, several minutes after starting the drying, the system seems to take a breath before it shrinks monotonously until its final state after about one day. This short period we call "v"-event because of the shape of the curve characterizing the lattice constant: a decrease followed by a counter-intuitive increase which ends after one hour. This event is found in time-dependent optical spectra. It is assigned to the start of a nano-dewetting process occurring at the colloidal particles.

[1] M. Muldarisnur and F. Marlow, Observation of Nano-Dewetting in Colloidal Crystal Drying, Angew. Chem. Int. Ed. 2014, 53 (33), pages 8761-8764

DY 13.3 Mon 16:15 PC 203

Solidification fronts in supercooled liquids: how rapid fronts can lead to disordered glassy solids — ●ANDREW ARCHER¹, MORGAN WALTERS¹, UWE THIELE², and EDGAR KNOBLOCH³ — ¹Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK — ²Westfälische Wilhelms-Universität Münster, Institut für Theoretische Physik, Wilhelm-Klemm-Str. 9, 48149 Münster, Deutschland — ³Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA

We determine the speed of a crystallization/solidification front as it advances into the uniform liquid phase after it has been quenched into the crystalline region of the phase diagram, for systems of soft particles. We calculate the front speed by assuming the system can be treated using dynamical density functional theory (DDFT). There are two mechanisms by which the front can advance, depending on whether the liquid state is linearly stable or not. When linearly unstable, the front speed can be calculated by applying a marginal stability criterion. As the solidification front advances, the density profile behind the advancing front develops density modulations, whose wavelength λ is a dynamically chosen quantity. For shallow quenches, λ is close to that of the crystalline phase and so well-ordered crystalline states are formed. However, when the system is deeply quenched, λ can be quite different from that of the crystal, so the solidification front naturally generates disorder in the system. Significant rearrangement and aging must subsequently occur for the system to form the regular well-ordered crystal that corresponds to the free energy minimum.

Invited Talk

DY 13.4 Mon 16:30 PC 203

Spontaneous symmetry breaking in 2D: Kibble-Zurek mechanism in colloidal monolayers at finite cooling rates — SVEN DEUTSCHLÄNDER, GEORG MARET, and ●PETER KEIM — Universität Konstanz

The Kibble-Zurek mechanism describes the evolution of defects and domains when a system is forced through a phase transition with spontaneously broken symmetry. It describes Higgs field in the early universe shortly after the Big Bang or condensed matter systems like quenched quantum fluids. For a system with second order phase transition, the domain structure naturally arises when it is cooled at a finite rate. Since diverging correlation length are accompanied with critical slowing down, the system has to fall out of equilibrium for any non-zero rate; At this so called fall out time the correlation length is frozen out before the transition can take place globally. Within this picture, we investigate the non-equilibrium dynamics in a soft-matter analogue, a two-dimensional ensemble of colloidal particles which in equilibrium obeys the Kosterlitz-Thouless-Halperin-Nelson-Young melting scenario with continuous phase transitions. The ensemble is exposed to finite cooling rates of the pair-interaction parameter (being an inverse system temperature) at very different rates from deep in the isotropic fluid into the polycrystalline phase. We analyse defect configurations as well as the evolution of orientationally ordered domains quantitatively via video microscopy and show that their frozen-out length scale follows an algebraic decay as function of the quench rate as predicted by the Kibble-Zurek mechanism.

15 min. break.

DY 13.5 Mon 17:15 PC 203

Molecular Dynamics Study of Colloidal Quasicrystals — ●HEIKO G. SCHOBERTH, HEIKE EMMERICH, and THOMAS GRUHN — Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth

Quasicrystals are of continuous interest due to their fascinating fundamental properties and their potential applications like advanced photonic materials. In the last years colloidal quasicrystals have been found in solutions with spherical polymer core-shell micelles [1]. Fundamental aspects have been investigated in theoretical studies in which the core-shell micelles are represented with a step-potential, in which the core-core interaction is modeled by infinite repulsion while the shell-shell interaction is modeled by a plateau at constant height ϵ and width λ [2]. The real interaction of the micelles is a continuous function which is more smeared out at the core and shell boundaries. Therefore, we perform coarse-grained molecular dynamics simulations to investigate the influence of the potential shape on the self-assembling structure. Varying the parameters we study systematically the phase diagram finding domains with 6-,10-,12-,24-fold symmetries. With increasing smoothness of the potential the phase diagram changes qualitatively and the geometry of the phase boundaries gets more regular.

[1] Fischer S. et al., PNAS, 108, 1810-1814 (2011)

[2] Dotera T. et al., Nature, 506, 208-2011 (2014)

DY 13.6 Mon 17:30 PC 203

Real-time study of multi-step nucleation in protein crystallization — ●ANDREA SAUTER¹, FELIX ROOSEN-RUNGE², FAJUN ZHANG¹, GUDRUN LOTZE³, ROBERT M. J. JACOBS⁴, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — ²Institut Laue-Langevin, Grenoble, France — ³European Synchrotron Radiation Facility, Grenoble, France — ⁴Department of Chemistry, University of Oxford, UK

We present a real-time study of protein crystallization of bovine β -lactoglobulin in the presence of the divalent salt CdCl_2 using SAXS and optical microscopy. Monitoring the crystallization kinetics, we demonstrate a multi-step crystallization mechanism particularly focusing on the role of the metastable intermediate phase (MIP). In the first step, an intermediate phase is formed, followed by the nucleation of crystals within the intermediate phase. In the next step, this intermediate phase is consumed by nucleation and slow growth and the crystals are exposed to the dilute phase. At this stage, the number of crystals stays nearly constant, whereas the crystals grow rapidly due to access to the free protein molecules in the dilute phase. The results suggest that increasing the salt concentration near the transition zone *pseudo-c*** reduces the energy barrier for both the MIP and crystal nucleation. The observed kinetics can be well described using a rate-equation model based on a clear physical multi-step picture. This real-time study not only provides direct evidence for a multi-step

process for protein crystallization, but also elucidates the role and the structural signature of the MIP in the non-classical process of protein crystallization.

DY 13.7 Mon 17:45 PC 203

All-atom MD simulation of fullerene dyads in water: Exploring hydrophobic hydration — ●OLGA GUSKOVA¹, SRINIVASA RAO VARANASI^{1,2}, and JENS-UWE SOMMER^{1,3} — ¹Leibniz-Institut für Polymerforschung Dresden e. V., Theorie der Polymere, Hohe Str. 6, 01069 Dresden, Deutschland — ²University of Queensland, School of Chemical Engineering, St Lucia QLD 4072, Australia — ³Technische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, 01069 Dresden, Deutschland

The nanometer-sized C60 fullerene, being a boundary case between small and large hydrophobes, represents an interesting object for the investigation of hydrophobic hydration. Extensive MD simulations are performed to study the solvation of pristine fullerene and fullerene dyads as well as their self-assembly in water [1]. The solute-solvent interactions, which reflect in the structure of solvation shells, translational and orientational dynamics of water molecules near the hydrophobic C60 cage and hydrophilic side chain, the H-bond networks and their defects, as dangling -OH bonds, are described. The agglomeration behavior of fullerenes is evaluated by determining sizes of the clusters, solvent accessible surface areas, and shape parameters. [1] O. Guskova, S.R. Varanasi, and J.-U. Sommer, *J. Chem. Phys.* 141 (14), 144303 (2014).

DY 13.8 Mon 18:00 PC 203

Phase field simulations of particle capture during directional solidification of photovoltaic silicon — HEIKE EMMERICH¹, ●HENNING HÖRSTERMANN¹, JULIA KUNDIN¹, JOCHEN FRIEDRICH², MARAL AZIZI², CHRISTIAN REIMANN², ARNE CRÖLL³, THOMAS JAUSS³, and TINA SORGENFREI³ — ¹University Bayreuth, Chair of Material and Process Simulations, Bayreuth, Germany — ²Fraunhofer IISB, Erlangen, Germany — ³University Freiburg, Institute for Geosciences, Freiburg, Germany

We study the interaction between the solidification front and SiC particles present in the melt during the growth process of silicon for solar cells. Particles of a given size are pushed in front of the interface for growth velocities below a critical value and are incorporated into

the crystal for growth velocities above this value. The existing theoretical models for particle capture find a relationship between critical particle size and critical growth velocity by assuming an equilibrium between a combination of gravity, drag, lift and other forces acting on the particle in the vicinity of the interface. For silicon these models predict significantly higher critical particle sizes than observed in experiments. We use a phase field model to test if these deviations can be explained by deviations from the spherical particle shape usually assumed in the theoretical models or effects like the deformation of the interface caused by the presence of the particle. In addition to testing and adapting existing theories, we narrow down the possible underlying mechanisms by identifying relevant length scales and other properties that are required to explain the experimental results.

DY 13.9 Mon 18:15 PC 203

Crystallization kinetics in printed active layers for organic solar cells — ●STEPHAN PRÖLLER¹, FENG LIU², CHENHUI ZHU³, PETER MÜLLER-BUSCHBAUM⁴, THOMAS P. RUSSELL², ALEXANDER HEXEMER³, and EVA M. HERZIG¹ — ¹Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — ²University of Massachusetts Amherst, Department of Polymer Science and Engineering, MA 01003 Amherst, Massachusetts, USA — ³Lawrence Berkeley National Laboratory, Advanced Light Source, CA 94720 Berkeley, California, USA — ⁴Technische Universität München, LS Funktionelle Materialien, 85748 Garching, Germany

Organic solar cells are a promising alternative to silicon based inorganic ones. Among other advantages like high absorption, a key advantage is the processability out of solution. This allows for printing of large area photovoltaic devices at low costs at low energy input. The morphology and crystalline properties of the active layer is of utmost importance for the functionality like exciton separation or charge carrier transport and thus for the performance of the produced devices. So far, not much is known on the crystallization kinetics of printed organic photoactive layers. Using an industrial slot-die printing process we studied the morphology evolution of a photoactive blend by in-situ X-ray scattering methods. With these experiments we are able to picture the process of crystallization of the polymer blend. We identified different stages during crystallization and propose a model for the crystal growth. This understanding is important to gain control over the morphology development of the system to improve organic solar cell performance.

DY 14: Focus Session: Chimera states: symmetry-breaking in dynamical networks (joint session DY/ BP)

Chimera states in dynamical networks consist of coexisting domains of spatially coherent (synchronized) and incoherent (desynchronized) behavior. They are a manifestation of spontaneous symmetry-breaking in systems of identical, nonlocally coupled oscillators, and have recently been found in different forms (phase chimeras, amplitude chimeras, multi-headed, 1D, 2D, or 3D). Such phenomena may occur in a variety of physical, chemical, biological, technological, or socio-economic systems, for instance in coupled optical systems, neural networks, mechanical, chemical or electrochemical oscillators, power grids, or communication networks. (Organizer: Eckehard Schöll)

Time: Tuesday 9:30–12:30

Location: BH-N 243

Invited Talk

DY 14.1 Tue 9:30 BH-N 243

Basins of Attraction for Chimera States — ●ERIK ANDREAS MARTENS^{1,2}, MARK PANAGGIO^{3,4}, and DANIEL ABRAMS^{4,5} — ¹Dept. of Biomedical Sciences, University of Copenhagen, Blegdamsvej 3, 2200 Copenhagen, Denmark — ²Dept. of Mathematical Sciences, University of Copenhagen, Universitetsparken 5, 2200 Copenhagen, Denmark — ³Dept. of Mathematics, Rose-Hulman Institute of Technology, Terre Haute, Indiana 47803 — ⁴Dept. of Engineering Sciences and Applied Mathematics, Northwestern University, Evanston, Illinois 60208 — ⁵Northwestern Institute on Complex Systems, Northwestern University, Evanston, Illinois 60208, USA

The coexistence of synchronized and desynchronized regions in populations of identical oscillators, known as chimera states, has received much attention following their recent experimental discovery. Chimeras occur only for special initial conditions; yet, despite numerous theoretical efforts their basins of attraction remain unexplored. We provide the first analysis of their basins of attraction by studying the simplest chimera system with two populations, allowing for three

configuration patterns: one fully synchronized and two partly synchronized patterns. The basins form a complex twisting motion around an invariant ray; our perturbative analysis allows the prediction of the asymptotic states and the associated destination maps. Understanding the precise nature of the basins is needed to develop control methods to switch between chimeric configuration patterns, which may be exploited for technological applications and serve function in neural biology.

Invited Talk

DY 14.2 Tue 10:00 BH-N 243

Hysteretic transitions and chaotic chimera states in networks of Kuramoto oscillators with inertia — ●SIMONA OLMI — CNR - Istituto dei Sistemi Complessi, Sesto Fiorentino, Italy — INFN sez. Firenze, Sesto Fiorentino, Italy

We report finite size numerical investigations and mean field analysis of a Kuramoto model with inertia for fully coupled and diluted systems. In particular, we examine for a Gaussian distribution of the frequencies the transition from incoherence to coherence for increasingly

large system size and inertia. For sufficiently large inertia the transition is hysteretic and within the hysteretic region clusters of locked oscillators of various sizes and different levels of synchronization coexist. A modification of the mean field theory developed by Tanaka, Lichtenberg, and Oishi [Physica D, 100 (1997) 279] allows to derive the synchronization profile associated to each of these clusters. By increasing the inertia the transition becomes more complex, and the synchronization occurs via the emergence of clusters of whirling oscillators. The presence of these groups of coherently drifting oscillators induces oscillations in the order parameter. We have shown that the transition remains hysteretic even for randomly diluted networks up to a level of connectivity corresponding to few links per oscillator. Finally an extension to a system of two symmetrically coupled networks of Kuramoto oscillators with inertia is reported. In this system the existence and the dynamical properties of novel chaotic chimera states are investigated, concentrating both on the microscopic dynamics and the macroscopic behavior.

Invited Talk DY 14.3 Tue 10:30 BH-N 243

Transient amplitude chimeras: the impact of time delay and noise — ●ANNA ZAKHAROVA¹, JULIEN SIEBERT¹, SARAH LOOS¹, ALEKSANDAR GJURCHINOVSKI², and ECKEHARD SCHÖLL¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, Germany — ²Institute of Physics, Faculty of Natural Sciences and Mathematics, Sts. Cyril and Methodius University, Skopje, Macedonia

For a network of Stuart-Landau oscillators with symmetry-breaking coupling we find chimera behavior with respect to amplitude dynamics rather than the phase (amplitude chimeras). We investigate the role of time delay and noise for these coherence-incoherence patterns. In more detail, we address the question of how time delay and noise influence the lifetime of transient amplitude chimeras.

15 min. break

DY 14.4 Tue 11:15 BH-N 243

Clusters, chimeras and localized turbulence under nonlinear global coupling — ●LENNART SCHMIDT, SINDRE W. HAUGLAND, and KATHARINA KRISCHER — Physik-Department, Nonequilibrium Chemical Physics, Technische Universität München, Garching, Germany

The coexistence of coherently and incoherently oscillating parts in a system of identical oscillators with symmetrical coupling, i.e. a chimera state, is even observable with uniform global coupling. We investigate the prerequisites for chimera states in globally coupled systems. It turns out that a clustering mechanism constitutes the first symmetry-breaking step as it splits the system into two groups. We demonstrate this by means of two different cluster solutions giving rise to two different chimera states. Consequently, essential features of the cluster solutions can be rediscovered in the corresponding chimera states. Furthermore, we compare the chimera states to localized turbulence and discuss their qualitative differences.

Given a chimera state with synchronized and desynchronized regions of the same size, interchanging both phases again yields a solution to the underlying equations. We observe this process of alternation emerging spontaneously. Studying different initial conditions, we could identify the growth of the turbulent domain as being responsible for the repeatedly occurring interchanges.

DY 14.5 Tue 11:30 BH-N 243

Amplitude-phase coupling drives chimera states in small globally coupled laser networks — FABIAN BÖHM¹ and ●KATHY LÜDGE² — ¹Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Institut f. Theo. Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany Berlin, Germany

Chimera states are an intriguing and widely discussed phenomenon, in which an ensemble of coupled systems self-organizes into spatially

separated regions of coherence and incoherence. While we still lack a complete understanding of this general phenomenon, three common existence criteria have been formulated in the past which demand large system sizes with non-local coupling and specially prepared initial conditions. For a network of globally coupled semiconductor lasers with time-delayed optical feedback, we show the existence of chimera states that defy these existence criteria. The typical regions of coherence and incoherence were found to exist for the amplitude and phase of the electrical field as well as the inversion of the electrons. Their stability does not depend on the system size which allows for the formation of chimera states in a system of only four coupled lasers. The formation of the chimera states can be linked to regions of multistability. Their occurrence is driven by the amplitude-phase coupling of the semiconductor lasers.

DY 14.6 Tue 11:45 BH-N 243

Chimera states in Van der Pol oscillators: Impact of local dynamics and time delay — ●IRYNA OMELCHENKO¹, ANNA ZAKHAROVA¹, JULIEN SIEBERT¹, PHILIPP HÖVEL^{1,2}, and ECKEHARD SCHÖLL¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin — ²Bernstein Center for Computational Neuroscience, Berlin

We discuss the phenomena of chimera states that exhibit spatial coexistence of regular synchronized and irregular incoherent regions in a network of nonlocally coupled Van der Pol oscillators. Tuning the bifurcation parameter of the individual units allows us to interpolate between regular sinusoidal and relaxation oscillations. We discuss the impact of these local dynamics on the occurrence of chimera states in the system, regimes of their stability in the parameter space, and analyze the influence of time delay introduced in the coupling.

DY 14.7 Tue 12:00 BH-N 243

Robustness of chimera states for coupled FitzHugh-Nagumo oscillators — ●PHILIPP HÖVEL^{1,2}, IRYNA OMELCHENKO¹, ECKEHARD SCHÖLL¹, JOHANNE HIZANIDIS³, and ASTERO PROVATA³ — ¹Technische Universität Berlin — ²Bernstein Center for Computational Neuroscience Berlin — ³National Center for Scientific Research "Demokritos", Athens

Chimera states are complex spatio-temporal patterns that consist of coexisting domains of spatially coherent and incoherent dynamics. This counterintuitive phenomenon was first observed in systems of identical oscillators with symmetric coupling topology. Can one overcome these limitations? To address this question, we discuss the robustness of chimera states in networks of FitzHugh-Nagumo oscillators. Considering networks of inhomogeneous elements with regular coupling topology, and networks of identical elements with irregular coupling topologies, we demonstrate that chimera states are robust with respect to these perturbations, and analyze their properties as the inhomogeneities increase. We find that modifications of coupling topologies cause qualitative changes of chimera states: additional random links induce a shift of the stability regions in the system parameter plane, gaps in the connectivity matrix result in a change of the multiplicity of incoherent regions of the chimera state, and hierarchical geometry in the connectivity matrix induces nested coherent and incoherent regions.

DY 14.8 Tue 12:15 BH-N 243

Chimera states and the interplay between initial conditions and non-local coupling — ●PETER KALLE^{1,2}, ANNA ZAKHAROVA¹, VLADIMIR GARCÍA-MORALES², KATHARINA KRISCHER², and ECKEHARD SCHÖLL¹ — ¹TU Berlin, Institut für Theoretische Physik — ²TU München, E19 - Chemische Physik fern vom Gleichgewicht

This talk addresses the impact of initial conditions and non-local coupling on the emergence of chimera states in networks of Stuart-Landau oscillators. An intuitive approach is presented by which it is possible to successfully predict and explain the occurrence of chimera states. Following this, some of the main properties of chimera states are discussed in the light of this approach.

DY 15: Statistical Physics - general

Time: Tuesday 9:30–12:30

Location: BH-N 334

DY 15.1 Tue 9:30 BH-N 334

Extracting Canonical Information from Grand Potential Density Functional Theory — •DANIEL DE LAS HERAS and MATTHIAS SCHMIDT — Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

Studying averaged quantities that compress the full many-body information into digestible, analyzable and experimentally measurable quantities lies at the core of essentially all condensed matter physics. Moreover, suitable averaging often simplifies theoretical treatments. An example is the use of the grand canonical ensemble, which permits fluctuations in the total number of particles, in the formulation of statistical mechanical liquid state theories. The structuring and self-assembly of real systems, however, can depend crucially on the precise number of particles in the system. In particular small systems, such as e.g. finite colloidal clusters, are better analyzed canonically, where the number of particles is fixed.

We present a general and formally exact method to obtain the canonical one-body density distribution and the canonical partition sums from direct decomposition of classical density functional results in the grand canonical ensemble [1]. The method is relevant for treating finite systems.

[1] D. de las Heras, and M. Schmidt. Accepted in Phys. Rev. Lett. (2014).

DY 15.2 Tue 9:45 BH-N 334

Canonical approach to equilibrium properties of interacting quantum gases — QUIRIN HUMMEL, JUAN DIEGO URBINA, and •KLAUS RICHTER — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

It is generally accepted that the equilibrium properties of quantum gases give the same results for the canonical and grand canonical ensemble. For finite systems well below the thermodynamic limit, however, this equivalence breaks down. The total number of particles cannot be fixed within the grand canonical formalism where this quantity is subject to thermal and quantum fluctuations. This poses a serious problem, as most of the powerful techniques to deal with quantum and interaction effects in quantum gases are based on the grand canonical formalism.

In this contribution we present a purely canonical approach, with the specific intention to obtain virial-type expansions for finite systems of interacting identical particles, including the equation of state and (local and non-local) pair correlations. In our formalism the canonical partition function is given by a finite expansion in the inverse temperature, thus providing a closed explicit form for the quantum equation of state. We also discuss the thermodynamic limit and the effect of interactions and particle symmetry on the many-body spectra.

DY 15.3 Tue 10:00 BH-N 334

Calculating the density of states for materials with nested sampling — •ROBERT BALDOCK¹, LIVIA BARTÓK-PÁRTAY², ALBERT BARTÓK-PÁRTAY³, MIKE PAYNE¹, and GÁBOR CSÁNYI³ — ¹Department of Physics, University of Cambridge — ²Department of Chemistry, University of Cambridge — ³Department of Engineering, University of Cambridge

We present the developed nested sampling algorithm for calculating the density of states of materials. Having obtained the density of states, one can calculate the partition function and perform statistical mechanics in full. We demonstrate calculation of the complete pressure-temperature phase diagram for aluminium (using an EAM potential), and a binary Lennard-Jones “alloy” that exhibits an order-disorder transition.

Thermal distributions for virtually any structural quantity can be calculated from the output of Nested Sampling. Such distributions are obtained in seconds at any temperature.

DY 15.4 Tue 10:15 BH-N 334

Weak thermal contact is not universal for work extraction — •HENRIK WILMING, RODRIGO GALLEGO, and JENS EISERT — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

The free energy difference to the equilibrium state limits the amount of work that can be extracted on average from a system out of thermal

equilibrium. This bound can be saturated by protocols putting the system and a bath into weak thermal contact (WTC), i.e., bringing the system into a Gibbs state at the bath’s temperature. Surprisingly, the same bound holds true when the contact to the heat bath is modelled by more general processes, which have the only restriction that when the system already is in equilibrium, it cannot be brought out of it. In that sense, WTC is universal for work extraction.

In this work, we introduce the study of work-extraction protocols under restrictions encountered in realistic devices at the nano-scale. We consider limitations on the maximum energies in the system and on the local structure of many-body Hamiltonians. Remarkably, we find that WTC then loses its universality: There is a gap between the work that can be extracted with WTC and with more general operations. Our work highlights the relevance of operational frameworks such as those of thermal operations and Gibbs preserving maps, as they can improve the performance of thermal machines, and provides a unifying framework of incorporating natural restrictions in quantum thermodynamics.

DY 15.5 Tue 10:30 BH-N 334

Ising model on two-dimensional unimodular Lattice Triangulations — •TONY WASSERKA, BENEDIKT KRÜGER, and KLAUS MECKE — Institut für Theoretische Physik, Staudtstr. 7, 91058 Erlangen

Unimodular triangulations of two-dimensional integer lattices can be used as real-space networks implementing certain amounts of order or disorder. We couple the well-known Ising model (which is a common prototype model for phase transitions and can be solved analytically for regular lattices) with such lattice triangulations so that nearest neighbours are defined by the edges of the triangulation. Using this setup the critical temperature and critical exponents can be measured numerically using Monte-Carlo-simulations. Introducing an order parameter for triangulations and interpreting it as an energy we determine micro-canonical and canonical averages and therewith the order-dependency of these critical observables.

DY 15.6 Tue 10:45 BH-N 334

Corrections to finite-size scaling in the φ^4 model on square lattices — •JEVGENIJS KAUPUZS — University of Latvia, LV-1459 Riga, Latvia

Corrections to scaling in the two-dimensional scalar φ^4 model are studied based on non-perturbative analytical arguments and Monte Carlo (MC) simulation data for different lattice sizes L ($4 \leq L \leq 1536$) and different values of the φ^4 coupling constant λ , i. e., $\lambda = 0.1, 1, 10$. According to our analysis, amplitudes of the nontrivial correction terms with the correction-to-scaling exponents $\omega_\ell < 1$ become small when approaching the Ising limit ($\lambda \rightarrow \infty$), but such corrections generally exist in the 2D φ^4 model. Analytical arguments show the existence of corrections with the exponent $3/4$. The numerical analysis suggests that there exists also a correction with the exponent $1/2$, which is detectable at $\lambda = 0.1$. The numerical tests clearly show that the structure of corrections to scaling in the 2D φ^4 model differs from the usually expected one in the 2D Ising model.

15 min. break

DY 15.7 Tue 11:15 BH-N 334

Multiply charged monopoles in cubic dimer model — •SREEJITH GANESH JAYA¹ and STEPHEN POWELL² — ¹MPI PKS, Dresden, Germany — ²University of Nottingham, UK

The classical cubic dimer model is a 3 dimensional statistical mechanical system whose degrees of freedom are dimers that occupy the edges between nearest neighbour vertices of a cubic lattice. Dimer occupancies are subject to the local constraint that every lattice point is associated with exactly one dimer. In the presence of an aligning interaction, it is known that the system exhibits an unconventional continuous thermal phase transition from a symmetry broken columnar phase to a Coulomb-phase. The transition is in the NCCP1 universality class, which also describes the Neel-VBS transition in the JQ model and the S=1/2 Heisenberg model with suppression of hedgehog defects. Using Monte-Carlo simulations of a pair of defects in a background of fluctuating dimers, we calculate the scaling exponents

for fugacities of monopole defects of charge $Q=2$ and 3 in this critical point. Our estimates suggest that $Q=3$ monopoles are relevant and could therefore drive the JQ model away from the NCCP1 critical point on a hexagonal lattice.

DY 15.8 Tue 11:30 BH-N 334

Critical adsorption and Casimir forces in systems with a globally constrained order parameter — ●MARKUS GROSS^{1,2}, OLEG VASILYEV^{1,2}, and SIEGFRIED DIETRICH^{1,2} — ¹Max-Planck-Institut für Intelligente Systeme, Heisenbergstrasse 3, 70569 Stuttgart, Germany — ²Institut für Theoretische Physik IV, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Typically, critical phenomena are investigated in the grand canonical ensemble, in which the order parameter is free to fluctuate without constraints. However, confining systems with a locally conserved order parameter – such as fluids in a closed environment – imposes a global constraint on the order parameter and thereby changes its fluctuation spectrum. This situation is naturally encountered in particle- or hydrodynamics-based simulations, such as Molecular Dynamics or Lattice Boltzmann methods. Here, we explore the consequences of the global order-parameter conservation on critical adsorption at walls and critical Casimir forces in a fluid film. Analytical calculations have been performed within mean-field theory as well as statistical field theory of a Ginzburg-Landau model. These results are confronted with Monte-Carlo simulations of the Ising model. Depending on the boundary conditions, the constraint is found to induce significant changes in the shape of the order-parameter profile of the adsorbed fluid. For instance, within mean field theory the divergence of the order parameter at the wall is cut-off. For certain boundary conditions, the Casimir force experienced by the critical film can have a drastically different temperature dependence as a consequence of the constraint.

DY 15.9 Tue 11:45 BH-N 334

Equilibrium of a mesoscopic system in a damping induced inhomogeneous space — ●ARIJIT BHATTACHARYAY — Indian Institute of Science Education and Research, Pune, India

Complex molecules like proteins, colloids etc can often have conformation dependent damping due to varied proximity of its constituents from each other at different conformational states. The dynamics of such systems in the conformation space, when in equilibrium with a homogeneous heat bath, is generally considered to be a stochastic dynamics with multiplicative noise. The origin of the multiplicative noise is related to the inhomogeneity of the conformation space caused by damping on top of which there can exist inhomogeneity of space caused by a conservative force field as usual. I would argue that, the equilibrium distribution of such systems has to be of a modified Maxwell-Boltzmann form resulting from a stochastic dynamics with additive noise. In this approach, putting the stochastic problem to an additive noise form would be the prerequisite for equilibrium. The results at the limit of constant damping would be recovered.

DY 15.10 Tue 12:00 BH-N 334

DY 16: Microswimmers - Part I (joint session DY/ BP/ CPP)

Time: Tuesday 9:30–12:30

Location: BH-N 128

DY 16.1 Tue 9:30 BH-N 128

Trapping of active particles in inhomogeneous systems — ●MARTIN P. MAGIERA, KEVIN SCHRÖER, and LOTHAR BRENDEL — Fakultät für Physik, Universität Duisburg-Essen

Inhomogeneities in a system containing active particles can lead to an inhomogeneous particle distribution if they influence the particles' velocities [Schnitzer, PRE **48**, 2553]. Those may be caused, e.g., by inhomogeneous tumble rates of bacteria or inhomogeneous drive of men-made microswimmers [e.g. Buttinoni et al, PRL **110**, 238301].

Using Brownian dynamics simulations we show that such inhomogeneities can lead to particle accumulation in a prescribed passivity region where the activity of particles is suppressed, an effect interesting for applications. We derive a corresponding accumulation parameter with an extended Fick's law for inhomogeneous systems. Depending on the overall particle density a complete particle trapping can be observed. However, even if only a minority of particles is trapped, a tiny yield can act as a nucleation seed for larger agglomerates generated by dynamical clustering [Fily and Marchetti, PRL **108**, 235702] and

Electrical charging effects on sliding lubrication properties of a model confined ionic liquid — ●ROSARIO CAPOZZA¹, ANDREA BENASSI², ANDREA VANOSSI^{3,1}, and ERIO TOSATTI^{1,4} — ¹International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy — ²Empa, Materials Science and Technology, Uberlandstrasse 129, 8600 Dübendorf, Switzerland — ³CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy — ⁴International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34014 Trieste, Italy

Ionic liquids lubricants, used under conditions of nanometric confinement between parallel plates or tip-surface gaps, explore the dependence of friction upon charging, suggestive of some electrical control of dynamics the friction between parallel plates under conditions of successive layering reached by squeezeout under an increasing inter-plate force. We then simulate the frictional changes brought about by different charging states of the plates, related to charging-induced switches corresponding to squeezeout (or suck-in) transitions between different layering states as predicted by local minima in the charge-dependent enthalpy curves. Although the actual frictional behavior obtained does depend upon the assumed features and parameters of the model liquid and its interaction with the plates, the broader scenario obtained for charging effects, its relationship to the equilibrium layering and its enthalpy characterization appear of general value.

DY 15.11 Tue 12:15 BH-N 334

Towards a General Theory of Extremes for Observables of Chaotic Dynamical Systems — ●VALERIO LUCARINI — Institute of Meteorology, University of Hamburg, Hamburg, Germany — Department of Mathematics and Statistics, University of Reading, Reading, UK

In this paper we provide a connection between the geometrical properties of a chaotic dynamical system and the distribution of extreme values. We show that the extremes of so-called physical observables are distributed according to the classical generalised Pareto distribution and derive explicit expressions for the scaling and the shape parameter. In particular, we derive that the shape parameter does not depend on the chosen observables, but only on the partial dimensions of the invariant measure on the stable, unstable, and neutral manifolds. The shape parameter is negative and is close to zero when high-dimensional systems are considered. This result agrees with what was derived recently using the generalized extreme value approach. Combining the results obtained using such physical observables and the properties of the extremes of distance observables, it is possible to derive estimates of the partial dimensions of the attractor along the stable and the unstable directions of the flow. Moreover, by writing the shape parameter in terms of moments of the extremes of the considered observable and by using linear response theory, we relate the sensitivity to perturbations of the shape parameter to the sensitivity of the moments, of the partial dimensions, and of the Kaplan-Yorke dimension of the attractor.

pinned to the passivity region.

DY 16.2 Tue 9:45 BH-N 128

Statistics of passive tracers in an active fluid — ●LEVKE ORTLIEB¹, MATTHIAS MUSSLER¹, CHRISTIAN WAGNER¹, THOMAS JOHN¹, PHILIPPE PEYLA², and SALIMA RAFAI² — ¹Universität des Saarlandes — ²Université Joseph Fourier - CNRS - LIPHY, Grenoble

In all aqueous suspension on earth there are various microswimmers, e.g. algae. In our experiments we tracked passive polystyrene particles with diameters from 1 to $3\mu\text{m}$ in suspension with the green alga *Chlamydomonas reinhardtii* at various concentrations. We used dark field microscopy for observations. The alga has a nearly spherical body of 5 to $10\mu\text{m}$ diameter and two flagella, which allow it to swims as a puller. We analysed the trajectories of the colloids statistically, in particular, the mean squared displacement and the probability density function (pdf) of position were computed. We found similarities to Brownian motion, as the mean squared displacement is proportional to time, but interestingly also a significant deviation was found: a non

gaussian pdf of the tracer particle positions.

DY 16.3 Tue 10:00 BH-N 128

Characterization of Swimming *Bacillus Subtilis* — ●JAVAD NAJAFI¹, THOMAS JOHN¹, GERT BANGE², and CHRISTIAN WAGNER¹ — ¹Experimental Physics, Saarland University, D-66123 Saarbrücken, Germany — ²LOEWE Center for Synthetic Microbiology (Synmikro), Marburg, Germany

Bacteria can use flexible appendages called flagella to swim in aqueous environment. Our goal is to understand the influence of the number of flagella on the swimming behavior and efficiency. We study wild type strain of *bacillus subtilis* as a model system to unravel a few fundamental questions on swimming behavior of bacteria. Our microorganism is a peritrichous bacterium with about 25 flagella, and uses run and tumble strategy to explore its surrounding. Using dark field microscopy and tracking of single cell movements, we calculate statistics of swimming velocity, running and tumbling times, turning angles, diffusion coefficients and the temporal auto-correlations in changes of swimming directions. In further steps, we will investigate the influence of number of flagella on genetically engineered *bacillus subtilis* in aforementioned quantities.

DY 16.4 Tue 10:15 BH-N 128

Non-linear dynamics of self-organized ciliary beats — ●PABLO SARTORI and FRANK JULICHER — Max Planck Institute for the Physics of Complex Systems, Noethnitzer Strasse 38, 01187, Dresden, Germany.

The dynamic bending of cilia is driven by forces generated by dynein motor proteins. These forces slide adjacent microtubule doublets within the cilium. To create oscillatory beating patterns the activities of the dyneins must be coordinated both spatially and temporally. It is believed that this coordination occurs via the self-organization of the motors along the cilium, which are regulated by local strains such as sliding or curvature. Yet which strain is the most relevant in regulation remains an elusive question.

In this work we show that self-organization of the motors is possible via a dynamic instability. We study the emerging beat patterns close and far from the critical point. By comparing two different motor regulatory mechanisms, sliding and curvature regulation, we conclude that the first only produces propulsion for long cilia, while the second does so also for short cilia. Our work thus suggests that short cilia may be regulated via curvature, and not sliding of the filaments.

DY 16.5 Tue 10:30 BH-N 128

Simulation of a microswimmer consisting of a four bead ring — ●HENDRIK ENDER and JAN KIERFELD — Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund

Bead-spring structures undergoing cyclic shape changes in a viscous liquid can serve as model systems for artificial microswimmers. Closed ring-like bead-spring models can propel by cyclic shape changes, for example, induced by cyclic expansion and contraction of springs. Using multi-particle collision dynamics, we simulate a four-bead swimmer model in which the spheres are linked into a square-shaped ring structure. We show that cyclic changes of linker lengths give rise to a net swimming motion. The model can be generalized by including more beads into the ring structure and represents the first step towards the simulation of bigger ring or spherical swimmers, which propel by cyclic swelling and shrinking.

DY 16.6 Tue 10:45 BH-N 128

Spontaneous chiral symmetry breaking in model bacterial suspensions — REBEKKA E. BREIER¹, ROBIN L. B. SELINGER², GIOVANNI CICCOTTI^{3,4}, STEPHAN HERMINGHAUS¹, and ●MARCO G. MAZZA¹ — ¹Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany — ²Chemical Physics Interdisciplinary Program, Liquid Crystal Institute, Kent State University, Kent, OH, USA — ³Department of Physics, University of Rome “La Sapienza”, P.le A. Moro 5, 00185 Rome, Italy — ⁴School of Physics, University College Dublin, Belfield, Dublin 4, Ireland

Chiral symmetry breaking is ubiquitous in biological systems, from DNA to bacterial suspensions. A key unresolved problem is how chiral structures may spontaneously emerge from achiral interactions. We study a simple model of bacterial suspensions in three dimensions that effectively incorporates active motion and hydrodynamic interactions. We perform large-scale molecular dynamics simulations (up to 10^6 par-

ticles) and describe stable (or long-lived metastable) collective states that exhibit chiral organization although the interactions are achiral. We elucidate under which conditions these chiral states will emerge and grow to large scales. We also study a related equilibrium model that clarifies the role of orientational fluctuations.

15 min. break

DY 16.7 Tue 11:15 BH-N 128

Velocity distributions in active Brownian suspensions — ●ZAHRA MOKHTARI and ANNETTE ZIPPELIUS — Institute for Theoretical Physics, Georg-August University of Göttingen

We study numerically a model of self-propelled polar disks in suspension. The active particles interact via hard-core elastic interactions and are driven along their axes, which are subject to rotational noise. We study the distribution of linear and rotational velocities, which are predicted to show strongly anomalous but largely universal features. We furthermore analyze the correlations due to the coupling of translational and rotational motion and show that the alignment of particles' velocities and orientations can be controlled by the damping.

DY 16.8 Tue 11:30 BH-N 128

Experimental setup for 3D tracking of artificial active microswimmers — ●GUNNAR KLÖS, CARSTEN KRÜGER, CORINNA C. MAASS, and STEPHAN HERMINGHAUS — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

During solubilisation in an aqueous surfactant solution well above the critical micelle solution, droplets of nematic liquid crystal show self-propelled swimming, driven by a Marangoni flow at the droplet interface [1]. These active pusher-type swimmers provide a potential physical model-system for micro-bioswimmers. We expect dimensional confinement to have a significant impact on their dynamics [2].

We have designed an experimental setup combining a microfluidic cell with a selective plane microscope using a scanning fluorescent light sheet [3]. At densities within the single scattering limit, trajectories of single swimmers or ensembles can be recorded under varying conditions of buoyancy, particle activity and cell geometry.

[1] S. Herminghaus et al., *Soft Matter* **10**, 7008 (2014). [2] E. Lauga et al., *Biophys. J.* **90**, 400 (2006). [3] J. Huisken et al., *Science* **305**, 1007 (2004).

DY 16.9 Tue 11:45 BH-N 128

Liquid crystal droplets as artificial microswimmers — CARSTEN KRÜGER, GUNNAR KLÖS, CHENYU JIN, CORINNA C. MAASS, ●CHRISTIAN BAHR, and STEPHAN HERMINGHAUS — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Droplets of common nematic mesogens show self-propelled motion (velocity up to $50 \mu\text{m/s}$, typical droplet diameter $10 - 100 \mu\text{m}$) when placed into aqueous phases containing ionic surfactants at concentrations considerably above the critical micelle concentration [1]. The self-propelled motion is fueled by the solubilization of the nematic droplet in the aqueous phase, resulting finally in the formation of a microemulsion in which all mesogenic molecules have been transferred from the initial droplet into the micelles of the ionic surfactant.

We report results concerning the dependence of the swimming behavior on various parameters (droplet size, surfactant concentration, etc.), the trajectories in different confinements, the collective behavior, and the influence of the nematic or isotropic state of the mesogenic droplets.

[1] S. Herminghaus, C. C. Maass, C. Krüger, S. Thutupalli, L. Goehring, and C. Bahr, *Soft Matter* **10**, 7008 (2014).

DY 16.10 Tue 12:00 BH-N 128

3D-tracking reveals how sperm find the egg — JAN F. JIKELI¹, LUIS ALVAREZ¹, ●BENJAMIN M. FRIEDRICH², and LAURENCE WILSON³ — ¹CAESAR, Bonn, Germany — ²MPI PKS, Dresden, Germany — ³University of York, York, UK

Sperm cells are guided to the egg by chemical cues in a process termed chemotaxis. We have previously put forward a theory of how sampling a concentration gradient along helical paths allows sperm of marine species to steer up-gradient [1]. Now, high-speed tracking in three space dimensions allows to probe sperm navigation live. We find that sperm display deterministic steering responses, which sets their chemotaxis strategy apart from those employed by most bacteria (biased random walk) or immune cells (spatial comparison). We

dissect the control logic that links sensation and motor actuation in sperm chemotaxis. We find that control delays are close to their theoretical optimum for up-gradient navigation. The resultant navigation strategy is particularly well suited for fast swimmers operating at the limits of chemical detection. The choice of optimal navigation strategy of a search agent is tightly linked to its susceptibilities for noise [2].

- [1] B.M. Friedrich *et al.*: Chemotaxis of sperm cells, *PNAS* **33**, 2007.
 [2] L. Alvarez *et al.*: The computational sperm cell, *Trends in Cell Biology* **24**, 2014.

DY 16.11 Tue 12:15 BH-N 128

Complex lane formation in a system of dipolar microswimmers — ●FLORIAN KOGLER and SABINE H. L. KLAPP — Institute of Theoretical Physics, Secr. EW 7-1, Technical University Berlin,

Hardenbergstrasse 36, D-10623 Berlin, Germany

We investigate the non-equilibrium structure formation of an experimentally motivated [1] two-dimensional (2D) binary system of dipolar colloids propelling in opposite directions. Using Brownian Dynamics simulations we find a transition towards a laned state, reminiscent of the laning transition in colloidal systems with isotropic repulsive interactions. However, the strongly anisotropic dipolar interactions induce two novel features: First, lanes are characterized by a complex internal structure. Second, the laning transition displays reentrance with respect to the interaction strength. We interpret our findings by simple theoretical arguments relating the observed behaviour to general equilibrium properties of phase-separating fluids [2].

- [1] S. Gangwal and O. J. Cayre and M. Z. Bazant and O. D. Velev, PRL 100 (2008) 058302.
 [2] F. Kogler and S. H. L. Klapp, preprint

DY 17: Modeling and Data Analysis

Time: Tuesday 9:30–12:00

Location: BH-N 333

DY 17.1 Tue 9:30 BH-N 333

Structure, equation of state and transport properties of molten calcium carbonate (CaCO₃) from atomistic simulations — RODOLPHE VUILLEUMIER¹, ●ARI PAAVO SEITSONEN^{1,2}, NICOLAS SATOR³, and BERTRAND GUILLOT³ — ¹Département de Chimie, École Normale Supérieure Paris, France — ²Institut für Chemie, Universität Zürich, Switzerland — ³Sorbonne Universités, Université Paris 6 et CNRS, UMR 7600, LPTMC, Paris, France

We have performed first-principle molecular dynamics (FPMD) simulations to evaluate the physical properties (liquid structure, density, atomic vibrational motion, diffusion coefficients and electrical conductivity) of liquid calcium carbonate (CaCO₃), which are up to now poorly known. As compared with silicate melts, molten CaCO₃ is characterized by a low density, a viscosity almost as low as that of water and a high conductivity. An empirical force field has been developed for predicting the properties of molten CaCO₃ at any state point in the liquid stability field and used in classical MD simulations, from which the equation of state and the phase diagram of the liquid phase have been obtained. The self diffusion coefficients, viscosity, and the electrical conductivity with pressure and temperature have been investigated and the results fitted to analytical forms. It is shown that the Stokes-Einstein equation, expressing the viscosity as a function of diffusion motion, is followed and that the Nernst-Einstein equation relating the electrical conductivity to the diffusion coefficients of charge carriers leads to an accurate prediction of the conductivity when a constant correcting factor is applied.

DY 17.2 Tue 9:45 BH-N 333

Optical detection of infrared and Raman modes in NdFeO₃ under pressure * theory and experiment — ●K. M. LEBECKI⁴, D. LEGUT⁵, M. MIHALIK JR.¹, M. MÍŠEK^{2,6}, M. VÁVRA^{1,3}, M. MIHALIK¹, K. V. KAMENEV², and M. ZENTKOVÁ¹ — ¹Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovak Republic — ²Centre for Science at Extreme Conditions, University of Edinburgh, Edinburgh, United Kingdom — ³Institute of Chemistry, Faculty of Science, P. J. Šafárik University, Košice, Slovak Republic — ⁴Nanotechnology Centre, VSB Technical University of Ostrava, Ostrava-Poruba, Czech Republic — ⁵IT4Innovations Centre, VSB Technical University of Ostrava, Ostrava-Poruba, Czech Republic — ⁶Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic

We determine lattice vibrations in NdFeO₃ crystal using first-principles calculations. We assign them to Raman- and infrared active modes according to the group theory. The direct method is used to obtain the Hellman-Feynman forces. The supercell approach with the finite displacement method is used to calculate phonon properties. Lattice vibrations, phonon density of states, dispersion curves, etc. are obtained by the PHONOPY program within harmonic approximation. Finally, our results are compared with other calculations using interatomic force constants and with our Raman experimental data for pressures up to 110 kbar.

DY 17.3 Tue 10:00 BH-N 333

Optimizing Large-Scale ODE Simulations — ●MARIO MULAN-

SKY — Institute for Complex Systems (ISC), CNR, Sesto Fiorentino, Firenze, Italy

Efficient computational methods are crucial in many parts of science. Here, we present a strategy to speed up Runge-Kutta-based ODE simulations of large systems with nearest-neighbor coupling. By introducing granularity we are able to transform the algorithm from bandwidth bound to CPU bound. By additionally employing SIMD instructions we are able to boost the efficiency even further. In total, a performance increase of up to a factor three is reached when using cache optimization and SIMD instructions compared to a standard implementation.

DY 17.4 Tue 10:15 BH-N 333

A Bayesian method for the analysis of deterministic and stochastic time series — ●CORYN BAILER-JONES — Max Planck Institute for Astronomy, Heidelberg, Germany

I introduce a general, Bayesian method for modelling univariate time series data assumed to be drawn from a continuous, stochastic process. The method accommodates arbitrary temporal sampling, and takes into account measurement uncertainties for arbitrary error models (not just Gaussian) on both the time and signal variables. Any model for the deterministic component of the variation of the signal with time is supported, as is any model of the stochastic component of the signal and time variables. The posterior probability distribution over model parameters is determined via Markov Chain Monte Carlo sampling. Models are then compared using the “cross-validation likelihood”, a version of the Bayesian evidence which is less sensitive to the prior. I illustrate the method on astronomical time series data using both deterministic models and a purely stochastic model, the Ornstein-Uhlenbeck process. This latter process appears to be a good description of several astronomical phenomena, including the flux variability of objects as different as brown dwarfs and active galactic nuclei.

DY 17.5 Tue 10:30 BH-N 333

Learning equations of motion from sparse observations — ●ANDREAS RUTTOR, PHILIPP BATZ, and MANFRED OPPER — Technische Universität Berlin

Equations of motion describe the dynamics of a system in terms of differential equations. These can be derived from theory if all the relevant properties are exactly known. But for real devices, e.g. robots, this is usually not the case. Instead one can drive the system applying a noisy control force and learn the equations of motion by observing its behavior. For that purpose we use a non-parametric approach based on Gaussian process regression, which does not require a detailed model of the dynamics, but still allows to include prior knowledge. As our method is based on estimating the probability distribution in phase space, it works with sparse observations, where the time intervals between data points are large.

DY 17.6 Tue 10:45 BH-N 333

State estimation and observability analysis employing delay coordinates — ●ULRICH PARLITZ^{1,2}, JAN SCHUMANN-BISCHOFF^{1,2}, and STEFAN LUTHER^{1,2} — ¹Max Planck Institute for Dynamics and Selforganization, Göttingen, Germany — ²Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Germany

For many dynamical processes in physics and other fields of science a model is known, but some of its variables and parameter values are difficult to observe or measure directly. In this case one may try to estimate the unknown quantities by adapting the model to time series generated by the process of interest. We shall revisit this problem by addressing the question whether the estimation problem is solvable in principle (observability) [1,2] and how synchronization based estimation methods can be improved to achieve good estimates based on few observables, only [3]. For both tasks delay coordinates will be employed and the main concepts will be illustrated using examples including the Lorenz-96 model and other chaotic systems.

[1] U. Parlitz, J. Schumann-Bischoff, and S. Luther, *Phys. Rev. E* 89, 050902(R) (2014).

[2] U. Parlitz, J. Schumann-Bischoff, and S. Luther, *Chaos* 24, 024411 (2014).

[3] D. Rey, M. Eldridge, M. Kostuk, H.D.I. Abarbanel, J. Schumann-Bischoff, U. Parlitz, *Physics Letters A* 378, 869-873 (2014).

15 min. break

DY 17.7 Tue 11:15 BH-N 333

A new typology of El Niño and La Niña phases based on evolving climate networks — ●MARC WIEDERMANN^{1,2}, ALEXANDER RADEBACH^{2,3}, REIK V. DONNER¹, JONATHAN F. DONGES^{1,4}, and JÜRGEN KURTHS^{1,2} — ¹Potsdam Institute for Climate Impact Research, Germany — ²Humboldt University, Berlin, Germany — ³Mercator Research Institute on Global Commons and Climate Change, Berlin, Germany — ⁴Stockholm Resilience Centre, Stockholm University, Sweden

The El Niño Southern Oscillation (ENSO) has a large impact on the global climate system. Its variability can roughly be categorized into El Niño (anomalously warm), La Niña (anomalously cold) and normal periods. Recently, it has been suggested that El Niño and La Niña can be further discriminated into two different types. However, no formal criterion for this distinction has been introduced so far. Here, we use evolving climate networks from daily surface air temperature fields and investigate the time-evolution of their structural properties. During certain El Niño and La Niña periods global network measures show distinct peaks indicating an induced reorganization of the global climate system. For ENSO events without such reorganization, we find substantially different spatial patterns of degree and other local measures than for the other events. This observation can be attributed to the general signature of normal vs. anomalous ENSO events. In

this spirit, characteristics involved in the assessment of evolving climate networks allow to detect structural similarities between different ENSO periods and systematically categorize these different stages.

DY 17.8 Tue 11:30 BH-N 333

Eigenvalue Density of the Doubly Correlated Wishart Model: Exact Results — ●DANIEL WALTNER, TIM WIRTZ, and THOMAS GUHR — Fakultät für Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

Data sets collected at different times and different observing points can possess correlations at different times *and* at different positions. The doubly correlated Wishart model takes both into account. We calculate the eigenvalue density of the Wishart correlation matrices using supersymmetry. In the complex case we obtain a new closed form expression which we compare to previous results in the literature. In the much more complicated real case we derive an expression for the density in terms of a fourfold integral. Finally, we calculate the density in the limit of large correlation matrices.

DY 17.9 Tue 11:45 BH-N 333

Entropy maps of complex excitable dynamics in cardiac cell cultures — ●ALEXANDER SCHLEMMER^{1,2}, T.K. SHAJAHAN¹, SEBASTIAN BERG^{1,2}, STEFAN LUTHER^{1,2}, and ULRICH PARLITZ^{1,2} — ¹Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany — ²Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Am Fassberg 17, 37077 Göttingen, Germany

The characterization of spatiotemporal complexity remains a challenging task. This holds in particular for the analysis of data from fluorescence imaging (optical mapping), which allows for the measurement of membrane potential and intracellular calcium at high spatial and temporal resolution. Hitherto methods include dominant frequency maps and the analysis of phase singularities. While these methods address some important aspects of cardiac dynamics, however they only consider very specific properties of excitable media.

We implemented several information-theoretical quantities derived from symbolic chains and wavelet-spectra. Using optical mapping from embryonic chicken cell culture experiments the methods have been validated and benchmarked. We discuss our findings with respect to dominant frequency maps and analysis of phase singularities. In this context we present a workflow to preprocess, filter and analyse large amounts of video data using the above techniques.

DY 18: Focus Session: Dynamics in Many-Body Systems: Equilibration and Localization (joint session TT/DY)

Much progress has recently been made in realizing controlled and coherent many-body systems, in the fields of condensed matter as well as ultra-cold atomic systems. One of the most exciting developments in recent years is the realization that disorder and interactions together can lead to an entirely new form of localization, “many-body localization”, the study of which is in its very infancy: nature, mechanism, and implications of many-body localisation are now subject of a rapidly developing field.

This Focus Session considers several aspects of many-body localisation: how to describe many-body localisation in a theoretical model; the roles of symmetry, topology, and of external driving; it also considers connections to the venerable field of Anderson localization. In addition, it features an account of recent experiments.

Organizers: Roderich Moessner and Frank Pollmann (MPI-PKS Dresden)

Time: Tuesday 9:30–13:00

Location: H 0104

Invited Talk DY 18.1 Tue 9:30 H 0104

Probing Non-Equilibrium Dynamics with Ultracold Atoms: from Quantum Magnetism to Many-Body Localization — ●IMMANUEL BLOCH — Fakultät für Physik, Ludwig Maximilians Universität, München, Germany — Max-Planck Institut für Quantenoptik, Garching b. München, Germany

Ultracold quantum gases are an ideal testbed to study non-equilibrium dynamics of closed quantum systems. Their isolation from the environment for example enables one to probe the dynamical evolution of high-energy states in strongly interacting quantum many-body system. In many of these cases, this can result in a breakdown of fundamen-

tal assumptions of statistical mechanics, leading to novel many-body paradigms such as, e.g., many-body localization. In my talk I will give several examples from recent experiments in our group where we have studied the quantum dynamics of spin-spirals in a Heisenberg ferromagnet, novel ordering phenomena in long-range interacting quantum magnets realized via Rydberg atoms and the observation of many-body localization in interacting fermionic quantum gases in disordered lattice potentials.

Invited Talk DY 18.2 Tue 10:00 H 0104

Many-Body Localization — ●DMITRY ABANIN — University of

Geneva, Switzerland — Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada

We are used to describing systems of many particles by statistical mechanics. However, the basic postulate of statistical mechanics – ergodicity – breaks down in so-called many-body localized systems, where disorder prevents particle transport and thermalization. In this talk, I will give an overview of recent developments in many-body localization. I will describe a phenomenological theory of the many-body localized (MBL) phase, based on new insights from quantum entanglement. I will argue that, in contrast to ergodic systems, MBL eigenstates are not highly entangled, but rather obey so-called area law, typical of ground states in gapped systems. I will use this fact to show that MBL phase is characterized by an infinite number of emergent local conservation laws, in terms of which the Hamiltonian acquires a universal form. Turning to the experimental implications, I will describe the response of an MBL systems to quenches: surprisingly, entanglement shows logarithmic in time growth, reminiscent of glasses, while local observables exhibit power-law approach to “equilibrium” values. I will support the presented theory with the results of numerical experiments, and close by discussing experimental implications and other directions in exploring ergodicity and its breaking in quantum many-body systems.

Topical Talk DY 18.3 Tue 10:30 H 0104
Long-Time Behaviour of Periodically Driven Many-Body Quantum Systems — ●ACHILLEAS LAZARIDES¹, ARNAB DAS², and RODERICH MOESSNER¹ — ¹Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — ²Indian Association for the Cultivation of Science, Kolkata, India

We study the long-time behaviour of closed quantum systems under temporally periodic driving, arguably the simplest deviation from equilibrium. Drawing inspiration from current understanding of equilibration and thermalisation in closed quantum systems with a time-independent Hamiltonians we study the long-time behaviour of free, interacting and (many-body) localised systems under periodic driving.

15 min. break.

Topical Talk DY 18.4 Tue 11:15 H 0104
Many Body Localization and Eigenstate Order — ●SHIVAJI SONDHI — Department of Physics, Princeton University, Princeton, NJ 08544, USA

Recent advances in our understanding of the quantum statistical mechanics of isolated quantum systems have focused attention on the properties of individual many body eigenstates of large systems. While these advances have deepened our understanding of thermal/ergodic systems, they are even more crucial for understanding the properties of many body localized systems where statistical mechanics breaks down. In particular, as I will describe, many body localized systems can exhibit phase transitions while remaining localized wherein the properties of their eigenstates change in singular fashion even as naive statistical mechanical averages are entirely smooth.

Invited Talk DY 18.5 Tue 11:45 H 0104
Anderson Transitions and Electron-Electron Interaction —

●ALEXANDER MIRLIN — Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Recent results on the interplay of Anderson localization and electron-electron-interaction effects will be reviewed.

DY 18.6 Tue 12:15 H 0104

Impact of the eigenstate thermalization hypothesis on the relaxation of significantly off-equilibrium initial states — ABDELLEH KHODJA¹, ROBIN STEINIGEWEG², and ●JOCHEN GEMMER¹ — ¹Department of Physics, University Osnabrück, Germany — ²Institute for Theoretical Physics, Technical University Braunschweig, Germany

We investigate the connection between (a precisely stated version) of the eigenstate thermalization hypothesis (ETH) and initial state independent (ISI) equilibration of chosen observables. The focus is on a class of initial states that render the addressed observables significantly off-equilibrium, rather than on initial states contrived by quenches. An extensive numerical study on spin systems that goes beyond exact diagonalization indicates that the smallness of a certain ETH related quantity is indeed imperative to the occurrence of ISI equilibration for the above class of initial states.

DY 18.7 Tue 12:30 H 0104

Typicality of Eigenstate Thermalization — ●PETER REIMANN — Theoretische Physik, Universität Bielefeld, Germany

Thermalization, i.e., the relaxation of a macroscopic system towards thermal equilibrium, is a very common and well-established experimental fact, but has still not been satisfactorily explained in terms of the basic laws of physics. Specifically, for isolated many-body systems, the so-called eigenstate thermalization hypothesis (ETH) has recently attracted much interest as a sufficient condition from which thermalization could be deduced. Here, this hypothesis is validated as a typicality property for the textbook example of a simple gas in a box: admitting some tiny uncertainty about the “true” value of a single model parameter, e.g. the particle interaction strength, ETH and thus thermalization are warranted for the overwhelming majority of those slightly differing model parameter values.

DY 18.8 Tue 12:45 H 0104

Nonsmooth and level-resolved dynamics illustrated with a periodically driven tight binding model — ●JIANG MIN ZHANG and MASUDUL HAQUE — Max-Planck-Institute-PKS, Dresden, Germany

We point out that in the first order time-dependent perturbation theory, the transition probability may behave nonsmoothly in time and have kinks periodically. Moreover, the detailed temporal evolution can be sensitive to the exact locations of the eigenvalues in the continuum spectrum, in contrast to coarse-graining ideas. Underlying this nonsmooth and level-resolved dynamics is a simple equality about the sinc function $\text{sinc}(x) \equiv \sin x/x$. These physical effects appear in many systems with approximately equally spaced spectra, and is also robust for larger-amplitude coupling beyond the domain of perturbation theory. We use a one-dimensional periodically driven tight-binding model to illustrate these effects, both within and outside the perturbative regime.

[1] J. M. Zhang and Masudul Haque, arXiv:1404.4280.

DY 19: Transport: Graphene (joint session TT/ CPP/ DS/ DY/ HL/ MA/ O)

Time: Tuesday 9:30–12:15

Location: A 053

DY 19.1 Tue 9:30 A 053
Observation of supercurrent in graphene-based Josephson junction — ●LIBIN WANG¹, CHUAN XU², SEN LI¹, WENCAI REN², and NING KANG¹ — ¹Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing 100871, China — ²Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

Josephon junctions with a normal metal region sandwiched between two superconductors (S) are known as superconductor-normal-superconductor (SNS) structures. It has attracted significant attention especially when changing the normal metal with graphene, which allow for high tunability with the gate voltage and to study the proximity effect of the massless Dirac fermions. Here we report our work on graphene-based Josephon junction with a new two dimensional su-

perconductor crystal, which grown directly on graphene, as superconducting electrodes. At low temperature, we observe proximity effect induced supercurrent flowing through the junction. The temperature and the magnetic field dependences of the critical current characteristics of the junction are also studied. The critical current exhibits a Fraunhofer-type diffraction pattern against magnetic field. Our experiments provided a new route of fabrication of graphene-based Josephon junction.

DY 19.2 Tue 9:45 A 053

Magnetoresistance of nanocrystalline and ion-irradiated graphene — ●PAUL LINSMAIER¹, LORENZ WEISS¹, ARMIN SHAUKAT¹, CHRISTIAN BÄUML¹, DANIEL STEININGER¹, INA SCHNEIDER¹, MATTHIAS BÜENFELD², NILS-EIKE WEBER², ANDREY TURCHANIN², MIRIAM GROTHE³, THOMAS WEIMANN³, FERDINAND

KISSLINGER⁴, HEIKO B. WEBER⁴, and CHRISTOPH STRUNK¹ — ¹Inst. f. Exp. and Appl. Physics, University of Regensburg — ²Fac. of Physics, University of Bielefeld — ³Physikalisch-Technische Bundesanstalt, Braunschweig — ⁴Fac. of Physics, F.-A. University Erlangen-Nürnberg

We investigate the magnetotransport in Hall bar structures of nanocrystalline graphene [1] compared to Ar⁺-bombarded epitaxial graphene [2]. We measured the resistance $R(T)$ and $R(B)$ for samples with different sheet resistance (10-40 k Ω /sq at $T = 300$ K). The I-V characteristics of both types show strong non-linear behavior at low temperatures. Low resistive samples of nanocrystalline graphene show positive magnetoresistance (MR) with values up to + 60 % in perpendicular magnetic field for temperatures below a crossover temperature. Above this temperature the MR becomes negative. The perpendicular MR in the ion-bombarded graphene was always negative. In parallel magnetic field the MR exhibits large positive values up to + 700 % in the nanocrystalline graphene. Strongly non-monotonic behavior of the MR was observed in the ion-bombarded sample in parallel field.

- [1] A. Turchanin et al., ACS Nano 5 (2011).
[2] K. V. Emtsev et al., Nat. Mat. 8, 203 - 207 (2009).

DY 19.3 Tue 10:00 A 053

Aharonov-Bohm effect in a graphene ring encapsulated in hexagonal boron nitride — ●JAN DAUBER^{1,2}, MARTIN OELLERS¹, ALEXANDER EPPING^{1,2}, KENJI WATANABE³, TAKASHI TANIGUCHI³, FABIAN HASSLER⁴, and CHRISTOPH STAMPFER^{1,2} — ¹JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany — ²Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany — ³National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan — ⁴JARA-Institute for Quantum Information at RWTH Aachen University, Aachen, Germany

Recent developments in the van der Waals assembly of heterostructures of two-dimensional materials enable the fabrication of graphene on substrate with very high quality. Outstanding charge carrier mobility and mean free path have been reported for micrometer sized samples of graphene encapsulated in hexagonal boron nitride (hBN). These unique electronic properties offer opportunities for the observation of rich mesoscopic transport phenomena in sub-micron sized graphene-hBN devices. Here, we present low-temperature magnetotransport measurements on a high mobility graphene ring encapsulated in hexagonal boron nitride. We observe the co-existence of weak localization, Aharonov-Bohm (AB) oscillations and universal conductance fluctuations. We investigate the periodicity of the AB oscillations as a function of charge carrier density and find clear evidence of the AB effect even at very low carrier densities. Finally, we report on the investigation of the AB oscillations in the cross over regime of emerging quantum Hall effect at reasonable magnetic fields.

DY 19.4 Tue 10:15 A 053

Ab-initio simulations of local current flows in functionalized graphene flakes and ribbons — ●MICHAEL WALZ¹, JAN WILHELM², ALEXEI BAGRETS¹, and FERDINAND EVERS³ — ¹Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — ²Institute of Physical Chemistry, University of Zürich, CH-8057 Zürich, Switzerland — ³Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

Using our DFT-based transport framework AITRANSS [1], we calculate the transmission and the local current density in graphene flakes functionalized by adsorbed atoms, such as nitrogen or hydrogen. We find that even a single nitrogen atom can almost completely suppress the conductance of a (gated) graphene armchair nano-ribbon. In this situation local ring currents emerge that result in local (orbital) magnetic moments.

In addition, the current flow shows a highly inhomogeneous structure. In the absence of any scatters, the current flows along parallel streamlines that exhibit a strong lateral modulation [2]. In the presence of scattering centers, such as 20% hydrogen adsorbants, we observe a filamentary pattern of streamlines. It exhibits local ring currents (“ed-dies”) that go along with sizeable local magnetic fields, $\mathbf{B}(\mathbf{r})$. [3]

In the future, we plan to study the statistics of local currents of such large flakes and its dependency on the impurity concentration.

- [1] A. Arnold, F. Weigend, F. Evers, J. Chem. Phys. 126 (2007)
[2] J. Wilhelm, M. Walz, F. Evers, Phys. Rev. B 89 (2014)
[3] M. Walz, J. Wilhelm, F. Evers, Phys. Rev. Lett. 113 (2014)

DY 19.5 Tue 10:30 A 053

Fabry-Pérot interference in monolayer and bilayer graphene devices — ●MING-HAO LIU and KLAUS RICHTER — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Recent progress on high-quality graphene device fabrications has made submicron- or even micron-scale phase-coherent phenomena in graphene experimentally observable. Hence reliable quantum transport simulations for ballistic graphene devices are nowadays highly demanded. In this talk we give an overview on how such simulations can be accurately and efficiently performed. Concrete examples of Fabry-Pérot interference in single pn junctions in suspended monolayer graphene [1], multiple pn junctions in monolayer graphene on substrate [2], and pnp junctions in bilayer graphene encapsulated by hexagonal boron nitride [3] will be briefly shown, as well as further studies of “electron optics” in graphene.

- [1] P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönberger, Nature Comm. 4, 2342 (2013); M.-H. Liu, et. al., arXiv:1407.5620 (2014).
[2] M. Drienovsky, F.-X. Schrettenbrunner, A. Sandner, D. Weiss, J. Eroms, M.-H. Liu, F. Tkatschenko, and K. Richter, Phys. Rev. B 89, 115421 (2014).
[3] A. Varlet, M.-H. Liu, V. Krueckl, D. Bischoff, P. Simonet, K. Watanabe, T. Taniguchi, K. Richter, K. Ensslin, and T. Ihn, Phys. Rev. Lett. 113, 116601 (2014).

DY 19.6 Tue 10:45 A 053

Substrate-Induced doping of supported graphene: an ab initio study — ●AREZOO DIANAT¹, RAFAEL GUTIERREZ¹, ZHONGQUAN LIAO², MARTIN GALL², EHRENFRIED ZSCHECH², and GIANAURELIO CUNIBERTI¹ — ¹Institute for Materials Science, Technische Universität Dresden, D-01062 Dresden, Germany — ²Fraunhofer Institute for Ceramic Technologies and Systems, D-01109 Dresden, Germany

A major challenge for applications of graphene in nanoelectronics is the absence of a band gap in its low energy spectrum. One possibility of gap opening is doping and there are various methods to achieve it: evaporation, thermal treatment, and plasma doping. In this study, using ab initio molecular dynamics, we investigate graphene doping mediated by substrate-induced mechanisms. More specifically, we address graphene on a B-doped Si(100) surface. Our ab initio total energy calculations show that B atoms prefer to locate on the surface layer of Si(100). Further, intercalation of B atoms into vacancy positions of graphene is only found for temperatures larger than 700 K. In a second step, the electrical transport properties of B-doped graphene are studied using the non-equilibrium Green’s function approach.

15 min. break.

DY 19.7 Tue 11:15 A 053

Density of states of graphene with vacancies — ●SOUMYA BERA — MPI-PKS, Dresden

We numerically calculate the density of states (DOS) of graphene in the presence of compensated vacancy disorder. The model belongs to the BDI class of Atland-Zirnbauer symmetry classification of disordered metals, where the non-linear Sigma model predicts a Gade-type singularity in the DOS $\rho(E) \sim E^{-1} \exp(-|\log(E)|^{-1/2})$. We show that in the pre-asymptotic regime this is indeed true, however, at even lower energies the Gade-type behavior gives away to a stronger singularity of the form $\rho(E) \sim E^{-1} |\log(E)|^{-x}$ with $2 > x \geq 1$ in agreement with recent analytical work (Ostrovsky et al., PRL 113, 186803). We conclude that the generic Sigma model of the BDI class does not apply for strong (unitary) scatterers; the nature of disorder is of important to determine the low energy behaviour of disordered graphene.

- [1] PRL 113, 186802 (2014).

DY 19.8 Tue 11:30 A 053

Nonlocal optical excitations and dynamic shear viscosity of graphene — ●JULIA LINK, PETER P. ORTH, and JÖRG SCHMALIAN — Institute for Theoretical Condensed Matter physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe

We study the dynamic shear viscosity of the interacting electronic fluid of graphene in the finite frequency, collision-less regime, relevant for nonlocal optical properties. We determine the frequency dependence of the dynamic shear viscosity for non-interacting graphene and study the influence of the long-range Coulomb interaction. Finally we discuss a setup where the viscosity can be spectroscopically measured.

DY 19.9 Tue 11:45 A 053

Transport phenomena in deformed graphene: Magnetic field versus curvature — THOMAS STEGMANN^{1,2} and NIKODEM SZPAK¹ — ¹Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — ²Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca, Mexico

The current flow in deformed graphene nanoribbons is studied theoretically. Using a tight-binding model, we apply the nonequilibrium Green's function (NEGF) method to investigate how a localized deformation and a perpendicular magnetic field affect the current flow. At long wavelengths, the eikonal approximation applied to the effective Dirac equation leads to the Mathisson-Papapetrou equations describing trajectories of a spinning point-like particle in a curved space. We show that these trajectories are compatible with the current flow paths of the NEGF calculations. The deformation has two-fold effect on them: First, via a pseudo-magnetic field, with sixfold symmetry of attractive and repulsive regions, which acts differently on electrons and holes, but changes its sign when going from the K to the K' point. Second, via an attractive force due to the curvature of the ribbon, which treats electrons and holes equivalently. We conclude with an outlook on how to use deformed graphene ribbons for geometrical focusing of the current flow.

DY 19.10 Tue 12:00 A 053

Merging of the Dirac points in electronic artificial graphene — ●JURAJ FEILHAUER^{1,2}, WALTER APEL¹, and LUDWIG SCHWEITZER¹ — ¹Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — ²Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava, Slovakia

Artificial graphene (AG) is a man-made electron system which has a similar bandstructure as normal graphene, i.e. in the low-energy part of the electronic spectrum, two bands touch and form a pair of Dirac cones. We study analytically and numerically the bandstructure of electronic AG under uniaxial strain. Here, AG is created from the two-dimensional electron gas by applying a repulsive triangular potential and the effect of strain is modeled by tuning the distance between the repulsive potentials along the armchair direction. In normal graphene, the theory based on nearest-neighbour tight-binding approximation predicts that due to the change of the hopping integrals by applying uniaxial strain, both Dirac cones are shifted away from the corners of the Brillouin zone and also becomes elliptical instead of circular. With increasing compressive strain, the Dirac cones move along the edge of Brillouin zone towards each other until they merge. We show that such a merging of the Dirac cones also exists in uniaxially compressed AG. With applied strain, we find the Dirac cones are also tilted and that can be simulated by the presence of a next-nearest-neighbour hopping in the tight-binding hamiltonian. We discuss a possible realization of our theoretical results in a recent experiment with molecular graphene.

DY 20: Focus Session: Complex Contagion Phenomena (joint session SOE/ DY/ BP)

Complex contagion is the phenomenon in nature in which multiple factors are required for an agent in order to adopt or/and change of a behavior. Generically pathogens, information, opinions, new technologies that spread and proliferate on networks (e.g. contact networks between individuals in single populations or in networks of populations that are coupled by means of transportation, etc) interact, coexist and coevolve. These can effectively change simple dynamical processes to complex contagion phenomena. This session addresses the theoretical approaches as well as empirical studies dealing with these phenomena. (Session compiled and chaired by Fakhteh Ghanbarnejad and Dirk Brockmann.)

Time: Tuesday 10:15–13:15

Location: MA 001

Topical Talk

DY 20.1 Tue 10:15 MA 001

Micro dynamics of social interactions — ●SUNE LEHMANN — Technical University of Denmark, Kgs Lyngby, Denmark

Over the past decade, we have made tremendous progress in understanding the complex networks in the world around us. In terms of social systems, we have recently developed the technological ability to measure the dynamics such networks with unprecedented accuracy, using smartphones as sensors.

For the past two years, my group has worked towards creating a dataset of unparalleled quality and size. We use smartphones as measurement devices to capture the complete network (face-to-face, telecommunication, online social networks, geolocation, etc) in a group of approximately 1000 individuals. In terms of size, this increases the number of study participants by a full order of magnitude compared to similar studies in the field.

I'll give an overview of our ongoing work with a particular focus on spreading processes as well as communities in face-to-face networks.

DY 20.2 Tue 10:45 MA 001

Cooperative SIS epidemics can lead to abrupt outbreaks — ●FAKHTEH GHANBARNEJAD¹, LI CHEN², WEIRAN CAI³, and PETER GRASSBERGER⁴ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Robert Koch- Institute, 13353 Berlin, Germany — ³TU Dresden, Germany — ⁴JSC, FZ Jülich, D-52425 Jülich, Germany

In this paper, we study spreading of two cooperative SIS epidemics in mean field approximations and also within an agent based framework. Therefore we investigate dynamics on different topologies like Erdos-Renyi networks and regular lattices. We show that cooperativity of two diseases can lead to strongly first order outbreaks, while the dynamics still might present some scaling laws typical for second order phase transitions. We argue how topological network features might be related to this interesting hybrid behaviors.

DY 20.3 Tue 11:00 MA 001

How to quantify the strength of factors in a contagion phe-

nomena? — FAKHTEH GHANBARNEJAD, MARTIN GERLACH, JOSE M. MIOTTO, and ●EDUARDO G. ALTMANN — Max Planck Institute for the Physics of Complex Systems, Dresden

Different factors contribute to the spreading of a process through a population. For instance, the adoption of an innovation may depend on factors such as peer pressure, agent specific beliefs, and the intrinsic fitness of the innovation. In this talk we (i) introduce a measure of the contribution of a factor to the overall spreading; (ii) show how this measure depends on the spreading dynamics (e.g., Bass or Threshold) and network topology; and (iii) propose methods to estimate the strength of factors from data.

[1] F. Ghanbarnejad, M. Gerlach, J. M. Miotto, and E. G. Altmann, "Extracting information from S-curves of language change", J. R. Soc. Interface 11, 20141044 (2014)

DY 20.4 Tue 11:15 MA 001

Competitive percolation: How cooperation can strengthen competitors — LI CHEN^{1,2} and ●DIRK BROCKMANN^{1,2} — ¹Robert-Koch Institute, Berlin, Germany — ²Humboldt University, Berlin, Germany

Competition and cooperation are ubiquitous in natural and social systems. Typically, both concepts are considered as antagonistic and mutually exclusive dynamic forces that typically enter systems as independent degrees of freedom with opposite signs. Direct interactions of both concepts, e.g. the benefit of cooperation among competitors and vice versa, is less well understood. Here we investigate a network system, in which two choices initially compete with for individual agents in a susceptible population. Cooperation enters the system by enhanced recruitment in a secondary contagion process for those individuals that recovered from the first reaction. A mean-field analysis supplemented with agent-based simulations shows that these systems can exhibit a discontinuous transition for the contagion process for strong cooperativity. We also show that one "infection" only survives in the presence of the other. Our model can shed light on the dynamics of systems in socio-economic contexts, sports and stability of fashion traits.

DY 20.5 Tue 11:30 MA 001

The good, the bad and the optimal: allocation of resources during emergent infectious diseases — ●OLGA BARANOV¹ and DIRK BROCKMANN^{1,2} — ¹Robert Koch Institut, Berlin — ²HU Berlin

The growing complexity of global mobility is a key challenge for the understanding of the worldwide spread of emergent infectious diseases and the design of effective containment strategies. Despite global connectivity, containment policies are based on national, regional and 'egocentric' assessments of outbreak situations that are no longer effective or meaningful in the development of efficient containment strategies. This was recently demonstrated by 2014 Ebola outbreak in West Africa where months passed before a concerted effort followed. Despite the importance of the matter, optimal strategies are poorly understood. We investigate a model for the optimal deployment of mitigation resources in a network of interacting countries. Each node can exercise a limited amount of resources among all nodes in the network to mitigate an outbreak. At each node costs are a combination of invested resources and effective susceptibility to import a disease. We treat the problem game theoretically and show that, contrary to common belief, purely selfish and cooperative actions do not differ considerably in a single outbreak scenario. Purely selfish behavior tends to invest resources at the outbreak location. However, in a scenario with multiple outbreak locations we find that resource allocation can follow more complex patterns and nodes can fall back on egocentric resource allocations. We will report on preliminary results obtained for a system when disease dynamics and resource allocation are modelled explicitly.

Topical Talk

DY 20.6 Tue 11:45 MA 001

Containing epidemics using limited resources and information — ●OLIVIA WOOLLEY-MEZA — Computational Social Science, ETH Zurich, Clausiusstrasse 37, CLD C6

Every action taken to contain disease spread carries a potential payoff but also a cost. Can we successfully contain epidemic spreading when resources are limited, and decisions on how to allocate these resources are based on imperfect information? I will discuss two cases where the interaction of economic constraints with disease spread transforms the spreading dynamics, usually making it harder to contain the disease. However, I will show that some constraints can work to our advantage. I first consider the dynamics of an epidemic when the recovery of sick individuals depends on the availability of healing resources that are generated by the healthy population. Epidemics spiral out of control into "explosive" spread if the cost of recovery is above a critical cost. The transition to this explosive regime is discontinuous – once there are signs of a transition it can no longer be prevented. In the second case I will show you how the information resolution available to individuals determines the effectiveness of voluntary vaccination decisions. Although an epidemic cannot be contained when individuals use global information, the successful eradication of a disease can occur in an intermediate region of information resolution between the local and the global.

DY 20.7 Tue 12:15 MA 001

Virus transmission on a network of injecting drug users — ●CORNELIA METZIG and PETER WHITE — Department of Infectious Disease Epidemiology, Imperial College London, UK

The Hepatitis C virus (HCV) is a virus that is most prevalent among injecting drug users, who transmit the virus by sharing their injecting equipment, a problem that receives much attention from healthcare providers. Several studies investigate the topology of drug injecting partners via snowball sampling methods with the goal of describing a static network. Typical networks are reported to be highly clustered, assortive and heavy-tailed in degree distribution. Transmission dynamics of the virus can be described by SIR or SIS-models, depending

whether treatment is considered.

In addition, virus transmission is affected by (i) change in sharing partners, and (ii) entry and exit from the community, which happen at shorter timescales than the duration of an untreated infection is. These phenomena can be captured in a network model where each connection describes only one sharing event. Simultaneous rewiring of the network and transmission are studied theoretically and numerically in a model. Assumptions on the network, HCV-incidence rate and HCV-prevalence are compared to data on drug users from the UK.

DY 20.8 Tue 12:30 MA 001

Spatio-temporal dynamics of the cholera epidemic of 1831/1832 in Austria — ●MICHAEL LEITNER¹ and GERO VOGL² — ¹Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany — ²Fakultät für Physik, Universität Wien, Boltzmanngasse 5, 1090 Wien, Austria

Caused by large-scale troop movements in the Russian empire, cholera reached Europe in 1830 and caused the first cholera pandemic to affect the western world. Within the confined region of Weinviertel in Lower Austria (approx. 5000 km²), first cases were registered in 1831, while major outbreaks followed in the summer months of 1832. We reconstructed the dynamics of the disease from the causes of death in the clerical burial records on the temporal scale of single days and spatial scale of single villages. We analyze the data in terms of connectivity, both concerning geographical distance and bodies of flowing water. In contrast to analyzes of recent epidemics, we hope to obtain finer-resolution information on the dynamics due to the lower human mobility in past times.

DY 20.9 Tue 12:45 MA 001

Containment of contagious processes on temporal networks via adaptive edge rewiring — ●VITALY BELIK^{1,2}, FLORIAN FIEBIG¹, and PHILIPP HÖVEL¹ — ¹Institut für Theoretische Physik, TU Berlin — ²Helmholtz-Zentrum für Infektionsforschung, Braunschweig

We consider a recurrent contagious process spreading on a time-varying network topology. As a containment measure we propose an adaptive rewiring mechanism: after detection of the disease, to temporary isolate infected nodes, rewiring the incoming edges away from those nodes. As a case study we use the network of animal trade in Germany. One of the main results reveals heterogeneous performance of adaptation in respect to different index nodes (where epidemic initially started): some index nodes lead to easily controllable epidemics and some not. Our findings are important for designing response strategies for infectious diseases management.

DY 20.10 Tue 13:00 MA 001

Spread of Infections on Temporal Networks — ●ANDREAS KOHER, LUCIAN WILLARETH, HARTMUT LENZ, and IGOR M. SOKOLOV — Humboldt University, Berlin

Social interactions can be naturally abstracted to temporal networks, where bonds appear as long as the corresponding contacts exist. In epidemiological studies the temporal dimension is usually projected out however, in order to apply the standard tools from (static) network analyses even though, a systematic error will be introduced thereby. We present an intuitive algebraic formalism by contrast, which is explicitly based on temporal networks and which allows to calculate potential paths of an infection. By applying the idea to a SIR (susceptible-infected-recovered) type of disease, we will present an elegant way to find all possibly affected nodes of an outbreak. The method can be efficiently implemented and will be demonstrated on a recorded data set.

DY 21: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 3 (joint session TT/ DY)

Time: Tuesday 14:00–16:00

Location: H 3010

DY 21.1 Tue 14:00 H 3010

Real-time decay of a highly excited charge carrier in the one-dimensional Holstein model — ●FLORIAN DORFNER¹, LEV VIDMAR¹, CHRISTOPH BROCKT², ERIC JECKELMANN², and FABIAN HEIDRICH-MEISNER¹ — ¹Ludwig-Maximilians-Universität München, Germany — ²Leibniz Universität Hannover, Germany

We study the real-time dynamics of a highly excited charge carrier coupled to quantum phonons via a Holstein-type electron-phonon coupling [1]. This is a prototypical example for the non-equilibrium dynamics in an interacting many-body system where excess energy is transferred from electronic to phononic degrees of freedom. We use an efficient numerical method, i.e., diagonalization in a limited functional space, to study the non-equilibrium dynamics on a finite one-dimensional chain. We perform a comprehensive analysis of the time evolution in different parameter regimes by calculating the electron, phonon and electron-phonon coupling energies, and the electronic momentum distribution function. For example, we demonstrate that in the weak coupling regime, the relaxation dynamics obtained from the Boltzmann equation agrees very well with the numerical data. We also study the time dependence of the eigenstates of the single-site reduced density matrix, the so-called optimal phonon modes, unveiling that their structure in non-equilibrium contains very useful information for the interpretation of the numerical data. Support from the DFG through FOR 1807 is gratefully acknowledged.

[1] Dorfner et al, arXiv:1411.5074 (2014).

DY 21.2 Tue 14:15 H 3010

Measure of equilibration in Luttinger liquids — ●MARIYA MEDVEDYEVA and STEFAN KEHREIN — Goettingen University, Goettingen, Germany

We consider the properties of the Luttinger liquid in the echo protocol (forward evolution in time followed by the backward evolution of slightly perturbed system) and explore the relation of the Loschmidt echo (the overlap of the initial and final wavefunctions) and the measurable properties of the system. We first study the linear Luttinger liquid as an example of an integrable system and find that the momentum distribution function exhibits almost complete recurrence while the Loschmidt echo does not, as the diagonal basis is different during the forward and backward time evolution. For a nonlinear Luttinger liquid the recurrence strength of the momentum distribution function drops as the nonlinearity of the fermion dispersion relation grows. We conclude that there is no simple relation of the Loschmidt echo to the behavior of the observables and that more work is needed to understand how to interpret the echo in the context of experiment.

DY 21.3 Tue 14:30 H 3010

Quantum Freezing Effect in 1D SU(N) Hubbard Systems — ●SALVATORE R. MANMANA, MARIYA V. MEDVEDYEVA, and JOHANNES M. OBERREUTER — Institut f. Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen

We investigate the time evolution of SU(N) Fermi-Hubbard systems by releasing initially trapped particles onto an empty lattice. Using the time-dependent DMRG and perturbative approaches, we find that in one spatial dimension for large enough filling and values of N, repulsive interactions cause the dynamics to develop a very strong freezing effect, i.e., on the time scales accessible, particle motion is essentially suppressed. We relate this finding to the quantum distillation effect previously reported for SU(2) Fermi-Hubbard systems and discuss its relevance for ongoing experiments with alkaline earth atom experiments on optical lattices.

DY 21.4 Tue 14:45 H 3010

Thermalization Dynamics in the Interacting Luttinger Model after a Quantum Quench — ●MICHAEL BUCHHOLD and SEBASTIAN DIEHL — Institut für Theoretische Physik, TU Dresden, 01062 Dresden

Interacting Luttinger Liquids form a paradigmatic example of one-dimensional interacting fermions with a weak integrability breaking non-linearity. The thermalization dynamics of this model after an interaction quench is studied in a Keldysh non-equilibrium framework

by means of Dyson-Schwinger equations.

After the quench, the ballistic dephasing of the phononic modes leads to correlations corresponding to a prethermal state, well described by a generalized Gibbs ensemble (GGE). This behavior is however overwritten on short distances by a sub-ballistically spreading thermal regime. While the GGE still features algebraic correlations in space and time with a corresponding non-equilibrium exponent, the thermal state shows the well-known exponential decay of correlations.

DY 21.5 Tue 15:00 H 3010

Spectral Properties of One-Dimensional Fermi Systems after an Interaction Quench — ●CHRISTIAN KLÖCKNER, DANTE MARVIN KENNES, and VOLKER MEDEN — Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA - Fundamentals of Future Information Technology, 52056 Aachen, Germany

We show that the single-particle spectral properties of gapless one-dimensional Fermi systems in the Luttinger liquid state reached at intermediate times after an abrupt quench of the two-particle interaction are highly indicative of the unusual nonequilibrium nature of this state. Analytical and numerical insights gained by applying bosonization are presented. The resulting line shapes of the momentum-integrated and -resolved spectral functions strongly differing from their ground state as well as finite temperature equilibrium counterparts.

DY 21.6 Tue 15:15 H 3010

Inhomogeneous Quantum Quenches in the 1D Hubbard Model — ●ERNST VON OELSEN¹, GÖTZ SEIBOLD¹, and JÖRG BÜNEMANN² — ¹BTU Cottbus-Senftenberg — ²Philipps-Universität Marburg

We investigate the dynamics of a many-electron system after a sudden quench of the single-particle potential and of the interaction strength. The calculation is based on the single-band Hubbard model and the time-dependent Gutzwiller theory. Our study is focussed on finite-size systems with lattice-site dependent on-site potentials and interaction strengths.

We compute the time-evolution of the electrons' density matrix and of the electrons double occupancy by fully integrating the equations of motion. Thus, our approach is not limited to small amplitudes but allows for a detailed study of the dependence of the electrons' excitation energies on both the interaction strength and the strength of the quench. Our results are compared to those from exact diagonalization techniques, from the small-amplitude limit and from a Hartree-Fock calculation.

DY 21.7 Tue 15:30 H 3010

Thermalization rates in a 1d Fermi-Hubbard model with slightly broken integrability for various fillings — ●FABIAN BIEBL and STEFAN KEHREIN — Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

Understanding relaxation in quantum systems is essential to determine whether an experimental setup can be described by equilibrium concepts. For example integrable systems do not thermalize, but develop into non-thermal steady states. By slightly breaking integrability, thermalization of such non-thermal (prethermalized) states becomes possible. An important question is to identify the corresponding timescale for thermalization due to the breaking of integrability.

We investigate this question for a fermionic Hubbard chain in the thermodynamic limit. The integrability breaking term is a small next to nearest neighbor hopping term [1,2]. The thermalization timescale is extracted from the quantum Boltzmann equation and depends strongly on temperature, especially when one goes away from half filling. The dependence on filling is connected to Umklapp-processes and we study this dependence systematically.

[1] M. L. R. Fuerst et al., Phys. Rev. E 86, 031122 (2012).

[2] M. L. R. Fuerst et al., Phys. Rev. E 88, 012108 (2013).

DY 21.8 Tue 15:45 H 3010

Time evolution of the ohmic spin boson model at finite bias in the weak coupling limit — ●CARSTEN LINDNER and HERBERT SCHOELLER — Institut für Theorie der Statistischen Physik, RWTH Aachen

The spin boson model is a prominent model which describes dissipation in a quantum mechanical two-state system caused by an energy exchange with the environment. Proposed for applications in various fields of condensed matter physics, it has been discussed widely for more than twenty years. However, a full systematic analysis of the weak coupling regime has not been done for a long time. Recently, the time evolution of the ohmic spin boson model at zero bias has been investigated in the case of weak coupling where the interaction with the environment can be regarded as a small perturbation [1]. Therefore, a non-equilibrium renormalization group (RG) method, which has come

to be known as the real-time RG (RTRG), has been employed to determine its time evolution. The chosen approach allows to obtain the time evolution in a controlled way which means that the renormalized coupling parameters stay small for arbitrarily long times. Beside predicting the dominant exponential time evolution, this method also enables us to address the time scaling behavior of the pre-exponential functions precisely. Based on this insight, we have investigated the ohmic spin boson model at finite bias accordingly, leading to new results on all time scales.

[1] O. Kashuba and H. Schoeller, Phys. Rev. B 87, 201402(R) (2013)

DY 22: Evolutionary Game Theory II (joint session SOE/ BP/ DY)

Time: Tuesday 14:00–16:15

Location: MA 001

DY 22.1 Tue 14:00 MA 001

Frequency-Dependent Selection at Rough Expanding Fronts — ●JAN-TIMM KUHR and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin

Microbial colonies are a formidable model system to study longstanding questions of population dynamics, ecology, and evolutionary dynamics. Growth on surfaces naturally allows to observe range expansions, where microbes colonize new territory. The small number of reproducing individuals introduces strong demographic fluctuations, which interact with mutation and selection at the front.

We use generalized Eden models to explore statistical properties of multi-species range expansions, where the front's geometry and evolutionary dynamics couple to each other. In earlier work we found that irreversible mutations entail a new type of non-equilibrium phase transition accompanied by enhanced surface roughening [1].

If reproduction rates depend on local species composition, we distinguish a variety of patterns. Focusing on social dilemmas, we obtain new exponents for both kinetic roughening and the transition between global defection vs. global cooperation. This is also reflected in the dynamics of single species domains which at large times show enhanced fluctuation statistics.

[1] J.-T. Kuhr, M. Leisner, and E. Frey, New J. Phys. **13**, 113013 (2011).

DY 22.2 Tue 14:15 MA 001

Evolutionary Fitness in Variable Environments — ●ANNA MELBINGER and MASSIMO VERGASSOLA — University of California San Diego

One essential ingredient of evolutionary theory is the concept of fitness as a measure for a species' success in its living conditions. Here, we quantify the effect of environmental fluctuations onto fitness by analytical calculations on a general evolutionary model and by studying corresponding individual-based microscopic models. We demonstrate that not only larger growth rates and viabilities, but also reduced sensitivity to environmental variability substantially increases the fitness. Even for neutral evolution, variability in the growth rates plays the crucial role of strongly reducing the expected fixation times. Thereby, environmental fluctuations constitute a mechanism to account for the effective population sizes inferred from genetic data that often are much smaller than expected.

DY 22.3 Tue 14:30 MA 001

Non-selective evolution of growing populations — ●KARL WIENAND¹, MATTHIAS LECHNER¹, FELIX BECKER², HEINRICH JUNG², and ERWIN FREY¹ — ¹Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians Universität, Munich, Germany — ²Biozentrum, Ludwig-Maximilians Universität, Munich, Germany

Evolution results from the interplay between directed selection and non-selective effects. Most theoretical analyses of non-selective evolution rely on constant population sizes and result in some trait taking over the entire population. However, bacterial populations both in nature and in the laboratory are often observed during their exponential growth. In this work we show that, during growth, populations "freeze" to a random steady state composition. To show this, we employed theoretical models based on Pólya urns and performed experiments on two *Pseudomonas putida* strains in non-selective conditions. We found excellent agreement between experiments and theory. We were also able to elucidate the importance of initial conditions on the steady state distribution on population compositions. In particular,

the initial size of the populations can tune the relative importance of initial assortment and growth as noise sources for the final distribution.

DY 22.4 Tue 14:45 MA 001

Counterintuitive findings for evolution on networks — ●LAURA HINDERSIN and ARNE TRAUlsen — Max Planck Institute for Evolutionary Biology, Plön, Germany

How does spatial population structure affect the fixation time of a novel mutation?

In the framework of evolutionary graph theory, individuals inhabit the nodes of a network. We study the Moran birth-death process, where reproduction happens with probability proportional to fitness. The links of a node determine which other individuals can be replaced by the offspring of that individual.

Intuitively, one might assume that adding a link to a given network would always decrease fixation time. However, a simple counterexample disproves this intuition. We show analytically for small networks, that adding a link can increase the fixation time. Simulating the stochastic process on larger lattices, we find a similar result. By adding links to a 2D-lattice without boundary conditions, the fixation time can increase as well. This shows the validity of our counterintuitive result even for larger populations.

[1] Hindersin L, Traulsen A. 2014 Counterintuitive properties of the fixation time in network-structured populations. J. R. Soc. Interface **11**: 20140606. <http://dx.doi.org/10.1098/rsif.2014.0606>

DY 22.5 Tue 15:00 MA 001

The Cost and Dynamics of Competence in *Bacillus subtilis* — ●JEFFREY POWER, MELIH YÜKSEL, and BERENIKE MAIER — Universität zu Köln, Cologne, Germany

When bacterial cells deplete all of the nutrients in their environment, they can enter a stationary growth phase. In *Bacillus subtilis*, the stationary phase is of particular interest as a fraction of a culture in the stationary phase will stochastically switch into a competent state, where cells can take up extracellular DNA. Competence presents the opportunity for the acquisition and implementation of new genes, but at the cost of a reduced growth rate.

To better understand the advantage of stochastic switching, stationary phase competition assays were carried out competing strains with various fractions of competent cells against the wild type. Flow cytometry was used to monitor changes in the mixed populations over time, and fitness advantages were quantified by means of selection coefficients. We found selection coefficients of $s = 0.04(1)$ for the non-competent *comK* strain and $s = -0.07(1)$ for the hypercompetent *rok* strain, indicating that competence development has a large cost.

This work is a fundamental start to better understanding the dynamics of the stationary phase and the evolutionary advantage of stochastically switching a population subset into a competent state.

DY 22.6 Tue 15:15 MA 001

A Two-Player Game with Linear State-Dependent Payoff Function — ●TIM HERRMANN¹, MARK KIRSTEIN², and KATHARINA FISCHER³ — ¹TU Dresden — ²TU Dresden, Chair of Managerial Economics — ³TU Dresden, Institut für mathematische Stochastik

In classic game theory all elements of a game (set of players, set of strategies, payoff function) are static. In contrary, real-world strategic interactions are often characterized by changes of at least one of the three elements of a game over time. In our model a game with state-dependent payoff functions is analysed. The payoff function of

the $(n + 1)$ -st round depends linearly on the payoff of the n -th round. Thereby the structure of the game can change, e.g. from prisoner's dilemma structure to a structure, where individual rationality coincides with collective rationality. Therefore, the concepts of short-term and long-term rationality are defined. It is shown for our game with a state-dependent payoff function, that the following criteria of long-term rationality are equivalent (besides a few special cases): Pareto optimality, collective rationality and the Nash equilibrium in recursive dominant strategies. For symmetric payoff functions these three criteria of (individual and collective) long-term rationality are additionally equivalent to the collective short-term rationality. The concept of ESS is refined to absolute ESS (ESSA) and relative ESS (ESSR). It is shown that ESSA-tuples are equivalent to the above mentioned criteria for symmetric payoff functions and long-term rationality.

DY 22.7 Tue 15:30 MA 001

Evolutionary Coalitional Games — •TADEUSZ PŁATKOWSKI — Faculty of Mathematics, Informatics, and Mechanics \ \ University of Warsaw, Warsaw, Poland

We introduce the concept of evolutionary coalitional games played in a large population. The members of the population play a strategy chosen from a finite set, and interact in randomly formed coalitions. The interactions are described by a multiplayer strategic game. Each coalition generates a total utility, identified with the value of the coalition, and equal to the sum of the payoffs of its all members from the multiplayer game. The total utility is distributed among the coalition members, proportionally to their Shapley values. Evolution of the whole population is governed by the replicator equations. Polymorphic stationary states of the population are studied for various types of the multiplayer social dilemma games. It is argued that application of coalitional game theory solution concepts to social dilemma models of evolutionary game theory can foster cooperation in the long run.

DY 22.8 Tue 15:45 MA 001

Evolutionary games of condensates in coupled birth-death processes — •JOHANNES KNEBEL, MARKUS F. WEBER, TORBEN KRÜGER, and ERWIN FREY — Ludwig-Maximilians-Universität, München, Deutschland

Condensation phenomena occur in many systems, both in classical and quantum mechanical contexts. Typically, the entities that constitute a system collectively concentrate in one or multiple states during condensation. For example, particular strategies are selected in zero-sum games, which are generalizations of the children's game Rock-Paper-

Scissors. These winning strategies can be identified with condensates.

In our work, we apply the theory of evolutionary zero-sum games to explain condensation in bosonic systems when quantum coherence is negligible. Only recently has it been shown that a driven-dissipative gas of bosons may condense not only into a single, but also into multiple non-degenerate states. This phenomenon may occur when a system of non-interacting bosons is weakly coupled to a reservoir and is driven by an external time-periodic force (Floquet system). On a mathematical level, this condensation is described by the same coupled birth-death processes that govern the dynamics of evolutionary zero-sum games. We illuminate the physical principles underlying the condensation and find that the vanishing of relative entropy production determines the condensates. Condensation proceeds exponentially fast, but the system of condensates never comes to rest: The occupation numbers of condensates oscillate, which we demonstrate for a Rock-Paper-Scissors game of condensates.

DY 22.9 Tue 16:00 MA 001

Length selection and replication in a thermal flow chamber — •SIMON A. LANZMICH¹, LORENZ M. R. KEIL¹, MORITZ KREYSING², and DIETER BRAUN¹ — ¹Systems Biophysics, LMU Munich, Germany — ²MPI of Molecular Cell Biology and Genetics, Dresden, Germany

The replication of long nucleic acids is central to life. On the early Earth, suitable non-equilibrium boundary conditions were required to surmount the effects of thermodynamic equilibrium such as dilution and degradation of oligonucleotides. One particularly intractable experimental finding is that short genetic polymers replicate faster and outcompete longer ones, leading to ever shorter sequences and the loss of genetic information. We show in theory and experiment that heat flux across an open chamber in submerged rock concentrates replicating oligonucleotides from a constant feeding flow and selects for longer strands. The thermal gradient triggers a complex interplay of molecular thermophoresis, external flow and laminar convection, where the latter drives strand separation and exponential replication. The measurements are understood quantitatively based on the calculation of stochastic trajectories inside the chamber using a two-dimensional random walk model. This allowed to derive lifetimes and thermal oscillation frequencies of the nucleic acids. In an intermediate range of external velocities, the superposition of flow fields retains strands of 75 bases, while strands half as long die out, inverting above dilemma of the survival of the shortest. The combined feeding, thermal cycling and positive length selection opens the door for stable molecular evolution in the long-term micro-habitat of asymmetrically heated porous rock.

DY 23: Reaction-Diffusion Systems

Time: Tuesday 14:30–16:15

Location: BH-N 243

DY 23.1 Tue 14:30 BH-N 243

Front and Turing patterns induced by Mexican-hat-like non-local feedback. — •JULIEN SIEBERT and ECKEHARD SCHÖLL — Technische Universität, Berlin, Deutschland

We consider the effects of a Mexican-hat-shaped nonlocal spatial coupling, i.e., symmetric long-range inhibition superimposed with short-range excitation, upon front propagation in a model of a bistable reaction-diffusion system. We show that the velocity of front propagation can be controlled up to a certain coupling strength beyond which spatially periodic patterns, such as Turing patterns or coexistence of spatially homogeneous solutions and Turing patterns, may be induced. This behaviour is investigated through a linear stability analysis of the spatially homogeneous steady states and numerical investigations of the full nonlinear equations in dependence upon the nonlocal coupling strength and the ratio of the excitatory and inhibitory coupling ranges.

DY 23.2 Tue 14:45 BH-N 243

Front propagation in channels with spatially modulated cross-section — •STEFFEN MARTENS, JAKOB LÖBER, and HARALD ENGEL — Technische Universität Berlin, Berlin, Germany

The problem of front propagation in a three-dimensional channel with spatially varying cross-section is reduced to an equivalent reaction-diffusion-advection equation with boundary-induced advection term [S. Martens et al., *PRE*, in press; arXiv:1406.7516]. Treating the advection term as a weak perturbation, an equation of motion for the

front position is derived. We analyze channels whose cross-sections vary periodically with L along the propagation direction of the front. Taking the Schlögl model as representative example, we calculate analytically the nonlinear dependence of the front velocity on the ratio L/l where l denotes the intrinsic front width. Our analytical results agree well with the results obtained by numerical simulations. In particular, the peculiarity of boundary-induced propagation failure for a finite range of L/l values is predicted by analytical calculations. Lastly, we demonstrate that the front velocity is determined by the suppressed diffusivity of the reactants for $L \ll l$.

DY 23.3 Tue 15:00 BH-N 243

Kinetics of a chemical clock reaction in a microflow — •ROBERT RAIMUND NIEDL¹, ALEXANDER ANIELSKI¹, IGAL BERENSTEIN², and CARSTEN BETA¹ — ¹Biological Physics, Universität Potsdam, Germany — ²Nonlinear Physical Chemistry Unit, Université libre de Bruxelles, Brussels

We study the dynamics of the autocatalytic iodate-arsenite reaction in PDMS-based microfluidic devices under continuous flow conditions. If a critical amount of initializer is present, a color reaction is triggered by a nonlinear autocatalytic process. We investigate the kinetics of the clock depending on the various input concentrations and in different channel geometries. We could show that due to delayed mixing in the microchannel, higher local initiator concentrations occur, so that the reaction runs up to seven times faster, than in a macroscopic well-mixed volume.

DY 23.4 Tue 15:15 BH-N 243

Three-Dimensional Autonomous Pacemaker in Excitable Media — ●ARASH AZHAND, JAN F. TOTZ, and HARALD ENGEL — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

In experiments with the photosensitive Belousov-Zhabotinsky reaction (PBZR) we found a stable three-dimensional organizing center that periodically emits trigger waves of chemical concentration. Our experiments are performed in a parameter regime with negative line tension using an open gel reactor to maintain stationary non-equilibrium conditions. The observed periodic wave source is formed by a scroll ring stabilized due to its interaction with a no-flux boundary.

Sufficiently far from the boundary, the scroll ring expands and undergoes the negative line tension instability before it finally develops into scroll wave turbulence. Our experimental results are reproduced by numerical integration of the modified Oregonator model for the PBZR. In the numerical simulations besides stationary also breathing self-organized pacemakers have been found where both the radius of the scroll ring and the distance of its filament plane to the no-flux boundary undergo stable limit cycle oscillations.

[1] Y. Kuramoto, *Chemical Oscillations, Waves, and Turbulence* (Dover Publications, 2003)

[2] M. Stich, I. Ipsen, and A.S. Mikhailov, *Phys. Rev. Lett.* 86, 4406 (2001)

[2] A. Azhand, J. F. Totz, and H. Engel, *EPL* 108, 10004 (2014)

DY 23.5 Tue 15:30 BH-N 243

Critical coupling and bifurcations in two-dimensional oscillator arrays undergoing the Belousov-Zhabotinsky reaction — ●CLAUDIA LENK and J. MICHAEL KÖHLER — Institut für Chemie und Biotechnologie, TU Ilmenau, Ilmenau, Deutschland

Spatio-temporal dynamics of many biological and chemical systems depend on coupling of individual oscillators e.g. catalyst particles, the heart cells during atrial fibrillation or neuronal networks. In these systems, irregular patterns and bifurcations of frequency are most often observed in regions of critical coupling strength. To elucidate the influence of local coupling of individual oscillators we perform on one hand experiments of the Ferrioin-catalyzed Belousov-Zhabotinsky reaction in silica gels and on the other hand numerical calculations of the FitzHugh-Nagumo (FHN) model, both with a catalyst distribution in form of a micro spot pattern. We observe transitions to multiple period oscillations and amplitude oscillations in dependence of spot distance and size. Furthermore, these transitions can also be observed due to gradients of the spot distance for parameter ranges, which otherwise do not show these bifurcations. The identification of bifurcation parameters is done in the numerical simulations. Experimental results

DY 24: Quantum Chaos (joint session DY/ TT)

Time: Tuesday 14:30–16:00

Location: BH-N 334

DY 24.1 Tue 14:30 BH-N 334

Regular phase-space structures and bifurcations in generic 4D symplectic maps — ●FRANZISKA ONKEN¹, STEFFEN LANGE¹, ARND BÄCKER^{1,2}, and ROLAND KETZMERICK^{1,2} — ¹TU Dresden, Institut für Theoretische Physik, Dresden — ²MPI für Physik komplexer Systeme, Dresden

The dynamics of Hamiltonian systems (e.g., planetary motion, electron dynamics in nano-structures, molecular dynamics) can be investigated by symplectic maps. While a lot of work has been done for 2D maps, much less is known for higher dimensions.

For a generic 4D map regular 2D-tori are organized around a skeleton of families of elliptic 1D-tori [1], which can be visualized by 3D phase-space slices [2]. We present an analysis of the different bifurcations of the families of 1D-tori in phase space and in frequency space by computing the involved hyperbolic and elliptic 1D-tori. Applying known results of normal form analysis, both the local and the global structure can be understood: Close to a bifurcation of a 1D-torus, the phase-space structures are surprisingly similar to bifurcations of periodic orbits in 2D maps. Far away the phase-space structures can be explained by remnants of broken resonant 2D-tori.

[1] S. Lange, M. Richter, F. Onken, A. Bäcker and R. Ketzmerick, *Global structure of regular tori in a generic 4D symplectic map*, *Chaos* 24, 024409 (2014)

confirm the numerical analysis.

DY 23.6 Tue 15:45 BH-N 243

Electrodissolution of silicon: Self-organized patterns in space and time — ●KONRAD SCHÖNLEBER, LENNART SCHMIDT, and KATHARINA KRISCHER — TU München, Deutschland

The oscillatory electrodisolution of silicon in fluoride containing electrolytes has been studied for decades. Still many basic aspects concerning this system remain unknown, most prominently the mechanism giving rise to the oscillations.

In the present work, some key features of this oscillatory mechanism will be presented. It will be specifically shown that the system seems to have a built-in memory of its current state even when perturbed drastically.

For n-doped silicon, pattern formation is observed under limited illumination. Remarkably, these patterns often consist of different dynamical states coexisting on the electrode, the most striking example of which are the so-called 'chimera states'. The pattern formation can be well understood in theory, when treating the silicon as an oscillatory medium close to the onset of oscillations. A comparison of theoretical simulations and experiments will be given.

DY 23.7 Tue 16:00 BH-N 243

Enhancement of dimerization in a 1D-out-of-equilibrium system — ●PHILIPP SEIFERT^{1,2}, PATRICK HILLENBRAND², VLADIMIR PALYULIN², and ULRICH GERLAND² — ¹Ludwig-Maximilians-Universität München, 80799 Munich, Germany — ²Theory of Complex Biosystems, Physik-Department, Technische Universität München, James-Frank-Strasse 1, D-85748 Garching, Germany

Mutual enhancement of polymerization and accumulation was recently found to be essential for spontaneous synthesis of long polynucleotides from nucleotide monomers, which is perceived as a substantial step in the emergence of early life [1]. The major driving force behind this effect is a thermally induced drift, which increases the concentration of monomer units in a certain volume and hence enhances the subsequent polymerization. Here we study a simple model of a drift-diffusion system coupled with a reversible dimerization process. We introduce a measure of the global chemical balance, which characterizes the enhancement of dimerization relative to a homogenous system. Numerical and analytical results show a nontrivial dependence of this enhancement on the physical properties of the system. Specifically, we find that the ratio of timescales between physical and chemical processes critically influences the steady state properties.

[1] Mast, C. B., Schink, S., Gerland, U., and Braun, D. (2013). *Proc. Natl. Acad. Sci. USA*, 110, 8030-8035.

[2] M. Richter, S. Lange, A. Bäcker, and R. Ketzmerick, *Visualization and comparison of classical structures and quantum states of four-dimensional maps*, *Phys. Rev. E* 89, 022902 (2014)

DY 24.2 Tue 14:45 BH-N 334

How to deform a dielectric microcavity to get a given emission directionality — ●MARCUS KRAFT and JAN WIERSIG — Otto-von-Guericke-Universität Magdeburg, 39016 Magdeburg

An important characteristic of dielectric microcavities is the far field emission pattern. Here, we present a method to find an optimized deformation of the boundary of a microcavity to get a predetermined far field pattern. We write the symmetric deformation of the boundary in a Fourier series and put this ansatz into a perturbation theory for weakly deformed microcavities. By minimizing the difference between the resulted and desired far field pattern we develop a system of linear equations for the Fourier coefficients of the deformed boundary. A comparison to full numerical calculations is also presented.

DY 24.3 Tue 15:00 BH-N 334

Quantum Ergodicity in Open Chaotic Systems? — ●KONSTANTIN CLAUSS¹, MARTIN KÖRBER¹, ARND BÄCKER^{1,2}, and ROLAND KETZMERICK^{1,2} — ¹TU Dresden, Institut für Theoretische Physik, Dresden — ²MPI für Physik komplexer Systeme, Dresden

In open quantum systems a fundamental question concerns the phase-space localization of resonance states. For a fully chaotic phase space the resonance states are supported on a fractal set of classically trapped orbits. We investigate the possibility of quantum ergodicity, i.e. semi-classical equidistribution with respect to suitable classical densities on this fractal set. We explain why these classical densities have to be chosen according to the quantum decay rate.

DY 24.4 Tue 15:15 BH-N 334

Frobenius-Perron operator for asymmetric backscattering in deformed microdisk cavities — ●JULIUS KULLIG and JAN WIERSIG — Institut für Theoretische Physik, Universität Magdeburg, Germany

Due to radiation and absorption optical microcavities cannot be described by hermitian but non-hermitian Hamiltonians of open quantum systems. This leads in general to non-orthogonal quasibound states. In case of asymmetric optical cavities this is related to an imbalance between clockwise (CW) and counter-clockwise (CCW) propagating waves which manifests in a finite chirality of quasibound states [1, 2, 3, 4]. This has applications e.g. in optical sensors [5], where so-called exceptional points in parameter space can be used to enhance sensitivity [6].

We study the backscattering process between CW and CCW waves from pure classical ray dynamics. To this end we construct a finite approximation of Frobenius-Perron operator \mathcal{F} to describe the time evolution of phase-space densities. The eigenstates of \mathcal{F} show interesting analogues to quasibound states, including non-orthogonality and chirality. Our method is demonstrated for a spiral geometry and the asymmetric Limaçon.

[1] J. Wiersig, S. W. Kim and M. Hentschel PRA 78, 053809 (2008); [2] J. Wiersig, A. Eberspächer, J.-B. Shim, J.-W. Ryu, S. Shinohara, M. Hentschel and H. Schomerus PRA 84, 023845 (2011); [3] J. Wiersig PRA 84, 063828 (2011); [4] J. Wiersig PRA 89, 012119 (2014); [5] F. Vollmer, L. Yang, Nanophotonics 1, 267 (2012); [6] J. Wiersig PRL

112, 203901 (2014)

DY 24.5 Tue 15:30 BH-N 334

Ray-path reversal and Loschmidt echo for light beams — ●PIA STOCKSCHLÄDER and MARTINA HENTSCHEL — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

A fundamental feature in classical geometrical optics is the reversibility of the light path. In reality, however, all light beams have finite width in contrast to the geometrical rays. This leads to corrections to ray optics – beam shift effects known as Goos-Hänchen shift and Fresnel filtering – which break ray-path reversibility. Here, we investigate in detail the influence of these corrections on the reversal of the optical path for a light beam reflected at a dielectric interface. As a measure of how much the reversed light path differs from the original one, we define and calculate a Loschmidt echo-like quantity in this context. As a possible technical application, we discuss the potential utilization of broken ray-path reversibility in optical sensors.

DY 24.6 Tue 15:45 BH-N 334

Quantum-classical correspondence in electronic transport through quantum point contacts — ●KAZUHIRO KUBO and MARTINA HENTSCHEL — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We investigate the propagation of electrons starting from a quantum point contact like source in a random potential. We present the density of classical trajectories which clearly shows the well-known branching pattern near the source and its gradual disappearance at larger distances. We calculate the semiclassical Green's function for each trajectory, and discuss how its amplitude is related to both the branching features and the conjugate points (caustics) along the trajectory. Furthermore, we complement these discussions by including quantum mechanical results.

DY 25: Nonlinear Stochastic Systems

Time: Tuesday 15:00–16:15

Location: BH-N 128

DY 25.1 Tue 15:00 BH-N 128

Stability induced by PT-symmetry breaking in stochastic oscillators — ●MIRKO LUKOVIC¹, PATRICK NAVEZ², THEO GEISEL^{1,3}, and GIORGOS TSIRONIS^{2,4} — ¹Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — ²Crete Center for Quantum Complexity and Nanotechnology, Heraklion, Greece — ³Institute for Nonlinear Dynamics, University of Goettingen, Germany — ⁴Department of Physics, University of Crete, Heraklion, Greece

We investigate the effects of dichotomous noise added to the harmonic oscillator in the form of stochastic time-dependent gain and loss phases, whose durations are sampled from two distinct exponential waiting time distributions. We show that this oscillator system is unstable in the special (symmetric) case where the two waiting time distributions are identical and that it stabilizes only after introducing a significant amount of asymmetry (bias), consisting of much longer periods of loss rather than gain. This concept could be applied in the stabilization of light propagation in metamaterials (optical fibres) with random regions of asymmetric active and passive media.

DY 25.2 Tue 15:15 BH-N 128

Noise-controlled bistability in an excitable system with positive feedback — ●JUSTUS ALFRED KROMER¹, REYNALDO DANIEL PINTO², BENJAMIN LINDNER^{1,3}, and LUTZ SCHIMANSKY-GEIER^{1,3} — ¹Department of Physics, Humboldt-Universität zu Berlin - Newtonstr. 15, 12489 Berlin, Germany — ²Laboratório de Neurodinâmica/Neurobiofísica, Universidade de São Paulo - São Carlos, SP, Brazil — ³Bernstein Center for Computational Neuroscience - Berlin, Germany

We study the interplay between noise and a positive feedback mechanism in an excitable system that generates events. We show that such a system can exhibit a bistability in the dynamics of the event generation (states of low and high activity). The stability of the two states is determined by the strength of the noise such that a change of noise intensity permits complete control over the probabilities with which the two states are occupied. The bistability also has strong implications for the regularity of the event generation. While the irregularity

of the interevent interval (short-time variability) and the asymptotic Fano factor of the event count (long-time variability) are limited if the system is only in one of the two states, we show that both measures of variability display giant values if both states are equally likely. The long-time variability is additionally amplified by long-range positive correlations of the interevent intervals.

DY 25.3 Tue 15:30 BH-N 128

Simulating stochastic differential equations using truncated Markov chains — ●RÜDIGER KÜRSTEN and ULRICH BEHN — Institut für Theoretische Physik, Universität Leipzig, Brüderstr. 16 D-04103 Leipzig

Markov chains with detailed balance are widely used to sample high-dimensional distributions, a prominent example is the Monte Carlo simulation. To sample critical phenomena or rare events with high precision modified techniques such as, for example, the multicanonical method are successfully applied. The methods use more or less tacitly a truncated Markov chain where transition probabilities between certain regions of state space are manipulated. Solution trajectories of stochastic differential equations (SDE) can be sampled naively for instance by an Euler-Mayurama scheme. Here we develop an efficient simulation technique for SDEs that is based on a variant of the truncated Markov chain. An extension for systems without detailed balance is proposed.

DY 25.4 Tue 15:45 BH-N 128

One single turbine to estimate fatigue within a wind farm — ●PEDRO LIND, IVAN HERRAEZ HERNANDEZ, MATTHIAS WÄCHTER, and JOACHIM PEINKE — ForWind, Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

We propose a procedure to estimate the fatigue loads on wind turbines, based on a recent framework used for reconstructing data series of stochastic properties measured at wind turbines. Through a standard fatigue analysis, we show that it is possible to accurately estimate fatigue loads in any wind turbine within one wind farm, using only the load measurements at one single turbine and the set of wind speed measurements. Our framework consists of deriving a stochastic differ-

ential equation that describes the evolution of the torque at one wind turbine driven by the wind speed. The stochastic equation is derived directly from the measurements and is afterwards used for predicting the fatigue loads at neighboring turbines. Such a framework could be used to mitigate the financial efforts usually necessary for placing measurement devices in all wind turbines within one wind farm.

DY 25.5 Tue 16:00 BH-N 128

1/f noise from the scaling and the nonlinear transformations of the variables — ●BRONISLOVAS KAULAKYS, MIGLIUS ALABURDA, and JULIUS RUSECKAS — Institute of Theoretical Physics and Astronomy, Vilnius University, A. Gostauto 12, LT-01108 Vilnius, Lithuania
Modeling of the low-frequency noise $1/f^\beta$ observable in different sys-

tems, from physics to financial markets, still remains a challenge. Different models and theories have been proposed for explanation of this phenomenon. Recently, the stochastic model of $1/f^\beta$ noise, based on the nonlinear stochastic differential equations has been proposed and analyzed [1]. Here we employ the self-similarity property of the nonlinear transformation of the nonlinear stochastic differential equations [2]. We show that processes with $1/f^\beta$ spectrum may yield from the nonlinear transformation of the variable of the widespread processes, e.g., from the Brownian motion, Bessel or similar familiar processes. Analytical and numerical investigations of such techniques for modeling processes with $1/f^\beta$ fluctuations will be presented.

[1] J. Ruseckas and B. Kaulakys, Phys. Rev. E **81**, 031105 (2010).

[2] J. Ruseckas and B. Kaulakys, J. Stat. Mech. P06005 (2014).

DY 26: Focus Session: Percolation and turbulent transition

(Organizers Björn Hof and Marc Avila)

Time: Wednesday 9:30–12:30

Location: BH-N 243

Invited Talk

DY 26.1 Wed 9:30 BH-N 243

Elusiveness of experimental evidence for directed percolation critical behavior — ●HUGUES CHATÉ — CEA-Saclay, Service de Physique de l'Etat Condensé, CNRS UMR 3680, Gif-sur-Yvette, France

The directed percolation universality class contains all generic continuous phase transitions into an absorbing state. It should in principle be observed in situations where an ‘active’ state is in an effectively-stochastic local competition with an ‘absorbing’ state from which no fluctuation allows to escape.

Such situations a priori abound: fires, epidemics, various invasion and front propagation processes, etc. In 1986, Pomeau even made the bold claim that the statistical, large-scale, properties of subcritical transitions to turbulence in shear flows, such as the plane Couette flow, should fall into the directed percolation class.

Hundreds of models have been shown to exhibit the universal critical behavior of directed percolation, which is also well understood at the field-theoretical level. Yet, comprehensive, unambiguous experimental evidence for it remains scarce.

In this talk, I will present this situation in more detail and discuss the reasons why experimental evidence for directed percolation scaling remains so elusive. I will describe the only fully-convincing case found by Takeuchi et al. in 2007. I will conclude with a cautious but optimistic viewpoint for the case of shear flows: almost thirty years after Pomeau’s conjecture, we may finally be near obtaining confirmation that his seminal insight was well-founded.

Invited Talk

DY 26.2 Wed 10:00 BH-N 243

Spatio-temporal dynamics in pipe flow and boundary layers — ●BRUNO ECKHARDT — Philipps-Universität Marburg

The transition to turbulence comes in two varieties: in one case, the laminar profile becomes linearly unstable, and a subsequent cascade of instabilities results in the spatially and temporally fluctuating turbulent state. A fluid heated from below (Rayleigh-Benard problem) is the paradigmatic example for this situation. In other cases, turbulence sets in even though the laminar profile remains linearly stable. This ‘bypass transition’ is typically observed in pipe flow, boundary layers and other shear flows. The turbulence is spatially heterogeneous and temporally transient, with the linearly stable laminar state as an absorbing state. Considerable numerical and experimental data support a model for the bypass transition that builds on localized exact coherent structures and their homoclinic and heteroclinic connections, the spatio-temporal dynamics of excitable media, and the statistical mechanics of directed percolation.

DY 26.3 Wed 10:30 BH-N 243

Transition to sustained turbulence in pipe flow: a second order phase transition? — ●VASUDEVAN MUKUND and BJÖRN HOF — Institute of Science and Technology Austria, Klosterneuburg, Austria

In a recent study, the critical point for sustained turbulence in a pipe was estimated to be $Re \approx 2040$, by balancing the times scales for turbulence growth and decay processes. This work brought into focus the spatio-temporal aspects of the transition and suggested the possibility that the transition is a second order non-equilibrium phase transition.

The present contribution aims to experimentally characterize the transition to sustained turbulence in pipe flow in greater detail and explore the analogy to a phase transition. However, the long time scales near the critical point ($\approx 10^7$ advective time units) pose a challenge in realizing this. We circumvent this problem by constructing a set-up with a quasi-periodic pipe, that exploits the memoryless nature of the turbulence spreading and decay processes in the vicinity of the critical point. In conjunction with an accurate control of the Reynolds number, it is then possible to monitor the spatio-temporal dynamics for arbitrarily long times, and obtain quantities such as the equilibrium turbulent fraction. We present evidence to support the idea that the transition to sustained turbulence in pipe flow is a phase transition of second order and provide first estimates of some of the associated critical exponents.

DY 26.4 Wed 10:45 BH-N 243

Critical exponents for the onset of turbulence in Couette flow — LIANG SHI and ●BJÖRN HOF — IST Austria, Klosterneuburg, Austria

At onset turbulence appears in localized patches surrounded by laminar flow. While individual spots eventually decay, they can also seed new ones in their neighbourhood. As the Reynolds number is increased turbulence becomes sustained once the rate of spot generation outweighs the decay rate of spots. In direct numerical simulations of Couette flow we determine the resulting turbulent fractions and size distributions close to this critical point. The exponents describing the scaling of the turbulent fraction, as well as those for correlation length and correlation times at critical are in excellent agreement with directed percolation.

15 min. break

DY 26.5 Wed 11:15 BH-N 243

About discontinuous laminar-turbulent transitions in planar shear flows — ●YOHANN DUGUET — LIMSI-CNRS, Université Paris-Sud, Orsay, France

The suggestion that transitional shear flows with a stable laminar state could be described as stochastic contact processes was formulated almost three decades ago. Recent progresses in pipe flow experiments and simulations have allowed for firmer claims about the universality class to which it belongs, with an emphasis on the universality class of directed percolation. In this flow we would like to discuss two planar flows also featuring competition between laminar and turbulent phases, by analysing the mechanisms for the collapse of turbulence from accurate numerical simulations in large domains. For the case of planar Couette flow, the question seems to remain open even judging from recent observations. The case of a parallel boundary layer flow with uniform suction, however, shows a clear example of brutal discontinuous phase transition. We will discuss the crucial differences between the local mechanisms in these two examples. This is joint work with the Mechanics department of KTH (Stockholm, Sweden).

DY 26.6 Wed 11:30 BH-N 243

Transition to turbulence in Couette-Taylor flow as a di-

rected percolation process ? — ●GRÉGOIRE LEMOULT¹, SHREYAS JALIKOP¹, KERSTIN AVILA², and BJÖRN HOF¹ — ¹IST Austria (Institute of Science and Technology, Klosterneuburg, Austria) — ²Institute for Multiscale Simulation at the Friedrich-Alexander Universität Erlangen-Nürnberg

In the counter-rotating regime of Couette-Taylor (CT) flow, turbulence appears abruptly through spatio-temporal intermittency (STI). STI is observed during the sub-critical transition to turbulence in many shear flows, most notably pipe flow and Couette flows. K. Avila *et al.* (Science 333, 2011) recently characterized the onset of sustained turbulence in pipe flow. Their work suggested that the transition could be a second order non-equilibrium phase transition. The present contribution aims to experimentally characterize the transition to sustained turbulence in CT flow and explore the analogy to a phase transition.

Our CT setup has an aspect ratio and an azimuthal length of more than 600 gap-widths. These large dimensions minimise the finite-size effects, and render the setup suitable to experimentally investigate the spatio-temporal dynamics. We present evidence to support the idea that the transition is a phase transition of second order and provide first estimates of some of the associated critical exponents: laminar gap size distributions and turbulent fraction.

DY 26.7 Wed 11:45 BH-N 243

Emerging spatiotemporal dynamics in fluid flow — ●MARC AVILA¹, PAUL RITTER¹, and FERNANDO MELLIBOVSKY² — ¹FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — ²UPC, 08860 Castelldefels, Spain

As of today, no theoretical framework fully describes the emergence of turbulent dynamics in shear flows. A dynamical-systems approach suggests that invariant solutions to the Navier-Stokes equations, like traveling waves and relative periodic orbits in pipe flow, act as building blocks of the disordered dynamics. While recent studies have shown how transient chaos arises from such solutions, the ensuing dynamics lacks the strong fluctuations in size, shape and speed of turbulent spots observed in experiments. In this talk I will show that the interaction of chaotic spots with distinct dynamical and kinematic properties gives rise to enhanced spatiotemporal fluctuations, providing a bridge from chaos toward turbulence. The link between the phase-space interpretation of the dynamics and percolation-like models will be discussed.

DY 26.8 Wed 12:00 BH-N 243

Localized periodic orbits in plane channel flow — ●STEFAN ZAMMERT and BRUNO ECKHARDT — Philipps-Universität Marburg

Exact solutions of the Navier-Stokes equation are assumed to form a skeleton for turbulent dynamics. Therefore, within the last two decades the study of exact solutions has attracted lots of attention. Nevertheless, until now there is a lack of localized solutions for plane shear flows that could help to understand the formation of turbulent spots. Using direct numerical simulation we were able to identify streamwise and doubly-localized relative periodic orbits that are exact solutions of the Navier-Stokes equations (Zammert& Eckhardt: J. Fluid Mech. 761, 348-359 (2014)) for plane channel flow. We will discuss the dependence of these structures on the Reynolds number and we will show that they are created in bifurcations of spatially extended travelling wave solutions.

DY 26.9 Wed 12:15 BH-N 243

Zeitaufgelöste High Speed PIV Untersuchung von Ablösepunkt und Transition in der Grenzschicht eines Tragflügels — ●TOM WESTER, DOMINIK TRAPHAN, GERD GÜLKER und JOACHIM PEINKE — ForWind, Institut für Physik, Universität Oldenburg, 26111 Oldenburg, Deutschland

Zur Optimierung von Windkraftanlagen ist der Umschlag von laminarer zu turbulenter Grenzschicht auf den Rotorblättern ein wichtiger Design-Parameter. Dieses Strömungsphänomen wird durch die Turbulenzintensität der Umgebung, sowie durch den Anstellwinkel des Profils stark beeinflusst. In der atmosphärischen Grenzschicht ist eine Windkraftanlage ständig wechselnden Anströmungsbedingungen ausgesetzt. Dies macht die Dynamik des laminar-turbulenten Umschlages, sowie des Strömungsabrisspunktes besonders interessant. Damit diese Phänomene zeitlich und räumlich gut aufgelöst werden können, wird in dieser Studie High-Speed Stereo Particle Image Velocimetry (HS-PIV) verwendet. Hierdurch wird weiter die Analyse der bisher noch nicht ausreichend untersuchten Dynamik der Transition und des Strömungsabrisses an Rotorblättern möglich. Dies soll unter verschiedenen Anströmbedingungen erforscht werden, wobei erste Ergebnisse eine deutliche Abhängigkeit von diesen zeigen und zur Lastminimierung an Windkraftanlagen, sowie zur Validierung von CFD-Simulationen beitragen können. Auch können die Ergebnisse zur Entwicklung neuer stochastischer Modelle für den laminar-turbulenten Umschlag beitragen.

DY 27: Statistical Physics far from Thermal Equilibrium - Part I

Time: Wednesday 9:30–12:15

Location: BH-N 334

Invited Talk

DY 27.1 Wed 9:30 BH-N 334

On the use and abuse of thermodynamic entropy — ●PETER HÄNGGI¹, JOERN DUNKEL³, and STEFAN HILBERT² — ¹Institute of Physics, University Augsburg, D-86135 Augsburg — ²Exzellenzcluster Universe, Boltzmannstr. 2, D-85748 Garching — ³Dept. Mathematics, MIT, 77 Massachusetts Avenue E17-412, Cambridge, MA 02139-4307 USA

Let us elaborate on the notion of thermodynamic entropy S (Clausius 1865) and its consequences. Gibbs put forward two notions of entropy for *isolated* systems that I commonly will refer to here as the volume entropy (involving the integrated density of states) and as the surface entropy, being proportional to the density of states, commonly also (incorrectly) known as the Boltzmann entropy. The absolute temperature, $T = \partial U / \partial S$, is related to thermodynamic entropy; but which one to use? – The consistency for thermodynamics, i.e. the validity for the celebrated 0-th, 1-st and 2-nd thermodynamic Law singles out the Gibbs-entropy [1].

I shall address shortcomings that relate to the thermodynamics of small systems when sticking to the (Boltzmann)-surface entropy [1-2]. This criticism applies also to the use of *absolute* negative temperatures in systems with an upper bound in energy, occurring in experiments in spin systems or experiments involving isolated ultra-cold atomic gases.

[1] S. Hilbert, P. Hänggi, and J. Dunkel, Thermodynamic Laws in Isolated Systems, Phys. Rev. E 90, 062116 (2014).

[2] J. Dunkel and S. Hilbert, Phase transitions in small systems: microcanonical vs. canonical ensembles, Physica A 370, 390 (2006).

DY 27.2 Wed 10:00 BH-N 334

Transverse waves discretize knot motion on a stretched poly-

mer — ●RAFFAELLO POTESTIO¹ and LUCA TUBIANA² — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Josef Stefan Institute, Ljubljana, Slovenia

In recent years topological properties of polymers, in particular biopolymers such as proteins or DNA, have been investigated by means of computer simulations. At the same time, the capability of performing single molecule experiments has tremendously grown, allowing a direct verification of theoretical results. Most of the investigation effort, though, both from the theoretical as well as experimental point of view, has been focused on equilibrium properties. Now that technology allows one to reach unprecedented levels of time and space resolution, it would be of great interest to investigate the behavior of knotted polymers under non-equilibrium conditions.

In this talk I will present and discuss the numerical study of a model polymer, knotted and stretched, subject to forced oscillations. By varying the oscillation period of one extreme of the polymer, different dynamical phases are identified, characterized by varying diffusive behaviors of the knot. Specifically, a transition between a free diffusion state to a discretized jump dynamics is observed.

DY 27.3 Wed 10:15 BH-N 334

Equivalence of Non-Equilibrium Ensembles and Representation of Friction in Turbulent Flows: The Lorenz 96 Model — ●VALERIO LUCARINI^{1,2} and GIOVANNI GALLAVOTTI³ — ¹Institute of Meteorology, University of Hamburg, Hamburg, Germany — ²Department of Mathematics and Statistics, University of Reading, Reading, UK — ³Department of Physics, Sapienza University of Rome, Italy

We construct different equivalent non-equilibrium statistical ensembles in a simple yet instructive N -degrees of freedom model of atmospheric turbulence, introduced by Lorenz in 1996. We construct a modified version of the model where viscosity varies with time, in such a way that energy is conserved, and the resulting dynamics is fully time-reversible. The statistical properties of the irreversible and reversible model are in excellent agreement. The phase space contraction rate of the reversible model obeys the fluctuation relation. The equivalence between the two non-equilibrium ensembles extends to dynamical properties such as the Lyapunov exponents. These results have relevance in motivating the importance of the chaotic hypothesis, in explaining that we have the freedom to model non-equilibrium systems using different but equivalent approaches, and, in particular, that using a model of a fluid where viscosity is kept constant is just one option, and not necessarily the only option, for describing accurately its statistical and dynamical properties.

DY 27.4 Wed 10:30 BH-N 334

The Second Laws for an Information driven Current through a Spin Valve — ●PHILIPP STRASBERG¹, GERNOT SCHALLER¹, TOBIAS BRANDES¹, and CHRISTOPHER JARZYNSKI² — ¹Institut für theoretische Physik, TU Berlin, Germany — ²Institute for Physical Science and Technology, University of Maryland, USA

We propose a physically realizable Maxwell's demon device using a spin valve interacting unitarily for a short time with electrons placed on a tape of quantum dots, which is thermodynamically equivalent to the device introduced by Mandal and Jarzynski [PNAS 109, 11641 (2012)]. The model is exactly solvable and we show that it can be equivalently interpreted as a Brownian ratchet demon. We then consider a measurement based discrete feedback scheme, which produces identical system dynamics, but possesses a different second law inequality. We show that the second law for discrete feedback control can provide a smaller, equal or larger bound on the maximum extractable work as compared to the second law involving the tape of bits. Finally, we derive an effective master equation governing the system evolution for Poisson distributed bits on the tape (or measurement times respectively) and we show that its associated entropy production rate contains the same physical statement as the second law involving the tape of bits.

REF: arXiv:1407.7679

DY 27.5 Wed 10:45 BH-N 334

Josephson effect and coherent energy transport in classical nonlinear oscillators — SIMONE BORLENGHI^{1,2}, ●STEFANO IUBINI³, STEFANO LEPRI⁴, LARS BERGQVIST¹, ANNA DELIN^{1,2}, and JONAS FRANSSON² — ¹Department of Material and Nano-Physics, School of Information and Communication Technology, KTH Royal Institute of Technology, Stockholm, Sweden — ²Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — ³Centre de Biophysique Moléculaire (CBM), CNRS-UPR 4301 Rue Charles Sadron, F-45071 Orléans, France — ⁴Istituto dei Sistemi Complessi, CNR Unità operativa di Firenze, Sesto Fiorentino, Italy

The standard approach to non-equilibrium thermodynamics describes transport in terms of generalised forces and coupled currents, a typical example being the Fourier law that relates temperature gradient to the heat flux. In this talk, we discuss the possibility to generate a persistent energy currents in a lattice of classical nonlinear oscillators with uniform temperature and chemical potential. In strong analogy with the well known Josephson effect, the currents are generated only by the phase differences between the oscillators. The phases play the role of additional thermodynamical forces, that drive the system out of equilibrium. Our results apply to a large class of oscillators and indicate novel ways to practically control the propagation of coupled currents and rectification effects in many different devices. They also suggest a simple, macroscopic setup for studying a phenomenon which hitherto have only been observed in microscopic, quantum-mechanical systems. (preprint arXiv:1411.5170)

15 min. break

DY 27.6 Wed 11:15 BH-N 334

Synchronization of moving oscillators — ●ROBERT GROSSMANN¹, FERNANDO PERUANI², and MARKUS BÄR¹ — ¹Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin, Germany — ²Université Nice Sophia Antipolis, Laboratoire J.A. Dieudonné, UMR 7351 CNRS, Parc Valrose, F-06108 Nice Cedex 02, France

We consider an extension of the Kuramoto model of noisy phase oscillators

with local interaction, where individual oscillators move randomly in D dimensional space. We study this model by using both analytical and numerical methods to answer the question how the synchronization is influenced by the motion of individual oscillators. Our model displays a non-equilibrium order-disorder transition from a desynchronized to a synchronized state depending on the noise acting on individual oscillators. The properties of the transition crucially depend on the spatial dimensionality and the diffusion-type of oscillators: We consider both normal diffusive motion as well as super-diffusively moving oscillators. We derive field equations which describe the large-scale dynamics of the system by means of Langevin equations for order parameters. By coarse-graining the model in this way, we are able to analyze the large-scale dynamics analytically. In particular, we study how fluctuations on the microscale (oscillator dynamics) enter the macroscopic dynamics (field theory) and calculate order-parameter correlation functions. Our theory suggests that a transition to long-range synchronization in $D \leq 2$ is not possible, if individual oscillators move diffusively. In contrast, long-range synchronization is possible in any spatial dimension for certain types of superdiffusive motion.

DY 27.7 Wed 11:30 BH-N 334

Condensation in asymmetric inclusion processes — ●MARKUS F. WEBER, JOHANNES KNEBEL, TORBEN KRÜGER, and ERWIN FREY — Ludwig-Maximilians-Universität München

Condensation occurs when the entities of a system collectively concentrate in one or multiple states. In our work, we study such a phenomenon for jump processes on networks. In these processes, many particles may occupy a node and jump rates depend linearly on the occupation of departure and arrival nodes. These kinds of processes are thus referred to as inclusion processes - an example being the totally antisymmetric inclusion process (TASIP) - and reflect bosonic analogues of fermionic exclusion processes (e.g., the TASEP). Not only do inclusion processes describe the interaction of strategies in zero-sum games but they also govern chemical kinetics in autocatalytic reaction networks. Furthermore, they were recently used to show that driven-dissipative bosonic systems may condense into multiple quantum states. We derived an algebraic method to determine which of the nodes in an inclusion process become condensates. We show that the vanishing of relative entropy production guides these systems into non-equilibrium steady states in which detailed balance is broken. For inclusion processes on large random networks, we find that the interplay between critical properties of networks and dynamically stable network motifs determines the selection of condensates. Our methods allow for the design of network topologies and jump rates that result in condensates with oscillating occupation.

DY 27.8 Wed 11:45 BH-N 334

Feedback control of interacting transport channels — ●TOBIAS BRANDES — Institut für Theoretische Physik, TU Berlin

Understanding the flow of information is crucial for interpreting feedback control of stochastic processes. Quantitative tools are available in the form of modified fluctuation relations, mutual information and flows in the framework of stochastic thermodynamics for discrete or continuous degrees of freedom [1].

In this talk, I present an extension of a previous non-autonomous feedback model for transport of particles that was based on the synchronization with an external clock [2]. The new autonomous model can be viewed as a paradigm for interacting feedback mechanisms or feedback in networks [3], where the control is achieved in a collective manner.

[1] J. M. Horowitz, M. Esposito, Phys. Rev. X 4, 031015 (2014); A. E. Allahverdyan, D. Janzing, G. Mahler, J. Stat. Mech. P09011 (2009); D. Hartich, A. C. Barato, U. Seifert, J. Stat. Mech. P02016 (2014).

[2] T. Brandes, Phys. Rev. Lett. 105, 060602 (2010).

[3] S. Ito, T. Sagawa, Phys. Rev. Lett. 111, 180603 (2013).

DY 27.9 Wed 12:00 BH-N 334

Phase Behaviour of Active Swimmers in Depletants — ●BENJAMIN TREFZ^{1,2}, SUBIR DAS³, SERGEI EGOROV⁴, PETER VIRNAU², and KURT BINDER² — ¹Graduate School Material Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — ²Johannes Gutenberg University Mainz, Department of Physics, Staudingerweg 7, 55128 Mainz, Germany — ³Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore 560064, India — ⁴Department of Chemistry, University of Virginia, Charlottesville, Virginia 22901, USA

We study the structure and phase behaviour of a binary mixture where one of the components is self-propelling in nature. The inter-particle interactions in the system were taken from the Asakura-Oosawa model, for colloid-polymer mixtures, for which the phase diagram is known. In the current model version the colloid particles were made active using the Vicsek model for self-propelling particles. The resultant active system was studied by molecular dynamics methods with a Langevin

thermostat. The Vicsek model based activity facilitates phase separation, and is thus broadening the coexistence region. Our findings have been published recently in [1].

[1] Subir K. Das, Sergei A. Egorov, Benjamin Trefz, Peter Virnau, and Kurt Binder, Phys. Rev. Lett., "Phase Behavior of Active Swimmers in Depletants: Molecular Dynamics and Integral Equation Theory", 2014

DY 28: Nonlinear Dynamics, Synchronization and Chaos - Part I

Time: Wednesday 9:30–12:00

Location: BH-N 128

DY 28.1 Wed 9:30 BH-N 128

Synchronization by Decoupling — ●MALTE SCHRÖDER¹, MANU MANNATIL², DEBABRATA DUTTA³, SAGAR CHAKRABORTY^{2,4}, and MARC TIMME¹ — ¹Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — ²Department of Physics, Indian Institute of Technology Kanpur, U.P. 208016, India — ³CGG Services UK, Crompton Way, Crawley, West Sussex RH10 9QN, UK — ⁴Mechanics and Applied Mathematics Group, Indian Institute of Technology Kanpur, U.P. 208016, India

Synchronization has a broad range of applications, from biological and ecological settings such as predator-prey dynamics and the migration of large populations, to technical systems such as lasers. In coupled chaotic systems, synchronization typically emerges only for a specific range of coupling parameters and is impossible otherwise. Here, we demonstrate that *restricting* the coupling to specific regions of phase space *widens* the range of coupling parameters where synchronization is achieved. This 'trick' works for simple master-slave systems of two coupled units as well as for larger networks of more complex interaction topologies.

DY 28.2 Wed 9:45 BH-N 128

Chaos synchronization by nonlinear coupling — ●JOHANNES PETERIT and ARKADY PIKOVSKY — Universität Potsdam, Potsdam, Germany

Synchronization of chaos is a well known phenomenon that occurs in ensembles of coupled chaotic systems. It presents itself in different forms depending on the dynamics and the coupling scheme of the interacting systems. Previous researches have focussed on pairwise coupling implemented by a linear coupling operator. We used *nonlinear* coupling methods to link at least three systems.

In detail we coupled three logistic maps using two different nonlinear coupling schemes in order to check general properties of nonlinear coupling. We analyze different synchronization patterns in dependence on coupling strength by calculating appropriate synchronization measures and Lyapunov exponents. Possible extensions are also briefly discussed.

DY 28.3 Wed 10:00 BH-N 128

Permutation symmetries and phase wave synchronization on networks of heterogeneous chemical oscillators — ●JAN FREDERIK TOTZ¹, HARALD ENGEL¹, and KENNETH SHOWALTER² — ¹Technische Universität Berlin, Berlin, Deutschland — ²West Virginia University, Morgantown, USA

Synchronization phenomena are observed in a wide variety of systems ranging from synchronizing fireflies through firing neurons to electrical power grids [1,2]. Recently it has been demonstrated that permutation symmetries of the underlying oscillator networks are of fundamental importance for zero-lag synchronization patterns [3]. In this contribution, we address the question: What role do network symmetries play, when the frequency detuning of the individual oscillators is too large to allow for zero-lag synchronization? Experiments and simulations on networks of discrete chemical relaxation oscillators [4] reveal transitions from incoherence through partial synchronization to phase waves following symmetry clusters as a function of coupling strength.

[1] P. C. Bressloff, *Waves in Neural Media: From Single Neurons to Neural Fields* (Springer, 2014)

[2] A. Pikovsky, M. Rosenblum, and J. Kurths, *Synchronization: A Universal Concept in Nonlinear Sciences* (Cambridge University Press, 2003)

[3] L. M. Pecora, F. Sorrentino, A. M. Hagerstrom, T. E. Murphy, and R. Roy, *Nat. Commun.* 5, 4079 (2014)

[4] M. R. Tinsley, S. Nkomo, and K. Showalter, *Nat. Phys.* 8, 662

(2012)

DY 28.4 Wed 10:15 BH-N 128

On the Arrest of Synchronized Oscillations — ●DARKA LABAVIĆ and HILDEGARD MEYER-ORTMANN — School of Engineering and Science, Jacobs University Bremen, Bremen, Germany

We study the mutual conversion of regimes of collective fixed-point behavior and collective synchronized oscillations in a system of coupled dynamical units, which individually can be in an excitable or oscillatory state. The conversion is triggered by the change of a single bifurcation parameter [1]. Of particular interest is the arrest of oscillations. We identify the criterion that determines the seeds of arrest and the propagation of arrest fronts in terms of the vicinity to the future attractor. Due to a high degree of multistability we observe versatile patterns of phase locked motion in the oscillatory regime. Quenching the system into the regime, where oscillatory states are metastable, we observe qualitatively distinct approaches of the fixed-point attractor, depending on the initial seeds. If the seeds of arrest are isolated single sites of the lattice, the arrest propagates via bubble formation, visually similar to nucleation processes; if the seed is extended along a line of lowest amplitudes, the freezing follows the spatial patterns of phase-locked motion with long interfaces between arrested and oscillating units. For spiral patterns of oscillator phases these interfaces are arranged along the arms of the spirals.

[1] D. Labavić and H. Meyer-Ortmanns, *Chaos* 24, 043118 (2014)

[2] D. Labavić and H. Meyer-Ortmanns, *On the Arrest of Synchronized Oscillations*, submitted

DY 28.5 Wed 10:30 BH-N 128

Synchronizing noisy and chaotic oscillators with non-uniform couplings — ●BERNARD SONNENSCHEN¹, THOMAS K. DM. PERON², FRANCISCO A. RODRIGUES³, JÜRGEN KURTHS^{1,4}, and LUTZ SCHIMANSKY-GEIER¹ — ¹Department of Physics, Humboldt-Universität zu Berlin, Germany — ²Instituto de Física de Sao Carlos, Universidade de Sao Paulo, Brazil — ³Departamento de Matematica Aplicada e Estatística, Instituto de Ciências Matemáticas e de Computação, Universidade de Sao Paulo, Brazil — ⁴Potsdam Institute for Climate Impact Research, Potsdam, Germany

It is well-known that coupled oscillatory units tend to synchronize. However, many open questions remain, if the couplings are heterogeneous, e.g. in their strengths or in their effects (attractive vs. repulsive). We investigate all-to-all coupled networks that are composed of two intertwined populations. All the oscillators are characterized by two individual coupling strengths and these are the same within the populations, but different between them. One of the coupling constants tells how strongly the single element feels the mean field, while the other one quantifies the strength of the contribution to the mean field. Furthermore, coupling constants are allowed to be negative. For the node dynamics we consider two very different models, chaotic Rössler systems and noisy Kuramoto phase oscillators. Intriguingly, in both models similar states of discordant synchronization can be found. We report so-called blurred pi states, chimera-like points and reentrant synchronization. For the noisy Kuramoto model we derive analytical results providing a deeper understanding of the numerical observations.

DY 28.6 Wed 10:45 BH-N 128

Kuramoto Dynamics in Hamiltonian Systems — DIRK WITTHAUT^{1,2} and ●MARC TIMME^{2,3} — ¹Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — ²Efficiency, Emergence and Economics of Future Supply Networks, FZ Jülich — ³Institute for Nonlinear Dynamics, University of Göttingen

The Kuramoto model constitutes a paradigmatic model for the dissipative collective dynamics of coupled oscillators, characterizing in particular the emergence of synchrony (phase locking). Here we present a classical Hamiltonian (and thus conservative) system with $2N$ state variables that in its action-angle representation exactly yields Kuramoto dynamics on N -dimensional invariant manifolds, <http://dx.doi.org/10.1103/PhysRevE.90.032917> (2014). We show that locking of the phase of one oscillator on a Kuramoto manifold to the average phase emerges where the transverse Hamiltonian action dynamics of that specific oscillator becomes unstable. Moreover, the inverse participation ratio of the Hamiltonian dynamics perturbed off the manifold indicates the global synchronization transition point for finite N more precisely than the standard Kuramoto order parameter. The uncovered Kuramoto dynamics in Hamiltonian systems thus distinctly links dissipative to conservative dynamics, with options of experimental realization (Witthaut et al., in prep.).

15 min. break

DY 28.7 Wed 11:15 BH-N 128

Nonlinear effects in semiconductor quantum dot microlasers — ●ELISABETH SCHLOTTMANN¹, STEFFEN HOLZINGER¹, SÖREN KREINBERG¹, LEON MESSNER¹, CHRISTIAN SCHNEIDER², SVEN HÖFLING^{2,3}, MARTIN KAMP², JANIK WOLTERS¹, and STEPHAN REITZENSTEIN¹ — ¹Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — ²Technische Physik, Universität Würzburg, W, Germany — ³Present address: SUPA, School of Physics and Astronomy, University of St Andrews, United Kingdom

Semiconductor microlasers with a few tens of quantum dots in the active layer exhibit ultra-low laser thresholds in the semiclassical limit, while showing genuine quantum effects below threshold. Today, it is well known that classical lasers under optical feedback or external injection possess highly non-linear behavior. However, the transition from classical to quantum chaos is hardly understood.

In our experiments we investigate non-linear effects in InGaAs/GaAs quantum dot micropillar lasers, aiming to expand the semiclassical Lang-Kobayashi physics to the quantum regime. To this end, we measured the influence of time-delayed feedback from a 2 m long external

cavity on the first and second order autocorrelation of the emitted radiation. With external injection of low intensity laser light, we pave the way for external quantum control of microlasers.

DY 28.8 Wed 11:30 BH-N 128

Synchronization in coupled organ pipes — ●JAKUB SAWICKI¹, MARKUS ABEL², and ECHEHARD SCHÖLL¹ — ¹Technische Universität Berlin, Berlin, Germany — ²University of Potsdam, Potsdam, Germany

We investigate synchronization in coupled organ pipes. Synchronization and reflection in the organ lead in special cases to undesired weakening of the sound. Experiments show that sound interaction is highly complex and nonlinear. As a model we consider two delay-coupled Van-der-Pol oscillators with distance-dependent coupling. Analytically, we investigate phenomena as synchronization frequency and bifurcation scenarios which occur at the boundaries of the Arnold tongues. We successfully compare our results to experimental data.

DY 28.9 Wed 11:45 BH-N 128

Coupled organ pipes - Numerical investigations and new synchronization experiments — ●JOST LEONHARDT FISCHER¹, ROLF BADER¹, and MARKUS ABEL^{2,3} — ¹Systematische Musikwissenschaft, Universität Hamburg, Deutschland — ²Institut für Physik und Astronomie, Universität Potsdam, Deutschland — ³Ambrosys GmbH, Potsdam, Deutschland

Motivated by recent synchronization experiments with slightly detuned organ pipes we show that mutual interaction between two organ pipes which lead to synchronization can be properly depicted by methods of numerical simulation. Therefore we integrated the fully compressible Navier-Stokes equations with suitable initial and boundary conditions using an LES-Model. This gives a deep insight into the fluid-dynamical and aeroacoustical first principles of sound generation and sound radiation of organ pipes. Furthermore we show first results of new synchronization experiments with equally tuned pairs of organ pipes. We observed abrupt switching between anti- and in-phase synchronization, depending on the distance of the pipes, respectively the time delay of the coupling.

DY 29: Statistical Physics of Biological Systems - Part II (joint session BP/DY/PPP)

Time: Wednesday 9:30–13:15

Location: H 1028

DY 29.1 Wed 9:30 H 1028

Pinned polymer loops in external field: how to align chromosomes for recombination? — YEN TING LIN¹, DANIELA FRÖMBERG¹, WENWEN HUANG¹, PETRINA DELIVANI², MARIOLA CHACÓN², IVA TOLIC², FRANK JÜLICHER¹, and ●VASILY ZABURDAEV¹ — ¹MPI for the Physics of Complex Systems, Dresden, Germany — ²MPI of Molecular Cell Biology and Genetics

Chromatin movement and structure are central to many processes in cells such as mitosis, replication, and transcription, where physical properties of the chromatin fiber play an essential role. Motivated by the problem of chromosome alignment and recombination during meiosis we solve for the statistics of a pinned polymer ring in an external force field. We predict how the contact probability between two rings depends on the ratio of the force to the intrinsic noise level and how it changes upon addition of new recombination spots. Due to the underlying loop topology, our theoretical results are readily applicable to the description of bacterial DNA and polymer brushes.

DY 29.2 Wed 9:45 H 1028

Statistical Inference of E.Coli's tumbling behavior and chemotaxis strategy using Kramers-Moyal coefficients — ●OLIVER POHL¹, MARIUS HINTSCHE², CARSTEN BETA², and HOLGER STARK¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin — ²Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam

The bacterium *Escherichia coli* moves with alternating runs and tumbles that occur with a mean tumble rate. In the presence of gradients of a chemoattractant, *E. coli* performs chemotaxis. We set up a time-continuous model that describes runs and tumbles as a stochastic process of the bacterium's swimming direction and speed. The swimming direction updates according to rotational Brownian motion and

additional shot noise, which initiates tumbling events. The speed is not constant as in previous models but decreases during the tumbling events.

By analyzing experimental data on swimming trajectories, we infer the parameters of our model. To this purpose generalized Kramers-Moyal coefficients are calculated for our shot-noise model and matched to the ones obtained from the trajectories. In contrast to common tumbling recognition algorithms no free parameters need to be pre-determined. Furthermore, we can identify the bacteria's chemotaxis strategy by exploiting the Kramers-Moyal coefficients.

DY 29.3 Wed 10:00 H 1028

In vitro Min protein patterns arise from self-controlled chaos — ●JACOB HALATEK and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität, München, Germany

The mass-conserving reaction-diffusion dynamics of Min proteins act as spatial regulator for the assembly of the cell division machinery. A plethora of experiments has demonstrated a remarkable adaptability of oscillatory Min protein patterns to variations of system geometry. As such, the Min system serves as ideal basis to study the theoretical concepts underlying a real pattern-forming system that can be found in nature. The classical picture for pattern-forming reaction-diffusion systems is rooted in two distinct concepts: The diffusion driven instability proposed by Turing, and the concept of diffusively coupled, self-sustained oscillators proposed by Kuramoto. Here, we investigate the spatio-temporal instabilities of Min protein dynamics that lead to characteristic patterns observed in vivo and in vitro. We find that the in vitro instability cannot be ascribed to any of the two classical concepts but gives rise to a new one. We find transient Turing patterns at onset that loose stability to a chaotic attractor. Further from onset this chaotic attractor condenses into a global limit cycle, passing a

regime with transient chimera states. As such, Min protein patterns arise in vitro from a state of self-controlled chaos, rather than from destabilization of uniform states. We find that such dynamics stem from generic properties of mass-conserved reaction-diffusion dynamics and are not specific to the Min system.

DY 29.4 Wed 10:15 H 1028

Stochastic Dynamics of IFN Type I Signaling — ●NIKOLAS SCHNELLBÄCHER^{1,2}, NILS BECKER³, THOMAS HÖFER³, and ULRICH SCHWARZ^{1,2} — ¹Institute for Theoretical Physics, University of Heidelberg, Heidelberg, Germany — ²BioQuant, University of Heidelberg, Heidelberg, Germany — ³German Cancer Research Center, Heidelberg, Germany

The signaling molecules interferon (IFN) of type I are secreted by many nucleated cells to signal the presence of an intracellular viral infection to their environment and to inhibit viral replication. Once in the extracellular environment, they bind to a heterodimeric cell surface receptor (IFNAR = Interferon Alpha Receptor) to form an active ternary signaling complex, which then triggers an intracellular response. The most prominent pathway activated by interferons is the canonical JAK/STAT signaling pathway, where STAT molecules dock at the receptor associated Janus kinases (JAKs) at their cytoplasmic domains.

A central question of this system is to explain the differential information processing of different interferons through the same transmembrane receptor system. Moreover notoriously low copy numbers of the receptors on the cell surface are a typical cause for a high degree of intrinsic stochasticity. We use stochastic computer simulations to analyze the activation dynamics in space and time. In particular we investigate spatial effects on the dose response behavior of the IFN type I signaling system.

DY 29.5 Wed 10:30 H 1028

Scaling Regimes for Confined Wormlike Chains under Tension — ●GREG MORRISON¹ and DAVE THIRUMALAI² — ¹IMT Lucca Institute for Advanced Studies, Lucca Italy 55100 — ²University of Maryland at College Park, College Park MD 20742

In this talk, we study the scaling behavior of a wormlike chain (WLC) with persistence length l_p confined to the surface of a cylinder of radius R under the application of an external tension. Inextensibility and confinement effects are treated on a mean field level, and we show that the stationary solution for the mean field parameters can be reduced simple equations that can be solved asymptotically. We are able to accurately recover the well known Odijk scaling of $F \sim L/l_d$, with the deflection length $l_d = (l_p R^2)^{1/3}$, for strongly confined chains and show that this scaling is robust to weak external forces. We show that the scaling regimes for both weakly and strongly confined polymers change drastically under application of large external tension, with $F \sim L/l_t$ for a tensile length scale $l_t \sim (l_p/\beta f)^{1/2}$. Our results may be relevant in the mechanical unbinding of histone-bound DNA as well as a variety of experimental situations involving DNA confined to nanochannels.

DY 29.6 Wed 10:45 H 1028

Single molecule measurement of the effective temperature in nonequilibrium steady states — ●ECKHARD DIETERICH¹, JOAN CAMUNAS-SOLER^{2,3}, MARCO RIBEZZI-CRIVELLARI^{2,3}, UDO SEIFERT¹, and FELIX RITORT^{2,3} — ¹II. Institut für Theoretische Physik, Universität Stuttgart, Germany — ²Departament de Física Fonamental, Universitat de Barcelona, Spain — ³CIBER-BBN de Bioingeniería, Biomateriales y Nanomedicina, Instituto de Salud Carlos III, Madrid, Spain

Temperature is a crucial concept for equilibrium systems. For glassy systems, it has been extended to the nonequilibrium regime as an effective quantity showing up in the fluctuation-dissipation theorem. However, direct supporting experimental evidence remains scarce. Here, we present the first direct experimental demonstration of the effective temperature by measuring correlations and responses in single molecules in nonequilibrium steady states generated under external random forces. We combine experiment, analytical theory and simulations for systems with different levels of complexity ranging from a single bead in an optical trap to two-state and multiple-state DNA hairpins. From these data, we can extract a unifying picture for the existence of an effective temperature based on the relative order of various time-scales characterizing intrinsic relaxation and external driving. Our study thus introduces driven small systems as a fertile ground to address fundamental concepts in statistical physics, condensed matter physics and biophysics.

30 min break

Invited Talk DY 29.7 Wed 11:30 H 1028
Efficiently extracting thermodynamics and kinetics from molecular simulation data at multiple thermodynamic states — ●FRANK NOE — FU Berlin, Arnimallee 6, 14195 Berlin

I will present novel methods based on Markov modeling for extracting statistical information (thermodynamics and kinetics) from molecular simulation data that has been generated at multiple thermodynamic states. Such data may be obtained from enhanced sampling protocols, such as umbrella sampling or replica-exchange dynamics, and by mixing one of these protocols with direct molecular dynamics data. Here I will propose ways to optimally extract information from such data, including the reconstruction of the kinetics of rare events that are not directly sampled in the data. An application of our approach is the estimation of rare unbinding kinetics of protein-ligand complexes when only the more frequent binding process can be sampled in direct MD simulations.

DY 29.8 Wed 12:00 H 1028

Stochastic dynamics of adhesion bonds for a rod propelled by both force and torque — ●ANNA BATTISTA and ULRICH SCHWARZ — Heidelberg University, Heidelberg, Germany

The stochastic dynamics of adhesion bonds has emerged as a powerful theoretical framework to explain many prominent features of sliding friction, including the stick-slip regimes often observed at intermediate driving velocity. Sliding friction occurs in a variety of physical contexts, ranging from tribology to cell motility. In particular, stochastic bonds have been employed to model the dynamics of adhesion between a cell and its substrate. Although much progress has been achieved with the help of stochastic bond models, up to now they have been restricted to sliding friction in one dimension. However, there are situations in which translation is coupled with rotation, as is the case of gliding cells with a shape asymmetry. Motivated by this observation, we develop a sliding friction model for a slider that is both translated and rotated, while being connected to the substrate by stochastic bonds. We find that torque enhances the tendency for stick-slip behaviour and that adhesive patches spontaneously form at the moving interface when the on-rate of the bonds has a velocity dependence. Interestingly, our results show an adhesion dynamics reminiscent of that observed during the migration of curved malaria parasites.

DY 29.9 Wed 12:15 H 1028

High stress levels lead to transition from heterogeneous timing to synchronized cellular response of the *E. coli* Colicin E2 operon — ●ANDREAS MADER¹, BENEDIKT VON BRONK¹, BENEDIKT EWALD¹, SARA KESEL¹, KARIN SCHNETZ², ERWIN FREY¹, and MADELEINE OPITZ¹ — ¹Faculty of Physics, LMU München, Germany — ²Institute for Genetics, Universität zu Köln, Germany

The production of bacteriocins, such as colicins, is one means of bacteria to outcompete other microorganisms. In a single cell study, we analyze the heterogeneous gene expression of Colicin E2, expressed from the SOS inducible *E. coli* Colicin E2 operon. We quantitatively study the expression dynamics of the Colicin E2 operon in *E. coli* using fluorescence time-lapse microscopy. Different fluorescence reporter proteins allow us to observe heterogeneity in Colicin production and Colicin release separately. At low exogenous stress levels all cells eventually respond after a given time (heterogeneous timing), high stress levels lead to a synchronized stress response of all cells about 75 min after induction via stress. A heterogeneous response in combination with heterogeneous timing can be biologically significant. It might enable a bacterial population to endure low stress levels, while at high stress levels an immediate and synchronized response may allow elimination of closely related bacteria competing for resources. Furthermore we could demonstrate that the amount of Colicin released is dependent on *cel* (lysis) gene expression. Future investigations will focus on transcriptional as well as post-transcriptional regulation affecting the dynamics of Colicin expression and release.

DY 29.10 Wed 12:30 H 1028

The fluidity of the cytoplasm is regulated by cytosolic pH — MATTHIAS MUNDER², ●DANIEL MIDTVEDT¹, ELISABETH NÜSKE², SHOVMAYEE MAHARANA², SONJA KROSCHWALD², DORIS RICHTER², VASILY ZABURDAEV¹, and SIMON ALBERTI² — ¹Max Planck Institut für Physik komplexer Systeme — ²Max Planck Institut für molekulare Zellbiologie und Genetik

Upon sub-optimal growth conditions, many cells enter a quiescent state characterized by lack of cell division, low metabolic activity and decreased intracellular pH. The mechanisms by which cells enter and leave quiescence are as of yet largely unknown.

Using single-particle tracking, we investigate the mobility of foreign tracer particles under different cytosolic pH conditions. We find a significant decrease in the mobility of the particles under acidic conditions.

Indicative of obstructed motion in a crowded solution, at short times the velocity autocorrelation function (VACF) of the tracer particles is negative. We relate these findings to a structural phase transition in the cytoplasm.

Our findings indicate that cells may use cytosolic pH to change the material properties of the cytoplasm. We are currently investigating possible consequences of these changes. Our findings could have broad implications for the understanding of alternative physiological states in cells, and promotes a view on the eukaryotic cytoplasm as a viscoelastic material with widely tunable properties.

DY 29.11 Wed 12:45 H 1028

Detailed balance violations in mesoscopic biological systems — ●CHRISTOPHER BATTLE¹, CHASE P. BROEDERSZ², NIKTA FAKHRI¹, FRED C. MACKINTOSH³, and CHRISTOPH F. SCHMIDT¹ — ¹Drittes Physikalisches Institut, Georg-August Universität, Göttingen, Germany — ²Lewis-Sigler Institute for Integrative Genomics and Department of Physics, Princeton University, Princeton, NJ, USA — ³Dept. of Physics & Astronomy, Vrije Universiteit, Amsterdam, Netherlands

Living systems exist far from thermal equilibrium, with active processes powering many of their functions. As such, they are expected to violate fundamental tenets of equilibrium, such as the principle of detailed balance. While some cellular processes show unmistakable non-equilibrium characteristics, e.g. persistent directed motion, others are more subtle, exhibiting non-thermal, random motion which is similar in appearance to Brownian motion, e.g. cortical stress fluctu-

ations or active cellular stirring. It is not a priori clear whether the active, random nature of the second class of motions will translate into observable violations of detailed balance on the mesoscopic, i.e. cellular, scale. Here we report experimental evidence of detailed balance violations for such a case. Such violations can be used to "fingerprint" non-equilibrium systems, and differentiate active processes from thermal ones without perturbing the system.

DY 29.12 Wed 13:00 H 1028

Genetic networks specifying the functional architecture of orientation domains in V1 — ●JOSCHA LIEDTKE and FRED WOLF — Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen (Germany)

Although genetic information is critically important for brain development and structure, it is widely believed that neocortical functional architecture is largely shaped by activity dependent mechanisms.

Here we show theoretically that mathematical models of genetic networks of principal neurons interacting by long range axonal morphogen transport can generate morphogen patterns that exactly prescribe the functional architecture of the primary visual cortex (V1) as experimentally observed. We analyze in detail an example genetic network that encodes the functional architecture of V1 by a dynamically generated morphogen pattern. We use analytical methods from weakly non-linear analysis [Cross & Hohenberg 1993] complemented by numerical simulations to obtain solutions of the model. In particular we find that the pinwheel statistics are in quantitative agreement with high precision experimental measurements [Kaschube et al. 2010].

This theory opens a novel perspective on the experimentally observed robustness of V1's architecture against radically abnormal developmental conditions such as a dark rearing [White et al. 2001]. Furthermore, it provides for the first time a scheme how the pattern of a complex cortical architecture can be specified using only a small genetic bandwidth.

DY 30: SYPS: Physics of Sustainability and Human-Nature Interactions (joint symposium SOE/ AKE/ BP/ DY/ jDPG)

Time: Wednesday 9:30–12:15

Location: H 0105

Invited Talk

DY 30.1 Wed 9:30 H 0105

Anticipating and avoiding tipping points — ●TIMOTHY M. LENTON — University of Exeter, Exeter, UK

A 'tipping point' occurs when a small change in forcing triggers a strongly non-linear response in the internal dynamics of a system, qualitatively changing its future state. Large-scale 'tipping elements' have been identified in the Earth's climate system that may pass a tipping point under human-induced global change this century. At the smaller scale of ecosystems, some tipping points have already been observed, and more are anticipated in future. Our capacity to forecast such abrupt, non-linear changes has historically been poor. However, much excitement has recently been generated by the theory that some approaching tipping points carry generic early warning signals. I will critically examine the prospects for gaining early warning of approaching tipping points. Promising methods are based on detecting 'critical slowing down' in the rate a system recovers from small perturbations, and on accompanying changes in the statistical distribution of its behaviour. I will show examples of early warning signals in paleo-data approaching past abrupt climate changes, and in models being gradually forced past tipping points. I will also consider the conditions under which the methods fail. Finally, I will discuss how we might respond to early warning to try and avoid tipping points, especially in the climate system.

Invited Talk

DY 30.2 Wed 10:00 H 0105

Climate investment under uncertainty: the two degree target and the desire for dynamic consistency — ●HERMANN HELD and DELF NEUBERSCH — Center of Earth System Research and Sustainability, University of Hamburg, Grindelberg 5, 20144 Hamburg

During the climate Conferences of the Parties 2009-2011 the global community developed a formal consensus to limit the anthropogenically induced increase of global mean temperature to 2K ("two-degree target" or "2°-target"). While the latest IPCC (Intergovernmental Panel on Climate Change) report (2014) summarizes cost estimates that can

be interpreted as rather low, suggesting some potential political feasibility of the 2°-target, some authors start to question the conceptual validity of the 2°-target: it might be too late to still comply with it, given the slow pace of mitigation policy. Moreover, it is pointed out that a strictly interpreted temperature target does not have a straightforward generalization when uncertainty is internalized in decision-making under anticipated future learning.

Here we present a generalization of the 2°-target that addresses both of these problematic aspects and that respects dynamic consistency under anticipated future learning. Consequences for climate policy are highlighted. We find that previous climate economic analyses of the 2K-target in terms of low cost for transforming the energy system are still valid, when being re-interpreted. Moreover, mitigation costs could be reduced by up to 1/3 if the climate response to greenhouse gas forcing were known with certainty, pointing to the expected economic value of geo-scientific information.

Invited Talk

DY 30.3 Wed 10:30 H 0105

What are the resources required to fulfil human needs? — ●JULIA STEINBERGER — Sustainability Research Institute, University of Leeds, UK

All human societies require environmental resources, in the form of energy and materials, to survive and flourish. However, the exact level of resource requirements may be difficult to estimate, since it can depend on many factors. These factors include: local biophysical conditions, such as climate or available crops for food; technological options and efficiencies for delivering key services; but also socio-economic parameters, including consumption levels and inequality in distribution. This talk will present recent advances in the international study of energy requirements for human needs. These results demonstrate that high levels of human wellbeing are attainable at moderate as well as very high energy use, and that the average level of energy use required to achieve high human wellbeing is declining over time. Moreover, it can be shown that energy itself does not play a dominant role in explain-

ing the considerable advances in human wellbeing over the past half century. An agenda for analysing the resource requirements to fulfil universal basic human needs will then be presented. This agenda must take into account socio-economic as well as technological choices, since fulfilling human needs at low levels of resource use most likely requires a re-organisation and re-orientation of many socio-economic activities.

15 min. break

Invited Talk DY 30.4 Wed 11:15 H 0105

Design of Sustainable Supply Chains for Sustainable Cities — ●ANNA NAGURNEY — Isenberg School of Management, University of Massachusetts Amherst

Supply chains provide the critical infrastructure for the production and distribution of goods and services in our Network Economy and serve as the conduits for the manufacturing, transportation, and consumption of products ranging from food, clothing, automobiles, and high technology products, to even healthcare products. Cities as major population centers serve not only as the principal demand points but also as the locations of many of the distribution and storage facilities, transportation providers, and even manufacturers. The sustainability of supply chains is, hence, a precursor to the sustainability of our cities.

In this presentation, we discuss a plethora of relevant supply chain networks for cities from food to energy ones. We provide the foundations of the methodologies in terms of variational inequality theory and projected dynamical systems theory and describe both an opti-

mization model for sustainable supply chain network design as well as a game theory one with multiple decision-makers and frequencies of the network economic activities.

Invited Talk DY 30.5 Wed 11:45 H 0105

Ecological econophysics for degrowth — ●SALVADOR PUEYO — Dept. d'Ecologia, Universitat de Barcelona, Barcelona, Catalonia, Spain — Research & Degrowth, Barcelona, Catalonia, Spain

Climate change, resource scarcity and ecosystem degradation suggest that we have already overshoot the sustainable level of economic throughput. One of the greatest challenges of our time is to move from a growth-based economy to a socially benign degrowth. The obstacles ahead are not only political and cultural but also technical: How to transform the economic system in depth without undesired emergent properties or loss of its basic functionality? How to shrink the economy without triggering uncontrolled recessions? How to effectively increase equality to compensate for a decreasing average consumption? Several of the involved features are best expressed as frequency distributions (of recession sizes, of individual income or resource consumption), thus demanding the kind of approach used in statistical physics, which links distributions to mechanisms. This econophysical approach should be combined with that of ecological economics, which treats the economy as a subsystem of the biosphere instead of an autonomous system. Researchers in econophysics or complexity economics are in a unique position to move beyond more mundane goals and apply their knowledge to help changing the system in favor of sustainability, equality and democracy while we still have the opportunity.

DY 31: Transport: Fluctuations and Noise (joint session TT/ CPP/ DY)

Time: Wednesday 11:30–12:45

Location: H 3005

DY 31.1 Wed 11:30 H 3005

Quantum transport, master equations, and exchange fluctuations — ●SIGMUND KOHLER and ROBERT HUSSEIN — Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain

We investigate to which extent a many-body Bloch-Redfield master equation description of transport in coupled quantum dots is consistent with the exact generalized equilibrium conditions known as exchange fluctuation theorems. Thereby we identify a class of master equations for which this is the case. Beyond this class, we find deviations which exhibit characteristic scaling laws as functions of the dot-lead tunneling, the inter-dot tunneling, and the temperature. These deviations are accompanied by an increase of lead energy fluctuations inherent in the Bloch-Redfield equation beyond rotating-wave approximation. We illustrate our results with numerical data for a double and a quadruple quantum dot attached to four leads.

[1] R. Hussein and S. Kohler, *Phys. Rev. B* **89**, 205424 (2014).

DY 31.2 Wed 11:45 H 3005

Waiting time-distribution of a quantum-dot spin valve — ●BJÖRN SOTHMANN — Département de Physique Théorique, Université de Genève, Genève, Switzerland

Recently, the study of waiting-time distributions of electron transport has received a lot of interest [1]. It can provide information about transport processes that is complementary to average current and noise. Here, we discuss the waiting-time distribution of a quantum-dot spin valve [2], i.e., a single-level quantum dot coupled to two ferromagnetic electrodes with magnetizations that can point in arbitrary directions [3]. We demonstrate that the rich transport physics of this setup, such as the dynamical channel blockade and spin precession in an interaction-driven exchange field, shows up in the waiting-time distribution, and we analyze the conditions necessary to observe the various effects.

[1] M. Albert, G. Haack, C. Flindt, M. Büttiker, *Phys. Rev. Lett.* **108**, 186806 (2012).

[2] B. Sothmann, *Phys. Rev. B* **90**, 155315 (2014).

[3] M. Braun, J. König, J. Martinek, *Phys. Rev. B* **70**, 195345 (2004).

DY 31.3 Wed 12:00 H 3005

Waiting-time distribution of light from superconducting resonators coupled to voltage-biased Josephson junctions — ●SIMON DAMBACH, BJÖRN KUBALA, VERA GRAMICH, and JOACHIM

ANKERHOLD — Institute for Complex Quantum Systems, Ulm University, Ulm, Germany

The interplay of the tunneling transfer of charges and the emission and absorption of light can be investigated in a set-up, where a voltage-biased Josephson junction is placed in series to a microwave cavity. In such devices measurements of the emitted microwave radiation can yield information about the Cooper pair current and its fluctuations and vice versa.

Due to the inherent nonlinearity of the Josephson junction tunneling Cooper-pairs can create a variety of non-classical states of light already at weak driving. Depending on experimental parameters and tuning, the device can be described by effective Hamiltonians, indicating specific photon creation mechanisms which lead to strongly bunched or anti-bunched light emission [1].

We will use the waiting-time distribution [2] of emitted photons to highlight how charge quantization of the Cooper pair current drives a crossover from a coherent light source to a single-photon source. Analytical results for the weak driving regime, based on a quantum regression approach, are complemented by numerical results for the full nonlinear quantum case.

[1] B. Kubala, V. Gramich, and J. Ankerhold, arXiv:1404.6259.

[2] T. Brandes, *Ann. Phys. (Berlin)* **17**, 477 (2008).

DY 31.4 Wed 12:15 H 3005

Input-output description of microwave radiation in the dynamical Coulomb blockade — JUHA LEPPÄKANGAS¹, GÖRAN JOHANSSON¹, ●MICHAEL MARTHALER², and MIKAEL FOGELSTRÖM¹ — ¹Microtechnology and Nanoscience, MC2, Chalmers University of Technology, SE-412 96 Göteborg, Sweden — ²Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

We study microwave radiation emitted by a small voltage-biased Josephson junction connected to a superconducting transmission line. An input-output formalism for the radiation field is established, using a perturbation expansion in the junction's critical current. Using output field operators solved up to the second order, we estimate the spectral density and the second-order coherence of the emitted field. For typical transmission line impedances and at frequencies below the main emission peak at the Josephson frequency, radiation occurs predominantly due to two-photon emission. This emission is characterized by a high degree of photon bunching if detected symmetrically around half of the

Josephson frequency. Strong phase fluctuations in the transmission line make related nonclassical phase-dependent amplitude correlations short lived, and there is no steady-state two-mode squeezing. However, the radiation is shown to violate the classical Cauchy-Schwarz inequality of intensity cross-correlations, demonstrating the nonclassicality of the photon pair production in this region.

DY 31.5 Wed 12:30 H 3005

Distribution of energy dissipated by a driven two-level system — ●PHILIP WOLLFARTH^{1,2}, ALEXANDER SHNIRMAN^{1,2}, and YASUHIRO UTSUMI³ — ¹Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — ²DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — ³Department of Physics Engineering, Faculty of Engineering, Mie University, Tsu, Mie, 514-

8507, Japan

In the context of fluctuation relations, we study the distribution of energy dissipated by a driven two-level system. Incorporating an energy counting field into the well known spin-boson model enables us to calculate the distribution function of the amount of energy exchanged between the system and the bath. We also derive the conditional distribution functions of the energy exchanged with the bath for particular initial and/or final states of the two-level system. We confirm the symmetry of the conditional distribution function expected from the theory of fluctuation relations. We also find that the conditional distribution functions acquire considerable quantum corrections at times shorter or of the order of the dephasing time. Our findings can be tested using solid-state qubits.

[1] P. Wollfarth, A. Shnirman, Y. Utsumi, Phys. Rev. B **90**, 165411 (2014).

DY 32: Focus Session: Statistics of fully developed turbulence

Despite its omnipresence and wide range of technical applications, a comprehensive understanding of fully developed turbulence remains elusive. Fully developed turbulence constitutes a paradigm of a complex system with a large number of strongly interacting degrees of freedom far from equilibrium. With coherent structures interacting in a complex manner, fully developed turbulence falls in between purely random and pattern-forming systems. It is this combination which makes it a challenging research field with connections to non-equilibrium statistical mechanics, pattern formation and stochastic processes. In this focus session we will cover various aspects of fundamental turbulence research from both the Eulerian and Lagrangian perspective. (Organizors M.Wilczek and O. Kamps)

Time: Wednesday 15:00–18:45

Location: BH-N 243

Invited Talk

DY 32.1 Wed 15:00 BH-N 243

Turbulence and Instantons — TOBIAS GRAFKE¹, ●RAINER GRAUER², TOBIAS SCHÄFER³, STEPHAN SCHINDEL², and ERIC VANDEN-EIJNDEN⁴ — ¹Dept. of Physics of Complex Systems, Weizmann Institute, Rehovot, Israel — ²Theor. Physik I, Ruhr-Universität Bochum, Bochum, Germany — ³Dept. of Math., College of Staten Island, CUNY, USA — ⁴Courant Institute, NYU, New York, USA

It is evident that coherent nearly singular structures play a dominant role in understanding the anomalous scaling behavior in turbulent systems.

We ask the question, which role these singular structures play in turbulence statistics. More than 15 years ago, for certain turbulent systems the door for attacking this issue was opened by getting access to the probability density function to rare and strong fluctuations by the instanton approach. We address the question whether one can identify instantons in direct numerical simulations of the stochastically driven Burgers equation. For this purpose, we first solve the instanton equations using the Chernykh-Stepanov method [2001]. These results are then compared to direct numerical simulations by introducing a filtering technique to extract prescribed rare events from massive data sets of realizations.

In addition, we solve the issue why earlier simulations by Gotoh [1999] were in disagreement with the asymptotic prediction of the instanton method and demonstrate that this approach is capable to describe the probability distribution of velocity differences for various Reynolds numbers.

DY 32.2 Wed 15:30 BH-N 243

The non-universality of magnetohydrodynamic turbulence — ●WOLF-CHRISTIAN MÜLLER¹, ROLAND GRAPPIN², ANDREA VERDINI³, and ÖZGÜR GÜRÇAN⁴ — ¹Technische Hochschule Berlin, Plasma-Astrophysik — ²LUTH, Observatoire de Paris and LPP, Ecole Polytechnique, France — ³Università di Firenze, Dipartimento di Fisica e Astronomia, Firenze, Italy and Royal Observatory of Belgium, SIDC/STCE, Brussels — ⁴LPP, Ecole Polytechnique, Paris, France

We present a new cascade scenario motivated by the three-dimensional energy spectrum observed in numerical simulations of incompressible MHD turbulence in a strong mean field. It is shown that the energy distribution is not in accord with standard critical balance and the associated scale anisotropy. In spite of this, a measurable anisotropy of structure-function scaling exists independent of taking spatial increments with respect to the mean or local direction of the magnetic field.

We, thus, propose a combination of weak Iroshnikov-Kraichnan dynamics governing energy transfer in the field-perpendicular plane and the ricochet process distributing energy quasi-resonantly along all other directions. This spectral transfer process asymptotically approaches the 2D IK-cascade as B_0 increases. The new transfer mechanism is at variance with the commonly accepted resonant weak-turbulence cascade as well as with the critically balanced strong turbulence cascade. It is shown that the non-universal spectral dynamics are determined by the large-scale ratio of kinetic and magnetic energy.

DY 32.3 Wed 15:45 BH-N 243

Markov closure for the Lundgren-Monin-Novikov hierarchy in turbulence — ●JAN FRIEDRICH and RAINER GRAUER — Institut für theoretische Physik I, Ruhr-Universität Bochum, Deutschland

A central, yet unsolved problem of hydrodynamic turbulence is the closure problem, which is due to the nonlinear character of the Navier-Stokes equation. We formulate the closure problem for the many-increment probability distributions and introduce a new method for closing the hierarchy. Here we use the experimental and numerically verified assumption that the turbulent cascade possesses a Markov property in scale [1] down to the so-called Einstein-Markov length. This approximation is far beyond a Gaussian approximation and allows a full description of intermittency effects. The procedure is explained on the example of the simpler Burgers equation corresponding to a fluid without pressure contributions whose singular structures are determined by so-called shocks. The proposed closure also opens up the way to a perturbative treatment of the Navier-Stokes equation beyond the Einstein-Markov length in successively taking into account a larger and larger scale "history" of the system.

[1] R. Friedrich, J. Peinke, Phys. Rev. Lett. **78** (5) (1997) 863-866

DY 32.4 Wed 16:00 BH-N 243

Stochastic description of a turbulent wake — ●NICO REINKE and JOACHIM PEINKE — ForWind, Institute of Physics, Carl v. Ossietzky University, Oldenburg, Germany

The presentation will give an insight in our experimental work to fractal generated turbulent flows and especially in the stochastic analysis of this turbulent flow. The stochastic approach allows to characterize the turbulent cascade process in scale r and in different distances x to the grid. This stochastic characterization shows the complexity of the flow and the transition between an non homogenous to a homogeneous turbulent flow. To characterize the wake of a fractal grid velocity measurements $v(t)$ (using hot wire anemometer) were performed on

the wind tunnel test section center line $x \rightarrow v(t, x)$. We analysis the wake in terms of velocity increments $u(r, x) = v(t + \frac{r}{\langle v \rangle}, x) - v(t, x)$. The velocity increments are consider as Markov chain, which is true for $r \geq l_{EM}$, where l_{EM} is the Einstein-Markov coherence length. The information of the turbulent cascade process is captured in the conditional probability distribution function $p(u(r, x)|u(r + \delta r, x))$, $\delta r \geq l_{EM}$. $p(u(r, x)|u(r + \delta r, x))$ changes for different scales r . This change is describe by the so called Fokker-Planck equation, which is governed by Kramers-Moyal functions $D^{(1)}(u(r, x))$ and $D^{(2)}(u(r, x))$. Finally, those functions characterize the turbulent cascade and allow us to understand the wake in scale and in distance to the grid.

DY 32.5 Wed 16:15 BH-N 243

Stochastic analysis of aerodynamic forces acting on airfoils in turbulent inflow — ●GERRIT KAMPERS¹, MICHAEL HÖLLING¹, ULRICH CORDES², KLAUS HUFNAGEL², CAMERON TROPEA², and JOACHIM PEINKE¹ — ¹ForWind, Institute of Physics, University of Oldenburg, 26111 Oldenburg, Germany — ²Institute of Fluid Mechanics and Aerodynamics, Technical University of Darmstadt, 64287 Darmstadt, Germany

Wind turbines work within the atmospheric boundary layer, which is dominated by turbulence. Such turbulent flows feature non-Gaussian statistics, that are currently not accounted for by industry standards. These intermittent statistics lead to heavy fluctuations in aerodynamic forces and mechanical loads, respectively. Active and passive flow control elements represent a promising approach for the reduction of fluctuating loads.

We present a new testing method for wind tunnel experiments, that allows an investigation of the force fluctuations on airfoil segments with and without flow control elements under realistic and reproducible conditions. The statistics of the desired inflow are defined by a scale dependent analysis of offshore wind data and then reproduced in the wind tunnel with an active grid. Aerodynamic quantities of interest are measured and subsequently studied using a stochastic Langevin approach, which separates the deterministic response of a system from its stochastic (noisy) part. This method enables for a quantitative analysis of the dynamical performance of flow control mechanisms in turbulent conditions.

15 min. break

DY 32.6 Wed 16:45 BH-N 243

Particle motion and irreversibility of turbulent flows — ●ALAIN PUMIR^{1,2}, HAITAO XU², JENNIFER JUCHA², and EBERHARD BODENSCHATZ² — ¹Laboratoire de Physique, Ecole Normale Supérieure de Lyon, F-69007, Lyon, France — ²Max-Planck Institut für Dynamik und Selbst-Organisation, D-37077, Göttingen, Germany

In three-dimensional turbulent flows, the flux of energy from large to small scales breaks time-reversal symmetry. I will discuss how this irreversibility can be observed by following the trajectories of tracers, moving with the fluid.

For the problem of relative particle dispersion, irreversibility implies that particles separate slower forward in time than backward (see Jucha et al, PRL 2014). This property can be understood in terms of an exact relation, established directly from the Navier-Stokes equations. A more surprising observation is that a tracer particle needs more time to build up large kinetic energy, than to dissipate it. This allows us to quantify the irreversibility of the turbulent fluid (Xu et al, PNAS, 2014).

DY 32.7 Wed 17:15 BH-N 243

The Time Irreversibility of Turbulence — ●JENNIFER JUCHA¹, ALAIN PUMIR², HAITAO XU¹, and EBERHARD BODENSCHATZ¹ — ¹Max Planck Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland — ²Ecole Normale Supérieure, Lyon, Frankreich

The dissipation of energy at the smallest scales of a turbulent flow leads to an increase in entropy and therefore renders the flow time-irreversible. This irreversibility also influences the transport and mixing processes at larger scales of the flow but the connection was unclear so far. In this talk, an analytical relation between the dissipation process and the dispersion of particle clusters will be presented. Experimental and numerical results will be shown that confirm our theoretical approach.

DY 32.8 Wed 17:30 BH-N 243

The stochastic description of non-Brownian particles in shear

flow by a colored-noise Fokker-Planck equation — ●LAURA LUKASSEN^{1,2} and MARTIN OBERLACK^{1,2} — ¹Chair of Fluid Dynamics, TU Darmstadt — ²Graduate School of Excellence Computational Engineering, TU Darmstadt

As described in literature, non-Brownian particles in shear flow show a diffusive behavior due to hydrodynamic interactions, namely shear-induced diffusion. The stochastic description by means of a Fokker-Planck equation is of major interest for non-Brownian particles in shear-induced diffusion. In contrast to Brownian diffusion, there is no separation of time scales in the context of shear-induced diffusion. The configuration of non-Brownian particles changes on the same time scale as the hydrodynamic velocity. This fact violates the Markov process assumption in pure position space. In order to assure the Markov process assumption, we derived a new Fokker-Planck equation in coupled position-velocity space (Lukassen, Oberlack, Phys. Rev. E 89, 2014). Under certain conditions, this new coupled Fokker-Planck approach can be reduced to a modified equation in pure position space. The new modified position space description exhibits additional correction terms when compared to other position space Fokker-Planck equations in that context known from literature. Our extended approach shall enable a better stochastic description of non-Brownian particle flows.

The work of L. Lukassen is supported by the "Excellence Initiative" of the German Federal and State Governments and the Graduate School of Computational Engineering at TU Darmstadt.

DY 32.9 Wed 17:45 BH-N 243

Universal properties of the intermittency generating function in fully developed turbulence — ●CHRISTOPH BERLING¹ and OLIVER KAMPS² — ¹Institut für Theoretische Physik, University of Münster, Germany — ²Center for Nonlinear Science, University of Münster, Germany

The understanding of the intermittent fluctuations of observables in fully developed turbulence is one of the central challenges in turbulence research. One example for intermittency is the non-self-similar evolution of the probability density functions (PDFs) of the Lagrangian velocity increments $v(\tau, t) = u(t+\tau) - u(t)$ with respect to the time lag τ . Based on the combination of an exact but unclosed PDF equation and experimental results it is possible to describe the non-self-similar evolution of the Lagrangian increment PDFs by a single function that itself is self-similar [1]. In this contribution we will show that within this framework Lagrangian intermittency can also be described for turbulent flows with different Reynolds numbers as well as for magneto-hydrodynamic and two-dimensional turbulence.

[1] Wilczek et. al., New Journal of Physics **15** (2013) 055015

DY 32.10 Wed 18:00 BH-N 243

the intermittent behavior of DDES simulation of fractal-generated turbulence — ●MOHAMED CHERIF MIHOUBI¹, BERNHARD STOEVESSANDT¹, and JOACHIM PEINKE^{1,2} — ¹Fraunhofer Institute for Wind Energy and Energy System Technology IWES, Oldenburg, Germany — ²ForWind, Center for Wind Energy Research, Oldenburg, Germany

In order to study the relevant sources of noise from wind turbines under real atmospheric inflow conditions, we investigate CFD simulations of fractal generated turbulence. The fractal grid used in this simulation is based on an experimental set-up to be able to validate the simulation results. The Results showed that in the production region of the turbulence the pdfs are roughly Gaussian, the deviation from the Gaussian distribution starts at 0.9m and lasts up to 2m behind the fractal grid. In this region the statistics show highly intermittent behavior with heavy tails which show similar behavior to atmospheric turbulence (please see [1],[2]). From 2m on, the pdfs become Gaussian again. Additionally, energy spectrum, integral length scale and other quantities are evaluated on the stream-wise directions. In comparison with wind tunnel data, the effect of turbulence model in analyzed

[1] Morales, A., Wächter, M. and Peinke, J. (2012), Characterization of wind turbulence by higher-order statistics, *Wind Energy*, 15: 391*406. doi: 10.1002/we.478

[2] Mücke, T., Kleinhans, D. and Peinke, J. (2011), Atmospheric turbulence and its influence on the alternating loads on wind turbines, *Wind Energy*, 14: 301*316. doi: 10.1002/we.422

DY 32.11 Wed 18:15 BH-N 243

Describing the heat transport of turbulent Rayleigh-Bénard convection by POD methods — ●JOHANNES LÜLFF — WWU Mün-

ster

Rayleigh-Bénard convection, which is the buoyancy-induced movement of a fluid enclosed between two horizontal plates, is an idealized setup to study thermal convection. We analyze the modes that transport the most heat between the plates by calculating the proper orthogonal decomposition (POD) of numerical data. Instead of the usual POD ansatz of finding modes that describe the energy best, we developed a method that is optimal in describing the heat transport. Thereby, we can determine the modes with the major influence on the heat transport and the coherent structures in the convection cell. We also show that in lower-dimensional projections of numerical convection data, the new developed modes perform consistently better than the standard modes.

DY 32.12 Wed 18:30 BH-N 243

2d-LCA - a new highly resolving anemometer — ●JAROSLAW PUCZYLOWSKI, MICHAEL HÖLLING, and JOACHIM PEINKE — University of Oldenburg / ForWind - Center for Wind Energy Research, Oldenburg, Germany

The 2d-Laser Cantilever Anemometer (2d-LCA) is a recently developed sensor for two-dimensional velocity measurements in fluids. It uses a micro-structured cantilever as a sensing element, which allows for extremely high resolved measurements. Hence, spatial structures of 140micrometer can be resolved at temporal resolutions of about 100kHz. The 2d-LCA can be applied in the same way as commercial x-wires, however, it can also be used in particle-laden flows and liquids. In addition, the angular acceptance range of the 2d-LCA comprises 90° , whereas standard x-wires are limited to 45° . Comparative measurements with the 2d-LCA and an x-wire have been carried out in a laboratory-generated turbulent wake flow. The data sets of both measurement techniques were analyzed using same stochastic methods. These include spectral analyses, inspection of velocity increments and analyses of extended self-similarity (ESS). Furthermore, key parameters, such as characteristic lengths, mean values of velocity and angles of attack were determined from both data sets. The evaluation shows great agreement between both anemometers. Therefore, we are able to show that the 2d-LCA is capable of providing data that is consistent with established sensors and theory.

DY 33: Critical Phenomena and Phase Transitions

Time: Wednesday 15:00–18:15

Location: BH-N 334

DY 33.1 Wed 15:00 BH-N 334

Fragmentation of fractal random structures — EREN M. ELÇI, ●MARTIN WEIGEL, and NIKOLAOS G. FYTAS — Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England

We analyze the fragmentation behavior of random clusters on the lattice under a process where bonds between neighboring sites are successively broken. Modeling such structures by configurations of a generalized Potts or random-cluster model allows us to discuss a wide range of systems with fractal properties including trees as well as dense clusters. We present exact results for the densities of fragmenting edges and the distribution of fragment sizes for critical clusters in two dimensions. Dynamical fragmentation with a size cutoff leads to broad distributions of fragment sizes. The resulting power laws are shown to encode characteristic fingerprints of the fragmented objects.

DY 33.2 Wed 15:15 BH-N 334

True asymptotics of self-avoiding walks on 3D percolation clusters. — ●NIKLAS FRICKE and WOLFHARD JANKE — Institut für Theoretische Physik and Centre for Theoretical Sciences (NTZ), Universität Leipzig, Postfach 100920, 04009 Leipzig, Germany

We study self-avoiding walks on three-dimensional critical percolation clusters using a new exact enumeration method. It overcomes the exponential increase in computation time by exploiting the clusters' fractal nature. We enumerate walks of over 10^4 steps, far more than has ever been possible. We found the scaling exponent ν for the end-to-end distance to be smaller than previously thought and the same on backbones and full clusters. Furthermore, we find strong evidence against the widely assumed scaling law for the average number of conformations and propose an alternative, which perfectly fits our data.

N. Fricke and W. Janke, arXiv:1410.5960, to appear in PRL (in print).

DY 33.3 Wed 15:30 BH-N 334

To return or not to return? Phase transition to transience and congestion in random walks and queueing systems — ●ANDREAS SORGE^{1,2,4}, JAN NAGLER^{3,4}, STEPHAN HERMINGHAUS^{1,2}, and MARC TIMME^{1,2,4} — ¹MPI for Dynamics and Self-Organization, Göttingen, Germany — ²Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Germany — ³Computational Physics, IFB, ETH Zürich, Switzerland — ⁴Organization for Research on Complex Adaptive Systems (or-cas), Göttingen, Germany

Will a random walker ever return to where she started, and keep returning forever? When we are unaware of the law governing the walk, wisdom has it that we cannot infer recurrence from a finite-time sample trajectory. In 1890, Henri Poincaré introduced the very idea of such recurrences as a stability criterion. This criterion also applies to stochastic dynamical systems: By tuning the system parameter, a random walk loses recurrence and becomes unstable at a critical point. Intriguingly, this constitutes a phase transition to transience in Markovian systems. Here, we present a practical method to determine the

critical point and the critical exponents of such systems in Monte-Carlo simulations. We also introduce the freely available Python implementation for effective and reproducible use of our method. Our findings and tools may be helpful in computational studies of stochastic systems, in particular queueing systems and dynamical congestion phenomena.

DY 33.4 Wed 15:45 BH-N 334

On the mixing of the single-bond dynamics for the random-cluster model — ●EREN M. ELÇI¹, TIMOTHY GARONI², ANDREA COLLEVECCHIO², and MARTIN WEIGEL¹ — ¹Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England — ²School of Mathematical Sciences, Monash University, Victoria, 3800, Australia

The Markov Chain Monte Carlo method is a ubiquitous tool in Statistical Physics. It is standard lore that close to a point of a second-order phase transition a phenomenon called critical slowing down hampers efficient sampling. A major breakthrough in reducing this slowing down for the random-cluster model has been the invention of the Swendsen-Wang-Chayes-Machta algorithm. Recently, however, it has been shown, that local chains can be as or even more efficient than non-local chains. Examples are the Worm algorithm for the Ising model and the single-bond dynamics for the random-cluster model. We present results of a numerical study of the coupling time of the single-bond chain dynamics for the random-cluster model. A careful analysis allows us to obtain high-precision (upper) bounds for auto-correlation, relaxation and mixing times for both critical and off-critical temperatures on square and simple-cubic lattices. The numerical results give strong evidence in favor of the rapid-mixing property of the single-bond dynamics for the random-cluster model, both at a second-order phase transition and off criticality. Furthermore we also present, to our knowledge, a novel heuristic method for detecting a first-order phase transition in the coupling-time distribution.

DY 33.5 Wed 16:00 BH-N 334

Nonstandard Finite-Size Scaling at First-Order Phase Transitions with Macroscopic Low-Temperature Phase Degeneracy — MARCO MUELLER¹, DESMOND A. JOHNSTON², and ●WOLFHARD JANKE¹ — ¹Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, 04009 Leipzig, Germany — ²Department of Mathematics, School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh EH14 4AS, Scotland, UK

We show that the standard inverse system volume scaling for finite-size corrections at a first-order phase transition (i.e., $1/L^3$ for an $L \times L \times L$ lattice in 3D) is transmuted to $1/L^2$ scaling if there is an exponential low-temperature phase degeneracy. The gonihedric Ising model which has a four-spin interaction, plaquette Hamiltonian provides an exemplar of just such a system. We use multicanonical Monte Carlo simulations of this model to generate high-precision data which provides strong confirmation of the nonstandard finite-size scaling law. The dual to the gonihedric model, which is an anisotropically coupled

Ashkin-Teller model, has a similar degeneracy and also displays the nonstandard scaling behaviour. A suitable “fuki-nuke” type order parameter and further potential applications of the transmuted finite-size scaling law will be briefly discussed.

M. Mueller, W. Janke, D.A. Johnston, *Phys. Rev. Lett.* **112** (2014) 200601;

M. Mueller, D.A. Johnston, W. Janke, *Nucl. Phys. B* **888** (2014) 214.

DY 33.6 Wed 16:15 BH-N 334

Phase transition of films in the Ising universality class — ●MARTIN HASENBUSCH — Humoldt-Universität zu Berlin, Deutschland

We study the phase transition of films with free and periodic boundary conditions. To this end we perform Monte-Carlo simulations of the Ising and the Blume-Capel model on the simple cubic lattice. Using a finite size scaling method, we determine accurately the transition temperature for thicknesses up to $L_0 = 64$. Since the transition is expected to share the universality class of the two-dimensional Ising model we can make use of exact and accurate numerical results obtained for this model. Our numerical results nicely confirm that the transition of the films indeed belongs to the universality class of the two-dimensional Ising model. We analyse how the transition temperature of the films approaches the transition temperature of the bulk system as the thickness increases. We confirm the power law behaviour predicted by finite size scaling.

15 min. break

DY 33.7 Wed 16:45 BH-N 334

Quantum phase transitions in networks of Lipkin–Meshkov–Glick models — ●ALEKSANDR SOROKIN, VICTOR BASTIDAS, and TOBIAS BRANDES — Technische Universität Berlin, Berlin, Germany

The Lipkin–Meshkov–Glick (LMG) model describes an ensemble of all-to-all-coupled two-level systems with anisotropic interactions, exhibiting quantum phase transitions. In this contribution we show that coupling of several LMG systems with the overall Hamiltonian

$$\mathcal{H} = \sum_{l=1}^N \left[gJ_l^z - \frac{\gamma}{2j} (J_l^x)^2 \right] - \frac{1}{2j} \sum_{l', l=1}^N \kappa_{ll'} J_l^y J_{l'}^y$$

gives rise to phases with different collective behaviour. Namely, the weak-coupling regime corresponds to the paramagnetic phase when the local field dominates the dynamics, but the local anisotropy leads to the existence of an exponentially degenerate ground state. In the strong-coupling regime, the ground state is twofold degenerate and possesses long-range magnetic ordering.

The calculations were performed in the mean-field (MF) approximation but taking into account quantum fluctuations around the MF solution. Within this approach analytical expressions for the ground-state and excitation energies as well as correlation functions in different phases were obtained for a network with the ring topology.

For details see [A.V Sorokin, V.M Bastidas and T Brandes, *Phys. Rev. E* **90**, 042141 (2014)]

DY 33.8 Wed 17:00 BH-N 334

Hypergeometric extrapolation of the strong coupling perturbation series of the Bose-Hubbard model — ●SÖREN SANDERS — Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg

Critical phenomena occurring at continuous phase transitions render a (low-order) perturbative description invalid. To overcome this a recently proposed scheme to obtain nonperturbative physics from low-order perturbation theory utilizing hypergeometric functions is studied and applied to the quantum phase transition from a Mott insulator to a superfluid undergone by the Bose-Hubbard model. The well-known phase diagram is reproduced and critical exponents obtained that are in remarkable agreement with the universality hypothesis.

DY 33.9 Wed 17:15 BH-N 334

Casimir force scaling functions in 2d Ising systems with open boundaries: The importance of corner contributions — ●FRED HUCHT and FELIX M. SCHMIDT — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

We consider the two-dimensional square lattice Ising model with free boundary conditions, aiming at universal critical Casimir force scaling functions. Surprisingly, no closed form solution exists for finite $L_{\parallel} \times L_{\perp}$ lattices due to the lack of translational invariance in both

directions. However, the exact partition function polynomial can be efficiently calculated from the determinant of a $(4L_{\parallel}L_{\perp})$ -dimensional sparse matrix using arbitrary-precision integer arithmetics. For infinite systems, we derive exact expressions for the bulk, surface and corner free energies at arbitrary temperatures using q -products [1]. Combining these results, we derive universal finite-size-scaling functions of the Casimir force and the residual free energy for different values of the aspect ratio $\rho = L_{\perp}/L_{\parallel}$. We find a unusual logarithmic divergence of the residual free energy scaling function at $x = tL_{\perp} \rightarrow 0$, which is directly related to the logarithmic L -dependence of the free energy at criticality predicted by Cardy and Peschel [2].

[1] E. Vernier and J. L. Jacobsen, *J. Phys. A: Math. Theor.* **45**, 045003 (2012).

[2] J. Cardy and I. Peschel, *Nucl. Phys. B* **300**, 377 (1988).

DY 33.10 Wed 17:30 BH-N 334

Thermodynamic properties of two-dimensional colloidal crystals with dipolar interactions — ●SVEN DEUTSCHLÄNDER¹, TOBIAS HORN², ANTONIO MANUEL PUERTAS³, HARTMUT LÖWEN², GEORG MARET¹, and PETER KEIM¹ — ¹University of Konstanz, Konstanz, Germany — ²Heinrich-Heine-University Düsseldorf, Düsseldorf, Germany — ³University of Almeria, Almeria, Spain

Colloidal suspensions provide the possibility to study a variety of classical many particle systems like glasses, gels, crystals or liquids on a microscopic scale by means of single particle resolution. Hence, macroscopically significant thermal and mechanical properties can be reasoned by the explicit structure and dynamics of the particles. By colloidal experiments and Monte Carlo simulations, we study the equilibrium melting scenario of two-dimensional systems with a repulsive dipole-dipole potential. Our results are largely in agreement with theoretical predictions of the continuous KTHNY melting scenario, but also indicate new prospects which are beyond the microscopic defect theory.

[1] S. Deuschländer, A. M. Puertas, G. Maret, and P. Keim, *Phys. Rev. Lett.* **113**, 127801 (2014).

[2] S. Deuschländer, T. Horn, H. Löwen, G. Maret, and P. Keim, *Phys. Rev. Lett.* **111**, 098301 (2013).

[3] T. Horn, S. Deuschländer, H. Löwen, G. Maret, and P. Keim, *Phys. Rev. E* **88**, 062305 (2013)

DY 33.11 Wed 17:45 BH-N 334

Thermal and nonthermal phase transitions in silicon induced by femtosecond free-electron laser pulse — ●NIKITA MEDVEDEV¹, ZHENG LI^{1,2}, and BEATA ZIAJA^{1,3} — ¹CFEL at DESY, Notkestr. 85, 22607 Hamburg, Germany — ²University of Hamburg, 20355, Hamburg, Germany — ³Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Krakow, Poland

Silicon under irradiation with intense femtosecond laser pulses can undergo a phase transition via two different channels: thermal and non-thermal. The first one occurs if the lattice is heated strongly enough with electron-phonon coupling to trigger silicon melting, while the second one results from the modification of the interatomic potential energy surface by excitation of electrons from the valence to the conduction band. We developed a model to include both channels. Tight-binding molecular dynamics (TBMD) is used to model atomic dynamics with the potential dependent on the state of electronic system. Simultaneously, electronic state is traced with the Boltzmann equation for low-energy electrons (the valence and the bottom of the conduction band), and with a Monte Carlo model for photoabsorption, high-energy electrons, and deep shell holes.

Our results show that electron-phonon coupling triggers phase transition into a low-density liquid phase for the deposited doses > 0.65 eV/atom. For deposited doses of over 0.9 eV/atom, silicon undergoes a phase transition into high-density liquid phase triggered via interplay of thermal heating and the nonthermal change of the atomic potential.

DY 33.12 Wed 18:00 BH-N 334

Line contribution to the critical Casimir force between a homogeneous and a chemically stepped surface — ●FRANCESCO PARISEN TOLDIN¹, MATTHIAS TRÖNDLE^{2,3}, and SIEGFRIED DIETRICH^{2,3} — ¹Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — ²Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — ³IV. Institut für Theoretische Physik, Universität Stuttgart, Germany

Recent experimental realizations of the critical Casimir effect have been implemented by monitoring colloidal particles immersed in a binary liquid mixture near demixing and exposed to a chemically structured substrate consisting of stripes with alternating adsorption pref-

erences, forming chemical steps between them. We analyze the contribution of such chemical steps to the critical Casimir force for the film geometry and within the Ising universality class. By means of Monte Carlo simulations, mean-field theory, and finite-size scaling analysis we determine the universal scaling function associated with the contribution to the critical Casimir force due to individual, isolated chemical steps facing a surface with homogeneous adsorption preference or with

Dirichlet boundary condition. These results allow one to compute the critical Casimir force in the presence of arbitrarily shaped, but wide stripes as a sum of the contributions due to the homogeneous parts of the surface and due to the chemical steps between the stripes. We assess this decomposition by comparing the resulting sum with actual simulation data in the presence of a chemically striped substrate.

Ref: F. Parisen Toldin, M. Tröndle, S. Dietrich, arXiv:1409.5536

DY 34: Nonlinear Dynamics, Synchronization and Chaos - Part II

Time: Wednesday 15:00–16:15

Location: BH-N 128

DY 34.1 Wed 15:00 BH-N 128

Unusually simple way to create spiral wave in an excitable medium — •VLADIMIR ZYKOV, ALEXEI KRECHOV, and EBERHARD BODENSCHATZ — Max-Planck-Institute for Dynamics and Selforganization, Goettingen, Germany

It is demonstrated that a spiral wave can be easily created in a nonuniform excitable media where a wave break is due to sufficiently strong jumps in the diffusion coefficient. Our analytical and numerical results indicate that in a one-dimensional medium such an inhomogeneity can result in a unidirectional propagation block. It is also illustrated how this phenomenon can be used to create spiral wave in a two-dimensional medium with a specific size and geometry of the inhomogeneity. It is important to stress that following this way the spiral wave is created simply after a single excitation stimulus while others known methods need at least two stimuli.

DY 34.2 Wed 15:15 BH-N 128

Entraining and eliminating spiral waves in excitable media by secondary excitations — •T K SHAJAHAN, SEBASTIAN BERG, and STEFAN LUTHER — Max Planck Institute for Dynamics and Self Organization, Am Fassberg, Göttingen, Germany

Excitable media comprises of a wide variety of physical, chemical, and biological systems made of coupled networks of excitable elements. Heart is an example of an excitable medium; the individual cardiac myocytes have a characteristic response, the action potential, to an external stimulus. Such excitations in a two-dimensional medium can form traveling wave patterns including spiral waves and target waves. These patterns in a physiological system have implications for the healthy functioning of the system. For example, spiral waves of cardiac excitation waves in the heart can override the natural rhythm of the heart and lead to cardiac arrhythmias. We study control and elimination of spiral waves using secondary excitations in monolayers of cultured cardiac cells. Free spiral waves can be eliminated with a local electrode by stimulating the medium at a higher frequency than the spiral. But this method fails if the spiral is pinned to tissue heterogeneities. A pinned spiral wave can be controlled by electric field stimulus. Our theoretical and experimental studies indicate that periodic field stimuli at a frequency lower than the spiral frequency is more efficient to eliminate pinned spiral waves. I will discuss the implications of this result for low energy defibrillation.

DY 34.3 Wed 15:30 BH-N 128

Exact linearization of nonlinear optimal trajectory tracking problems — •JAKOB LÖBER — Institut für Theoretische Physik, TU Berlin

We consider the task of forcing a phase space trajectory of an affine dynamical system as closely as possible along a desired trajectory. Using the regularization parameter of an appropriately formulated optimal

control problem as the small parameter, we develop a perturbation approach which allows to interpret a singular optimal control problem as a singularly perturbed system of ODEs. Surprisingly, for a certain class of nonlinear control systems as e.g. one-dimensional mechanical systems, the perturbative treatment of this ODE reduces to exclusively linear equations. The nonlinearity is eaten by the control while the solution for the controlled trajectories, being independent of the nonlinearity, is universal for the control system at hand.

DY 34.4 Wed 15:45 BH-N 128

Route to chaos in optomechanics — LUTZ BAKEMEIER, •ANDREAS ALVERMANN, and HOLGER FEHSKE — Institut für Physik, Ernst-Moritz-Arndt-Universität, Felix-Hausdorff-Str. 6, 17487 Greifswald

We establish the emergence of chaotic motion in optomechanical systems. Chaos appears at negative detuning for experimentally accessible values of the pump power and other system parameters. We describe the sequence of period doubling bifurcations that leads to chaos, and state the experimentally observable signatures in the optical spectrum. In addition to the semi-classical dynamics we analyze the possibility of chaotic motion in the quantum regime. We find that quantum mechanics protects the optomechanical system against irregular dynamics, such that simple periodic orbits reappear and replace the classically chaotic motion. In this way observation of the dynamical signatures makes it possible to pin down the crossover from quantum to classical mechanics.

DY 34.5 Wed 16:00 BH-N 128

Quantum synchronization of driven self-sustained oscillators — •CHRISTOPH BRUDER¹, ANDREAS NUNNENKAMP^{1,2}, and STEFAN WALTER^{1,3} — ¹Department of Physics, University of Basel, Klingelbergstr. 82, CH-4056 Basel — ²Cavendish Laboratory, J J Thomson Avenue, Cambridge CB3 0HE — ³Institute for Theoretical Physics, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

Synchronization is a universal phenomenon that is important both in fundamental studies and in technical applications. Here we study synchronization of two dissipatively coupled Van der Pol oscillators in the quantum regime and analyze synchronization in terms of frequency entrainment and frequency locking [1]. Due to quantum noise strict frequency locking is absent and is replaced by a crossover from weak to strong frequency entrainment. The differences to the behavior of one quantum Van der Pol oscillator subject to an external drive [2] are discussed. Moreover, a possible experimental realization of two coupled quantum Van der Pol oscillators in an optomechanical setting is described.

[1] S. Walter, A. Nunnenkamp, and C. Bruder, *Ann. Phys.* DOI: 10.1002/andp.201400144 (2014)

[2] S. Walter, A. Nunnenkamp, and C. Bruder, *Phys. Rev. Lett.* 112, 094102 (2014)

DY 35: Complex Fluids and Soft Matter - Part I (joint session DY/ CPP / BP)

Time: Wednesday 15:00–16:45

Location: BH-N 333

DY 35.1 Wed 15:00 BH-N 333

Particle segregation in a sedimenting bidisperse soft sphere system — MATTHIAS KOHL and ●MICHAEL SCHMIEDEBERG — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

We explore the sedimentation process of a binary soft colloidal sphere system. In case of large overlaps of the particles the segregation dynamics differs significantly from that of hard particles. By using Brownian dynamics simulations and theoretical predictions, we find new complex states [1]. For example, multiple-phase-stackings where large particles gather both at the top and the bottom of the system or metastable network-like structures occur. We analyze the comprehensive dynamics of the segregation process. Usually, we observe a multiple-step process: First there is local segregation, then clusters are formed, and finally the clusters sink to their equilibrium position.

[1] M. Kohl and M. Schmiedeberg, *Soft Matter* 10, 4340 (2014).

DY 35.2 Wed 15:15 BH-N 333

Suppression of Ostwald Ripening by Chemical Reactions in Active Emulsions — ●DAVID ZWICKER^{1,2}, ANTHONY A. HYMAN³, and FRANK JÜLICHER² — ¹Harvard University, Cambridge MA, USA — ²Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ³Max Planck Institute of Cell Biology and Genetics, Dresden, Germany

Ostwald ripening is a coarsening process of droplets in an emulsions that is driven by the surface tension of the droplets. This coarsening must be suppressed to stabilize emulsions, e.g. to control the properties of pharmaceuticals, food, or cosmetics. Ostwald ripening must also be suppressed in biological cells, which contain liquid-like compartments, e.g. germ granules, Cajal-bodies, and centrosomes. Such systems are often driven away from equilibrium by chemical reactions and can thus be described as active emulsions.

Here, we show that non-equilibrium chemical reactions can suppress Ostwald Ripening, leading to stable, monodisperse emulsions. Using a coarse-grained description of the droplet dynamics, we derive analytical approximations of the typical droplet size, droplet count, and time scale of the dynamics. We also compare these results to numerical simulations of the continuous concentration fields. We thus show how chemical reactions can be used to stabilize emulsions and control their properties.

DY 35.3 Wed 15:30 BH-N 333

Binary mixtures of hard rod-like colloids: mesoscopic equilibrium theory and shear-driven instabilities — ●RODRIGO LUGO FRIAS and SABINE KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Mixtures of rod-like particles occur in a wide range of biological contexts and technological applications, and their equilibrium phase behavior has been intensely studied in recent years. Here we investigate a binary mixture of rod-like colloidal particles driven out of equilibrium by means of a steady shear flow (Couette geometry).

Using classical density functional theory (DFT), we first derive a mesoscopic free energy functional for a mixture of hard spherocylinders with different length-to-length ratio in terms of tensorial order parameters that describe their alignment. The resulting free energy displays a strong dependence on the microscopical properties of the system. Based on the equilibrium analysis, we then discuss the dynamical behavior of the mixture using a natural extension of the mesoscopic Doi-Hess theory. In particular we analyze the orientational dynamics under shear for varying shear rate, concentration and aspect ratio.

[1] F. Tardani, L. Gentile, G. A. Ranieri and C. La Mesa, *J. Phys. Chem. C*, **117**, 8556 (2013).

[2] S. Hess, *Z.Naturforsch. A* **31a**, 1034 (1976). M. Doi, *J. Polym. Sci., Polym. Phys. Ed.* **19**, 229 (1981).

[3] R. Lugo-Frias and S. H. L. Klapp, in preparation (2015).

DY 35.4 Wed 15:45 BH-N 333

Dynamics of the Critical Casimir Effect in a Binary Fluid — ●SUTAPA ROY, FELIX HÖFLING, and S. DIETRICH — Max-Planck-Institut für Intelligente Systeme, Stuttgart and Institut für Theoretische

Physik IV, Universität Stuttgart, Germany

A binary fluid mixture near its consolute point exhibits critical fluctuations of the local composition. While the static properties of the mixture are well described by the 3D Ising universality class [1], the dynamic properties involving conservation of particle number and concentration, energy, and momentum are classified as model H' [2]. Confinement of critical fluctuations in such a mixture leads to critical Casimir forces (CCF) [3] acting on the confining surfaces.

We present results for the CCF in a symmetric binary Lennard-Jones model fluid, confined in a slit pore, close to its bulk critical point. Utilizing the computing resources of GPUs [4], molecular dynamics (MD) simulations were performed for system sizes of up to 216,000 particles and 5 orders of magnitude in time which is well beyond common computational efforts. Our results from MD and Monte Carlo simulations, for various static and dynamic quantities, both in bulk and in confinement, are compared to theory and experimental observations.

[1] S.K. Das *et al.*, *J. Chem. Phys.* **125**, 024506 (2006).

[2] P.C. Hohenberg and B.I. Halperin, *Rev. Mod. Phys.* **49**, 435 (1977).

[3] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich and C. Bechinger, *Nature* **451**, 172 (2008).

[4] P. Colberg and F. Höfling, *Comput. Phys. Commun.* **182**, 1120 (2011).

DY 35.5 Wed 16:00 BH-N 333

Simulating many-body Casimir interactions in colloidal suspensions — ●HENDRIK HOBRECHT and FRED HUCHT — Fakultät für Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg

We study the fluctuation-induced (Casimir) interactions in colloidal suspensions, especially between colloids immersed in a binary liquid close to its critical demixing point for two-dimensional systems. To simulate those systems, we present a Monte Carlo cluster algorithm based on geometric symmetries of the Hamiltonian. Utilizing the principle of universality, the suspension is represented by an Ising system while the colloids are areas of spins with fixed orientation. Our results for the Casimir interaction potential between two particles agree quantitatively with the theoretical predictions [1], where we find that the behavior depends strongly on whether the order parameter is held fixed or is allowed to fluctuate. Finally we present our results for the three-body interaction Casimir potential.

[1] T. W. Burkhardt and E. Eisenriegler, *Phys. Rev. Lett.* **74** (1995) 3189.

DY 35.6 Wed 16:15 BH-N 333

Flow induced deflection of a liquid-crystal topological defect — TILLMANN STIEGER¹, MARTIN SCHOEN¹, and ●MARCO G. MAZZA² — ¹Technische Universität Berlin — ²Max-Planck-Institut für Dynamik und Selbstorganisation

We perform nonequilibrium molecular dynamics simulations of a nematic liquid crystal flowing around a colloidal particle. We study the flow-induced modifications of the Saturn ring defect and the surface ring defect in the liquid crystal. By varying the strength of the interaction between liquid crystal and colloid we can produce Saturn rings of different sizes. We study the deflection of the topological defect as a function of applied stress, and find a linear, that is Hookean, stress-strain dependence. We relate this finding to the elastic properties of the nematic liquid crystal and to the properties of the core of the topological defect.

DY 35.7 Wed 16:30 BH-N 333

Modeling drying droplets on porous substrates — ●CHRISTIAN DIDDENS¹, HANS KUERTEN¹, CEES VAN DER GELD¹, and HERMAN WIJSHOFF^{1,2} — ¹Eindhoven University of Technology, The Netherlands — ²Océ Technologies B.V., Venlo, The Netherlands

We investigate the drying of an inkjet-printed picoliter droplet on a porous substrate in the framework of a numerical model. The evolution of the droplet is governed by evaporation at the liquid-air interface and absorption of the liquid into the porous substrate.

When a binary mixture is considered, an interplay of preferential evaporation, composition-dependent viscosity and the absorption dynamics can interestingly result in a slower drying for faster evaporation rates.

Since solute particles and their deposition to the surface are also taken into account, the present model can be utilized as predictive

tool for deposition patterns in ink-jet printing processes.

DY 36: SYHM Higgs Modes in Condensed Matter and Quantum Gases

Time: Wednesday 15:00–17:45

Location: H 0105

Invited Talk DY 36.1 Wed 15:00 H 0105
Amplitude or Higgs Modes in Condensed Matter — ●CHANDRA VARMA — University of California, Riverside, CA, USA

Spurred by some strange experimental observations in some superconductors, the theory of a new collective mode in superconductors and how it can be experimentally found under certain circumstances was provided in 1981. It was called the “Amplitude Mode” to distinguish it from the “Phase Modes” which provide Josephson effects and which in homogeneous superconductors are coupled to charge fluctuations and are at the energies of the plasmons. More generally, this mode is the amplitude mode of a particle-hole symmetric U(1) field, i.e., the model treated by Higgs and others in the 1960’s whose generalizations have played an important role in the standard model of particle physics.

I will tell the story of the above and why such modes were missed in the theory of superconductivity for so long and the applications of the ideas about such modes for cold bosons and fermions in optical lattices and in quantum anti-ferromagnets. I will also comment, as a very interested outsider and an enthusiast, on the Higgs in particle physics being discovered at LHC from the point of view of the theory of superconductivity.

Invited Talk DY 36.2 Wed 15:30 H 0105
Higgs Particles for Systems with U(1) Symmetry in Two Dimensions — ●LODE POLLET — Arnold Sommerfeld Center, Theoretical Physics, LMU Munich, Germany

We present solid evidence for the existence of a Higgs boson in two-dimensional relativistic field theories based on analytically continued results from quantum Monte Carlo simulations of the Bose-Hubbard model in the vicinity of the superfluid-Mott insulator quantum critical point, featuring emergent particle-hole symmetry and Lorentz-invariance. The Higgs boson, seen as a well-defined low-frequency resonance in the spectral density, is quickly pushed to high energies in the superfluid phase and disappears by merging with the broad secondary peak at the characteristic interaction scale. Simulations of a trapped system of ultra-cold Rb-87 atoms demonstrate that the low-frequency resonance feature is lost for typical experimental parameters, while the characteristic frequency for the onset of strong response is preserved. We compute the universal scaling function and comment on the agreements and disagreements with three dimensions and observations of Higgs particles in more traditional solid state experiments.

Invited Talk DY 36.3 Wed 16:00 H 0105
Massive Photons and the Anderson-Higgs Mechanism in Superconductors — ●DIRK VAN DER MAREL — University of Geneva, Geneva, Switzerland

When we tune the temperature or the pressure of a solid transitions can occur between different states of matter. Usually such a phase transition is accompanied by a symmetry breaking and the emergence of one or several collective modes of the material. A superconducting gap has collective oscillations of its amplitude -equivalent to the Higgs particle- and of its phase. As shown by Anderson in 1958, coupling to the electromagnetic field creates an energy gap in the longitudinal oscillations of the charge density, and in the transverse oscillations of mixed photon-matter character. The energy-momentum dispersion of the latter can be measured experimentally, and reveals the mass acquired by the photons due the coupling to the superconducting order parameter. In certain superconductors two or more condensates coexist. Weak coupling between the condensates gives rise to the so-called

Leggett-exciton, and the coupling to the electromagnetic field makes that two or more massive photon-branches coexist. Experimental examples of this will be discussed in this talk.

15 min. break.

Invited Talk DY 36.4 Wed 16:45 H 0105
Amplitude Higgs Mode in 2H-NbSe₂ Superconductor — ●MARIE-AUDE MÉASSON¹, ROMAIN GRASSET¹, YANN GALLAIS¹, MAX CAZAYOUS¹, ALAIN SACUTO¹, PIERRE RODIÈRE², and LAURENT CARIO³ — ¹LMPQ, Université Paris 7-CNRS, France — ²Institut Neel, Grenoble, France — ³IMN, Université de Nantes, France

When a spontaneous breaking of a continuous symmetry takes place, as happens during a superconducting transition, collective excitations such as the amplitude Higgs mode of the order parameter emerge. The existence of such Higgs mode was proposed in the charge density wave (CDW) superconductor (SC) 2H-NbSe₂, after the first experimental observation by Raman scattering. The Higgs mode could be unraveled via its coupling to the coexisting charge density wave mode. We will address here the questions of the nature of this mode as well as the mechanism of its observability.

We report experimental evidences for the Higgs mode scenario in 2H-NbSe₂ using Raman scattering. By comparing 2H-NbSe₂ and its iso-structural partner 2H-NbS₂ which shows superconductivity but lacks the charge density wave order and by destroying the coexisting CDW order under high pressure in 2H-NbSe₂, we demonstrate that the superconducting mode owes its spectral weight to the presence of the coexisting charge density wave order. In addition a full spectral weight transfer between both modes operates in 2H-NbSe₂ upon entering the superconducting phase. All these observations are consistent with a superconducting Higgs mode. Intriguing symmetry dependent results under pressure will be discussed.

Invited Talk DY 36.5 Wed 17:15 H 0105
The Higgs Mode in Disordered Superconductors Close to a Quantum Phase Transition — ●AVIAD FRYDMAN¹, DANIEL SHERMAN^{1,2}, UWE S. PRACHT², BORIS GORSHUNOV^{2,3}, and MARTIN DRESSEL² — ¹Department of Physics, Bar Ilan University, Ramat Gan, 52900, Israel — ²Physikalisches Institut, Universität, Stuttgart, 70550 Stuttgart, Germany — ³Moscow Institute of Physics and Technology, 141700, Dolgoprudny, Moscow Region, Russia

The Higgs theory, which generates mass for elementary particles, was inspired by screening of magnetic fields in superconductors. It is somewhat disappointing that in superconductors, the Higgs-amplitude mode has not yet been observed, partially because it can rapidly decay into unpaired electrons. Nevertheless, recent theories show that if the Higgs mass could be softened below the pairing gap it should be visible in two dimensions. Such conditions can be met by tuning a superconducting film towards a quantum critical point (QCP). We report on spectroscopic studies in the terahertz frequency regime of thin superconducting films for which the superconductor to insulator transition (SIT) is tuned by disorder. Tunneling spectroscopy determines the pairing gap 2Δ which remains finite on both sides of the SIT. In contrast, the threshold frequency for dynamical conductivity, which in BCS theory is associated with the gap, vanishes critically toward the SIT. The excess optical spectral weight below 2Δ is identified as an unambiguous observation of the Higgs mode in a superconductor.

DY 37: Fluctuating Electricity Supply: Modelling of Generation, Backup and Storage (joint session AKE / DY / SOE)

Time: Wednesday 15:00–16:30

Location: A 151

Invited Talk

DY 37.1 Wed 15:00 A 151

Fluctuations from photovoltaic and wind power systems

— •DETLEV HEINEMANN¹, GERALD LOHMANN¹, MOHAMMED REZA RAHIMI TABAR², and MEHRNAZ ANVARI² — ¹Universität Oldenburg, Institut für Physik, AG Energiemetereologie & ForWind — ²Universität Oldenburg, Institut für Physik, AG TWiSt & ForWind

Solar and wind resources vary considerably in time and space, and changes in their magnitude are almost immediately translated into output power variations of wind and solar power plants. Analyzing the stochastic properties of wind and solar resources in different temporal and spatial scales is therefore a necessary step towards a proper representation of these contributions to large scale power systems.

This presentation describes known stochastic properties of wind and solar resources as well as reports on current studies of (i) their conditional probability distribution functions in different time lags and (ii) increment statistics of large-scale wind and solar production.

Conditional distribution functions show severe deviations from Gaussian statistics and possess positive skewness, while the risk of flickering events in both wind and solar generally increases with parameters as wind speed and solar elevation, respectively. Spatial averaging significantly influences this behavior. The comparison of wind and solar power fluctuations is strongly affected by the presence of a deterministic contribution in the solar part. Applying a detrending approach for the solar data results in a significant improvement of the solar increment statistics.

DY 37.2 Wed 15:30 A 151

Facing Europe: Revised wind power upscaling algorithms

— •BRUNO SCHYSKA, LÜDER VON BREMEN, and ALEXANDER KIES — University Oldenburg - ForWind, Oldenburg, Germany

In the wind energy sector, upscaling models are used to estimate the total wind energy production within a certain region from a small number of reference sites. Each reference site is considered to be representative for a certain sub-region. Upscaling models therefore include selection schemes for the reference sites as well as statistical, partly non-linear, models to estimate the energy production in the sub-regions. Until now, upscaling models are mainly used on country level. For larger areas such as Europe no operational model and no research model exist.

In this study, revised upscaling models for the estimation of near real-time wind energy production in Europe are presented. These models include different approaches for the estimation of the energy production in the sub-regions as well as different selection schemes for the reference sites using cluster analyses. Cluster analyses are based on wind speed data from the MERRA reanalysis data set as well as on the geographical distribution of installed wind energy capacities in Europe. From the comparison, the selection scheme, which requires the minimal number of reference sites, is selected for long-term investigations of the wind energy production in Europe.

DY 37.3 Wed 15:45 A 151

Backup flexibility classes in complex renewable energy networks

— •DAVID SCHLACHTBERGER¹, SARAH BECKER¹, STEFAN SCHRAMM¹, and MARTIN GREINER² — ¹Frankfurt Institute for Advanced Studies, Uni Frankfurt, Frankfurt am Main, Germany — ²Department of Engineering, Aarhus University, Aarhus, Denmark

How large will be the demand for more flexible backup plants in an European power system with an increasing share of fluctuating renewable energies? We use eight years of high resolution weather-based wind

and solar power generation data to split the backup systems required to cover the residual load into three flexibility classes for daily, weekly, and seasonal time-scales. They are distinguished by the maximum rates of change of their power output. We find that a large fraction of seasonally and weekly flexible backup systems can no longer be reasonably integrated above a penetration of renewables of around 50% and 90% of the mean load, respectively. We also find that the total required backup capacity can only be reduced if countries share their excess generation and backup power.

DY 37.4 Wed 16:00 A 151

Dimensioning the Minimal Storage Needs in Renewable Power Systems

— •STEFAN WEITEMEYER, DAVID KLEINHANS, and CARSTEN AGERT — NEXT ENERGY · EWE Research Centre for Energy Technology at the University of Oldenburg, Germany

Integrating a high share of electricity from non-dispatchable Renewable Energy Sources (RES) in a power supply system is a challenging task; it will likely require large-scale installations of costly storage capacities.

We present a modelling approach to investigate which storage characteristics are most adequate for scenarios with high shares of RES. Adapted from an optimization approach, the model allows to systematically study the influence of important storage parameters (size, efficiency, power) on the integration of RES. In particular, the implications of simultaneously using multiple storage classes in combination with fossil back-up power plants can be investigated.

Applying our model to data for Germany, our simulations show how an extensive integration of RES requires different storage characteristics during different phases of the pathway towards a 100% RES scenario. The results also imply that a balance between installing storage capacities and additional generation capacities is required.

DY 37.5 Wed 16:15 A 151

The temporal development of storage needs in the European energy transition

— •ALEXANDER KIES, LÜDER VON BREMEN, and BRUNO SCHYSKA — ForWind, Universität Oldenburg, Oldenburg

Europe is on the way towards a highly renewable energy system. In 2012 23.5% of the gross electricity consumption in the EU-28 was produced from renewable sources. This share is expected to increase further up to very high penetration levels close to 100% in the next decades. To ensure reliability and stability of the power system several solutions to the generation-load-mismatch problem have been proposed like over-installation of renewables, transmission capacity extensions and the use of storages. In this work we investigate the development of storage needs in 34 European countries for different transmission grid scenarios until 2050. A large weather data set with a spatial resolution of 7 x 7 km and a hourly temporal resolution covering Europe is used to model the fluctuating feed-in from the renewables, i.e. wind, photovoltaics, hydro, concentrated solar power and wave. Additionally the controllable renewable generation types biomass and geothermal were considered. Starting from the renewable shares in the year 2012 we model the increase in renewable capacities in a linear and a logistic way until levels of 100% in 2050 for different transmission grid scenarios and calculate the storage needs for every year. The remaining generation shares to cover the load are assumed to come from conventional generation. We show that storage needs are unlikely to grow rapidly until 2030, but thereafter are of high importance. However, this process can be slowed down considerably by transmission grid extensions.

DY 38: Wetting, Micro and Nanofluidics (joint session CPP/ DY)

Time: Wednesday 15:00–18:15

Location: C 243

DY 38.1 Wed 15:00 C 243

Lateral adhesion force of superhydrophobic surfaces — ●DORIS VOLLMER, DOMINIK PILAT, NAN GAO, PERIKLIS PAPADOPOULOS, FRANK SCHELLENBERGER, RÜDIGER BERGER, and HANS-JÜRGEN BUTT — MPI for Polymer Research, Mainz, Germany

We designed an instrument to measure the lateral adhesion force of drops on surfaces (1). The forces required to slide a sessile drop over a surface was measured by means of the deflection of a capillary that stuck in the drop. This allows the investigation of the dynamic lateral adhesion force of water drops on superhydrophobic surfaces. The movement of the drop relative to the surfaces enabled us to resolve the pinning of the three-phase contact line. This was related to the shape of the drop profile, which was recorded by video microscopy. The lateral adhesion of a drop on a superhydrophobic pillar array was quantified in dependence of pillar spacing and drop velocity.

(1) D.W. Pilat, P. Papadopoulos, D. Schaeffel, D. Vollmer, R. Berger, and H.-J. Butt, *Langmuir* 2012, 28, 16812.

DY 38.2 Wed 15:15 C 243

Drying and Wetting transitions on irregular rough substrates. — ●SEGUN GIDEON AYODELE, CIRO SEMPREBON, RENAUD DUFUR, STEPHAN HERMINGHAUS, and MARTIN BRINKMANN — Max-Planck Institut für Dynamik und selbstorganisation, 37077 Göttingen.

Drying and wetting transitions on non-flat solids of homogeneous wettability are studied employing a sharp interface model. Interfacial configurations in the Grand canonical ensemble and corresponding numerical energy minimizations for a non-zero microscopic contact angle are compared to predictions based on the statistical model proposed in Refs. [1,2]. This mean field model considers exclusively local descriptors of the substrate topography such as the distribution of heights, as well as averages of the slope and its square at a given height. In contrast to the continuous desorption isotherm of a zero microscopic contact angle, we observe an increasingly discontinuous decay of the average film thickness in our numerical simulations during a desorption as the microscopic contact angle is increased. The pressure of the final drying transition as observed in the simulated annealing and numerical energy minimization is in agreement with predictions of the ‘Wenzel prewetting’ transition in the mean field model [1,2].

1. S. Herminghaus, *Eur. Phys. J. E* 35, 43 (2012).
2. S. Herminghaus, *Phys. Rev. Lett.*, 109,236102 (2012).

DY 38.3 Wed 15:30 C 243

Dynamic Trapping of Sliding Drops on Wetting Defects — ●ANDREA CAVALLI¹, MICHIEL MUSTERD², RUDY LAGRAAUW¹, DIETER 'T MANNETJE¹, DIRK VAN DEN ENDE¹, and FRIEDER MUGELE¹ — ¹University of Twente, MESA+ Institute for Nanotechnology; Physics of Complex Fluids, Enschede, The Netherlands — ²Delft University of Technology, Delft, The Netherlands

We present a numerical analysis of the dynamic interaction of sliding drops on an inclined plate with wetting defects. Our three-dimensional model, developed with OpenFOAM allows us to describe inertial and viscous effects, as well as the internal degrees of freedom of the droplet. We observe that the ability of a drop to deform and stretch enhances the strength and range of the wetting defect, as compared to a simplified analytic description of a non-deformable drop. Yet, the key physical parameters, namely the ratio between trapping strength and driving force as well as the ratio between inertial and viscous time scale prevail as governing control parameters. We further investigate the role of the strength, size and steepness of the wetting defect in retaining the drop. Finally, we compare our simulations with trapping experiments on electrowetting obstacles. The quantitative agreement shows that the trapping of sliding drops follows a universal behavior, which is largely independent of the specific nature of the defect.

DY 38.4 Wed 15:45 C 243

Sub-nanometric substrate structural changes enhance the solid/liquid slip boundary condition — ●JOSHUA MCGRAW, ANTOINE BRIDET, SAMUEL GRANDTHYLL, HENDRIK HÄHL, FRANK MÜLLER, and KARIN JACOBS — Experimental Physics, Saarland University, 66041 Saarbrücken, Germany

Alkylsilane self-assembled monolayers (SAMs) have long been used as model substrates for their ease of preparation and hydrophobic prop-

erties. We have long observed that these monolayers also provide a slip boundary condition for dewetting polymer films, and that the slip condition is switchable if the alkyl chain length is changed (from 12 to 18 backbone carbons, for example). Typically, this change is affected in a quantized way, using one or the other chain length, thus obtaining one or the other slip condition. It has been suggested that the specific structure of the resulting SAM controls the slip condition. Here, we present results in which this structure is changed in two continuous ways. First, we prepare SAMs containing bidisperse mixtures of alkyl silanes, with the composition as a control parameter. Second, we thermally anneal the SAMs, resulting in an irreversible loss of carbon from the monolayer. In both cases, we find an enhanced slip condition which is tuneable over a certain range.

DY 38.5 Wed 16:00 C 243

Universal Regimes in the Relaxation of Stepped Liquid Interfaces near Contact Lines — ●MARCO RIVETTI¹, THOMAS SALEZ², MICHAEL BENZAQUEN², ELIE RAPHAEL², and OLIVER BAEUMCHEN¹ — ¹Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — ²Laboratoire de Physico-Chimie Theorique, UMR 7083 CNRS & ESPCI ParisTech, Paris, France

A liquid droplet on a perfectly smooth surface wets or dewets the substrate according to the difference between initial and equilibrium contact angles [1]. Such a scenario, however, becomes less intuitive whenever the initial shape of the interface is non-spherical. Indeed, the capillary-driven relaxation of the liquid surface may be in competition with the relaxation of the contact angle at the three-phase contact line. Here, we study the dynamics of stepped interfaces of thin polystyrene films on hydrophilic substrates. Annealing the polymeric film above its glass transition temperature induces flow which is precisely monitored using ex- and in-situ atomic force microscopy. Both pinned and receding contact line regimes are observed. Rescaling with regard to the viscosity, surface tension and film thickness collapses the data on a master curve, providing a universal time for the transition between both regimes. In addition, we prove that the pinned interface exhibits self-similar height profiles which are captured by a thin film model in lubrication approximation [2].

[1] S.L.Cormier et al, *PRL* 109, 154501 (2012); [2] J.D.McGraw et al, *PRL* 109, 128303 (2012)

DY 38.6 Wed 16:15 C 243

Dynamic Contact Angle of a Soft Linear Viscoelastic Solid — ●STEFAN KARPITSCHKA¹, SIDDHARTHA DAS², MATHIJS VAN GORCUM¹, HUGO PERRIN³, BRUNO ANDREOTTI³, and JACCO H. SNOEIJER^{1,4} — ¹Physics of Fluids Group, Faculty of Science and Technology, MESA+ Institute, University of Twente, 7500 AE Enschede, The Netherlands — ²Department of Mechanical Engineering, University of Maryland, College Park, MD 20742, USA — ³Physique et Mécanique des Milieux Hétérogènes, UMR 7636 ESPCI -CNRS, Univ. Paris-Diderot, 10 rue Vauquelin, 75005, Paris, France — ⁴Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands

The wetting motion of a liquid over a rigid solid gives rise to a dynamic liquid contact angle. Here we show that on a soft, viscoelastic substrate, a moving contact line leads to a dynamic contact angle of the solid. The initially flat solid surface is deformed elastically into a sharp ridge. The ridge shape and the orientational angle of its tip depend on the contact line velocity. We present a theory based on linear response that reveals how the dynamics of the wetting ridge emerges from the substrate rheology. The theory is validated experimentally with measurements of the dynamic contact angle on a silicone gel.

15 min. break

DY 38.7 Wed 16:45 C 243

Capillary force acting on a particle correlated with the shape of the meniscus — ●FRANK SCHELLENBERGER, PERIKLIS PAPADOPOULOS, STEFAN WEBER, MICHAEL KAPPL, DORIS VOLLMER, and HANS-JÜRGEN BUTT — Max Planck Institute for Polymer Research, Mainz, Germany

Capillary bridges play a important role for the stability of colloidal

systems. The forces of these bridges strongly correlates with their shape. It is possible to measure capillary forces with an Atomic Force Microscope (AFM), but it is impossible with such a device to image the shape of the capillary bridge at the same time.

Analytical and numerical calculations exist that correlates the force of the capillary bridges with the shape of the liquid. However experimentally capillary bridges could not directly be imaged with the corresponding force in the micrometer range so far. A Laser Scanning Confocal Microscope (LSCM) can visualize the shape of a liquid bridge on solid surface in a three-dimensional form. We built a combined LSCM and AFM device and measured the forces with colloidal probes on liquid surfaces. The combination of force spectroscopy and confocal microscopy allows us to image capillary bridges and simultaneously measure the corresponding force.

With our setup we can now verify the theoretical forces, calculated from the shape of the meniscus, and the corresponding force curves. We present our results of the simultaneous AFM and LSCM measurements of capillary bridges.

DY 38.8 Wed 17:00 C 243

Wettability-independent bouncing on flat surfaces — JOLET DE RUITER, RUDY LAGRAAUW, DIRK VAN DEN ENDE, and •FRIEDER MUGELE — University of Twente; MESA+ Institute for Nanotechnology, Physics of Complex Fluids, Enschede, The Netherlands

The impingement of drops onto solid surfaces plays a crucial role in a variety of processes, including inkjet printing, fog harvesting, anti-icing, dropwise condensation and spray coating. Recent efforts in understanding and controlling drop impact behaviour focused on superhydrophobic surfaces with specific surface structures enabling drop bouncing with reduced contact time. Here, we report a different universal bouncing mechanism that occurs on both wetting and non-wetting flat surfaces for both high and low surface tension liquids. Using high-speed multiple-wavelength interferometry, we show that this bouncing mechanism is based on the continuous presence of an air film for moderate drop impact velocities. This submicrometre air cushion slows down the incoming drop and reverses its momentum. Viscous forces in the air film play a key role in this process: they provide transient stability of the air cushion against squeeze-out, mediate momentum transfer, and contribute a substantial part of the energy dissipation during bouncing.

DY 38.9 Wed 17:15 C 243

Surfactants in droplet-based microfluidics – Adsorption, Exchange and Biocompatibility — •BIRTE RIECHERS^{1,2}, PHILIPP GRUNER², FLORINE MAES^{1,2}, and JEAN-CHRISTOPHE BARET^{1,2} — ¹Center de Recherche Paul Pascal, Bordeaux, France — ²Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Emulsions are omnipresent in industry, research and daily life. They are widely used in painting materials, cosmetics as well as for medical and biotechnology applications [Bremond et al. *Soft Matter* 2012]. Emulsions are multiphase liquids stabilised using surfactants. These amphiphilic molecules adsorb to interfaces changing their properties (e. g. surface tension, interfacial rheology) [Baret *Lab Chip* 2012]. They also chemically or physically interact with the dispersed aqueous phase effecting solubility of solutes in all phases [Skhiri et al. *Soft Matter* 2012].

Here, we analyse the properties of surfactants which result in undesirable reactions and interactions with the interior of the droplets. We present a microfluidic method to determine the adsorption kinetics of surfactants. The principle is based on miniaturised pH measurements at the micron-scale. We show that the surfactant exchange between the droplet interface and the continuous phase occurs within seconds and significantly effects the loss of chemicals from droplets. Our method provides new means to analyse surfactant interfaces and their interactions with the aqueous phase of emulsion droplets. We anticipate that our approach can be used to optimise surfactants and formulations for applications in emulsion-based biochemical analysis.

DY 38.10 Wed 17:30 C 243

Coexistence of Various Instabilities on a Single Liquid Filament — MICHAEL HEIN¹, •JEAN-BAPTISTE FLEURY¹, and RALF SEEMANN^{1,2} — ¹Saarland University, Experimental Physics, Saarbruecken, Germany — ²Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Droplet based microfluidics exploits the decay of a liquid filament or cylinder into droplets of micrometric size. While the physics of droplet breakup on small scales remains a field of vivid interest, droplet based microfluidic systems have become widely used both in fundamental science and application such as (bio-)analytics or micro-chemistry. We present experimental research on the formation of droplets by breakup of a squeezed liquid filament surrounded by an immiscible phase that flows over a topographic step. This non-equilibrium process arises from the interplay between flow properties and interfacial instabilities when the filament is suddenly released from confinement at the step. In contrast to previous studies, a rich variety of different droplet breakup regimes was observed for the used geometry which are characterized by the coexistence of multiple liquid instabilities on a single filament. Surprisingly, these instabilities can be of different type while the filament is exposed to a symmetric flow-field. This spontaneous symmetry breaking is a nontrivial consequence of volume throughput constraints of each individual instability and allows for the specific production of heterogeneous droplet families from one single filament under constant flow rates.

(Michael Hein, Jean-Baptiste Fleury and Ralf Seemann, Submitted)

DY 38.11 Wed 17:45 C 243

Inertial microfluidics: control of lift forces and dynamics of microfluidic crystals — •CHRISTOPHER PROHM and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

At intermediate Reynolds numbers, particles in microfluidic channels assemble at fixed distances from the channel axis and bounding walls [1]. This Segré-Silberberg effect can be described in terms of an inertial lift force acting on the particles. At increasing densities the particles form microfluidic crystals due to an interplay of hydrodynamic interactions and inertial lift forces [2]. Microfluidic devices utilizing inertial migration have recently been demonstrated for biomedical tasks such as particle sorting or separation [1].

Here, we investigate the motion of colloidal particles in microfluidic channels using the lattice Boltzmann method [3]. First, we show how the geometry of the channel influences inertial focusing of a single particle. We also demonstrate that manipulating the axial or angular velocity of the particle modifies its lift-force profile, which permits control of the lateral particle position. Second, we investigate suspensions of particles. We describe how they self-assemble into microfluidic particle crystals and discuss the dynamic properties of these crystals.

[1] H. Amini, W. Lee, and D. Di Carlo, *Lab Chip* **14**, 2739 (2014).

[2] W. Lee, H. Amini, H. A. Stone, and D. Di Carlo, *Proc. Natl. Acad. Sci. U.S.A.* **107**, 22413 (2010).

[3] C. Prohm and H. Stark, *Lab Chip* **14**, 2115 (2014).

DY 38.12 Wed 18:00 C 243

High-throughput and passive trapping of nano-objects using electrostatic forces — •MICHAEL ADRIAN GERSPACH^{1,2,3}, NASIR MOJARAD², YASIN EKINCI², and THOMAS PFOHL^{1,3} — ¹Swiss Nanoscience Institute, Basel, 4056, Switzerland — ²Paul Scherrer Institute, Villigen, 5323, Switzerland — ³Department of Chemistry, University of Basel, Basel, 4056, Switzerland

Contact free trapping of nano-objects in solution is of broad interest. Although several methods have been developed, like optical tweezers, stable and high throughput trapping of nanometer-sized particles remains challenging. Our approach of trapping charged nano-objects is geometry induced electrostatic trapping [1], a method based on altering the surface topology of nano-channels that are negatively charged when exposed to water. Here we present the on chip contact free trapping of single 40 to 80 nm gold particles in nanometer-sized pockets without the use of any externally applied forces. The particles in the solution are pushed into the pockets and trapped only because of the difference in electrostatic potential between the nanofluidic channel walls and the finer pocket structures. Increasing the salt concentration of the solution leads to screening of the surface charges by free counter ions and therefore, weakens the trap strength and shortens the average time a particle dwell in a trap. Thus by changing the concentration of the solution or the height of the nanofluidic channels, the particles can be trapped from microseconds to several minutes. In future we plan to extend this method to trap and investigate the dynamics of biological entities such as DNA or large proteins. [1] *Nature* **457** (2010), 692-695

DY 39: Flow-Induced Structures in Complex Fluids (joint session CPP/ DRG, Deutsche Rheologische Gesellschaft/ DY)

Annual Meeting of the German Rheological Society together with the Spring Meeting of the Condensed Matter section of German Physical Society

Time: Wednesday 15:00–18:30

Location: C 264

Invited Talk DY 39.1 Wed 15:00 C 264

A new perspective of materials processing — ●KYUNG HYUN AHN — Seoul National University, Seoul, Korea

With recent advances in emerging technologies, materials design encounters new challenges. With more nano particles inside, processing experiences thinner and faster deformations than ever, which should be reflected in materials design. However, little is known about the flow characteristics of such complex fluids and less is known about how to design and control the process. Industrial coating materials such as ink, slurry and paste form heterogeneous microstructure as they contain various components. Therefore, it is necessary to incorporate the concept of heterogeneity into materials processing and to develop the methodology to quantitatively analyze the heterogeneous nature observed in both materials and processing. It will be a big challenge to establish a systematic protocol to characterize the materials and maintain uniform quality during manufacturing. In this talk, I will show illustrative examples that prove the heterogeneous nature in different length scales, covering the length scale from nano, micro to macro. With many illustrative examples of both system and methodology, I will deliver my idea on the perspective and strategy of the researches, which will be a new paradigm of materials processing as well as of materials design.

DY 39.2 Wed 15:30 C 264

Slow dynamics in sheared DGEBA/SiO₂ suspensions — ●RICK DANNERT, ROLAND SANCTUARY, and JÖRG BALLER — University of Luxembourg, Laboratory for the Physics of Advanced Materials, Grand-Duchy of Luxembourg

Investigations of concentrated and semi-diluted colloidal suspensions of spherical silica nanoparticles in Diglycidyl Ether of Bisphenol A (DGEBA) with oscillatory shear rheology have recently shown an anomaly at low frequencies, which was interpreted as Brownian stress relaxation resulting from strain-induced perturbations of the isotropic filler distribution [1]. To complete the study of the concentration dependency we extend the rheological investigation of the low-frequency anomaly to ultra-diluted DGEBA/silica suspensions. We illustrate that the Brownian relaxation process depends in a complex manner on the volume concentration: the relaxation frequency exhibits a maximum at low filler contents. This non-monotonic dependency of the relaxation frequency can no longer be modelled by classical Peclet frequencies. Including a structural, concentration dependent parameter allows for an accurate description of the Brownian relaxation process for all concentrations.

[1] R. Dannert, R. Sanctuary, M. Thomassey, P. Elens, J.K. Krüger, J. Baller, *Rheologica Acta*, 53 (2014) 715-723.

DY 39.3 Wed 15:45 C 264

Microstructure and nonlinear signatures of yielding in a heterogeneous colloidal gel under large amplitude oscillatory shear — JUNTAE KIM¹, ●DIMITRI MERGER², MANFRED WILHELM², and MATTHEW E. HELGESON¹ — ¹Department of Chemical Engineering, University of California Santa Barbara, Santa Barbara, California 93106 — ²Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

We investigate yielding in a colloidal gel that forms from a nanoemulsion by polymer mediated aggregation. Combining large amplitude oscillatory shear measurements with simultaneous small and ultra-small angle neutron scattering (rheo-SANS/USANS), we characterize both the nonlinear mechanical processes and strain amplitude-dependent microstructure underlying yielding. We observe a broad, three-stage yielding process that evolves over an order of magnitude in strain amplitude between the onset of nonlinearity and flow. Analyzing the intracycle response stress reveals a transition from elastic straining to elastoplastic thinning which eventually leads to yielding and flow. The instantaneous nonlinear parameters associated with yielding are correlated with time-averaged rheo-USANS measurements. This shows how the material passes through a cascade of structural breakdown

from large to progressively smaller length scales. All significant structural changes occur on the micron-scale, suggesting that large-scale rearrangements of hundreds or thousands of particles, rather than the homogeneous rearrangement of particle-particle bonds, dominate the initial yielding of heterogeneous colloidal gels.

DY 39.4 Wed 16:00 C 264

Rheological behavior of a highly concentrated colloidal dispersion on different length scales — ●CLARA WEIS and NORBERT WILLENBACHER — Karlsruhe Institute for Technology (KIT), Karlsruhe, Germany

Multi particle tracking and bulk mechanical rheometry have been used to study rheological properties of concentrated, colloidal suspensions. Using fluorescent tracer particles with particle sizes between 100nm and 1000nm enables MPT even in turbid systems and provides rheological information on the microscale. Following systems have been investigated: 1. Fluid suspensions with short range repulsive interactions at $\Phi_{\text{eff}} < 0.5$, in this case perfect agreement between bulk and microrheology is found. 2. Hard sphere type crystallizing dispersions in the liquid/crystalline coexistence regime with and without added non-adsorbing polymer. A large variation in mean square displacement (MSD) of different tracer particles with slopes $\delta\text{MSD}/\delta\tau$ between 0 and 1 is found. The heterogeneity of the samples can be directly imaged based on this rheological contrast. The broadening of the coexistence region due to weak attractive depletion forces induced by added polymer is directly proven by MPT. 3. Variation of tracer particle mobility is investigated for systems approaching the colloidal glass transition. 4. The change of particle mobility and the variation of sample heterogeneity is analyzed in the so-called re-entry regime at $\Phi > \Phi_g = 0.58$ where the system transitions from glassy to fluid and from fluid to gel-like when attractive interaction controlled by non-adsorbing polymer increases from 0 to about 10 kT.

DY 39.5 Wed 16:15 C 264

Microstructural studies of colloidal glasses using forced probe particles — ●MARKUS GRUBER¹, GUSTAVO ABADE¹, ANTONIO PUERTAS², and MATTHIAS FUCHS¹ — ¹Universität Konstanz, Germany — ²Universidad de Almería, Spain

Driving a colloidal probe particle through a complex fluid provides unique insights into local viscoelastic properties. For soft solids there is a delocalization transition when the force on the probe particle is large enough to pull it free [1]. We study the spatial probability distribution of a tracer particle as seen by active microrheology in constant force mode. As model system, we consider a bath of hard spheres performing Brownian motion in the glassy state and an actively pulled hard sphere tracer particle. The spatial probability distribution is accessed within mode-coupling theory (MCT) refining the previous model [2] by decomposing the mobility-tensor kernel as suggested by [3] to obtain physical results for even larger forces.

Highly nonlinear effects for example in mean and mean square displacements are seen already below the critical force. One reason is the emergence of an exponential tail of the probability distribution in the direction of the applied force, which can also be found in molecular dynamic computer simulations (MDS). In addition we compare other MCT predictions with results from MDS.

[1] I. Gazuz, et al. *Phys. Rev. Lett.* 102 (2009) 248302.

[2] Ch. J. Harrer, et al. *Z. Phys. Chem.* 226 (2012) 779.

[3] S. Lang et al. *J. Stat. Mech.* P12007 (2013).

DY 39.6 Wed 16:30 C 264

Rheological properties of temporarily cross-linked microcapsules — ●SARAH DEMAND and HEINZ REHAGE — Chair of Physical Chemistry II, TU Dortmund, 44227 Dortmund, Germany

Microcapsules have a broad spectrum of different applications and can be used as simple model systems for understanding the mechanical properties and controlled release processes of biological cells, e. g. erythrocytes. Capsules consist of a tiny fluid droplet which is surrounded by an ultra-thin, flexible membrane. Temporary networks,

which simply emerge from self-organization processes of surfactants, are of special interest. These coherent films exhibit striking viscoelastic properties which are influenced by dynamic fluctuations and the average life-time of cross-linking points. A typical emulsifying compound, showing this special ambivalent behavior, is the polysaccharide surfactant Span 65. In order to measure the kinetics of crosslinking and the stability of Span 65-films, we performed different types of rheological investigations. The shear and dilatational behavior of microcapsules was obtained from deformation studies in external fields. Capsule deformations in centrifugal fields were studied in a spinning-drop tensiometer. The deformation and orientation behavior in simple shear flow was investigated by means of an optical rheoscope. The results of all the studies showed a high ability of temporarily cross-linked surfactant films to stabilize emulsion droplets. Due to their processes of self-organization, this provides new and interesting perspectives for simple and effective micro- and nano-capsule technologies.

DY 39.7 Wed 16:45 C 264

Clusters formation in microcirculation — OTHMANE AOUANE^{1,2,3}, MARINE THIEBAUD², CHAOUQI MISBAH², and CHRISTIAN WAGNER¹ — ¹Department of Experimental Physics, Saarland University, 66123 Saarbrücken, Germany — ²Université Grenoble Alpes, LIPHY, F-38000 Grenoble, France — ³LMPHE, URAC 12, Faculte des Sciences, Rabat, Morocco

We investigate numerically the flow of deformable objects such as vesicles and red blood cells (rbc) in micro-channels. We focus on understanding the phenomena behind the formation of small train of cells (called clusters) that occurs in the microcirculation. We consider the rbc in 2D as a closed deformable and non-permeable membrane encapsulating an inner fluid and suspended in an outer fluid. The membrane total force is composed from a bending force, a tension force to fulfill the area conservation constraint, and a cell-cell interaction force to reproduce the depletion forces due to the effect of the plasma macromolecules such as fibrinogen. The cells are placed in a confined geometry (two parallel walls) and subjected to a Poiseuille flow. The inner and outer fluids obey to Stokes equations. This equations are solved using the boundary integral formulation. We observe that two kind of clusters exist namely: i) hydrodynamical clusters, and ii) polymer induced clusters. We notice that there is an interplay between the confinement and the formation/destruction of hydrodynamical clusters. The polymer induced clusters are more robust and remain stable independently from the confinement.

15 min. break.

DY 39.8 Wed 17:15 C 264

Red blood cells in intimate contact — ACHIM GUCKENBERGER and STEPHAN GEKLE — Biofluid Simulation and Modeling, University of Bayreuth, Germany

Red blood cells in confined flow exhibit an effective hydrodynamic attraction: At low volume fractions, they tend to form pairs of cells (clusters). Understanding this effect is important for designing microfluidic devices. Furthermore, agglomeration of erythrocytes plays a major role in biological processes ranging from clotting to cardiovascular diseases. We study this phenomenon with the help of a three-dimensional periodic boundary integral method for various parameter sets. Amongst other things, the cell to cell distance is found to depend on the channel geometry and the flow rate. However, it is independent of the initial configuration of the cells.

DY 39.9 Wed 17:30 C 264

Flow of complex fluids into porous media — VIVIANE LUTZ BUENO¹, MARIANNE LIEBI², and PETER FISCHER¹ — ¹ETH, Zürich, Switzerland — ²Paul Scherrer Institute, Villigen, Switzerland

The dynamic behavior of complex fluids is studied by controlling flow-geometry-fluid interactions. Quantitative information on flow-induced structures (FIS) and in-situ rheological response are reported. Wormlike micelles (WLMs) flowing through porous media lead to a highly transient and localized rheological signature, composed by shear-banding and FIS due to micellar alignment, stretching, and breaking down. The porous media is simplified by a single contraction for initial studies on shear/extensional rates, microstructure organization, and velocity fields. Flow confinement provokes shear banding and viscoelastic instabilities, which dependent on channel's geometry. Micro-designed channels provide extreme fluid confinement and tailored flow-geometry, which are investigate by flow-induced birefringence, micro-

particle image velocimetry, and scanning small-angle x-ray/neutron scattering. High shear/extensional rates in the flow through an array of cylinders cause permanent fluid gelation. By decoupling extensional and shear contributions, some of the critical factors, which influence this FIS formation, are reported.

DY 39.10 Wed 17:45 C 264

A thermodynamic study of shear banding in polymeric solutions — NATALIE GERMANN — Technische Universität München, Freising, Deutschland

Shear banding is an ubiquitous phenomenon occurring in soft matter. The mechanisms behind this type of flow instability is not fully understood. It has been hypothesized (1) that the formation of localized shear bands in polymeric solutions is caused by the diffusion of the polymers. In the first part of this talk, we will introduce a new model for polymeric solutions. A new thermodynamically consistent two-fluid approach (2-3) was employed to account for Fiction diffusion and shear-induced migration effects. In this two-fluid approach, the differential velocity resulting from local variations in concentration and conformation is treated as a state variable. The additional boundary conditions arising from the spatial derivatives of the diffusion terms in the time evolution equations are now directly imposed with respect to that state variable. Hence, it is not anymore necessary to make assumptions about the polymeric microstructure on the boundaries. In the second part of this talk, we will discuss the transient behaviour of the model. The influence of the viscoelasticity of the polymers and the flow geometry on the shear band formation will be examined. The uniqueness of the numerical results and the conditions under which multiple banded states develop will also be elaborated. (1) M. Cromer, G.H. Fredrickson, and L.G. Leal, *Phys. Fluids*, 26, 063101, 2014. (2) N. Germann, L.P. Cook, and A.N. Beris. *JNNFM*, (207):21-31, 2014. (3) N. Germann, L.P. Cook, and A.N. Beris, in preparation.

DY 39.11 Wed 18:00 C 264

Evidence for simultaneous appearance of gradient and vorticity shear bands using time-resolved Rheo-SANS and laser light transmittance measurements — ANNEKATHRIN MÜTZE¹, PEGGY HEUNEMANN¹, LIONEL PORCAR², and PETER FISCHER¹ — ¹ETH Zürich, Schmelzbergstr. 9, 8092 Zürich, Switzerland — ²Institute Laue-Langevin, 6 rue Jules Horowitz, B.P.156, F-38042 Grenoble Cedex 9, France

The flow properties of wormlike micellar surfactant solutions play an important role in applications like drag reduction in turbulent flows, fracturing fluids, and encapsulation agents. Such systems are studied with respect to the applied shear stress, concentration, temperature and composition of the salt counter ions. A combination of rheological measurements, laser-light transmittance, video analysis, and rheo-small angle neutron scattering allow a detailed exploration of number and types of shear bands. Typical flow curves of the solutions show Newtonian, shear-thinning, and shear-thickening flow behavior. In the latter regime, the solutions show vorticity and gradient shear bands simultaneously, in which vorticity shear bands dominate the visual effect, while gradient shear bands always coexist and predominate the rheological response. We show that gradient shear bands change their phases (turbid, clear) with the same frequency as the shear rate oscillates, whereas in-time vorticity shear bands change their phases with half the frequency of the shear rate [1].

[1] A. Mütze, P. Heunemann, P. Fischer. *Journal of Rheology* 58(6): 1647

DY 39.12 Wed 18:15 C 264

Soft Solid Rheology Near the Gel Point — HORST HENNING WINTER — University of Massachusetts Amherst

For most amorphous materials that undergo gelation, the powerlaw relaxation time spectrum, $H(\tau) \sim \tau^{-n}$ for $\tau_{\min} < \tau < \tau_{\max}$, governs the rheology only in a narrow window very close to the gel point. Soon beyond the gel point, the soft solid develops a very rich viscoelastic behavior for the evolving material states with increasing connectivity. Typical rheological features of the evolving soft solid are a growing relaxation modulus and accelerated relaxation processes for the structural components that can still relax. Time-resolved rheology measurements, in combination with time-cure superposition, on two model materials show this soft solid behavior. One model material (self-exfoliating clay-polymer composite) represents physical gelation and the other one (crosslinking polyurethane) represents chemical gelation. The relaxation characteristics near the gel point are different for

the two materials. For the physically gelling material, the modulus growth was found to be inversely proportional to the relaxation time decay. For chemical gelation, the modulus grows only with a factor of

about 0.7. During the next couple of months, more gelling materials are going to be included in the study since it is unclear how widespread the observed viscoelastic pattern occurs.

DY 40: Physics of Sustainability and Human-Nature Interactions - Part I (joint session SOE/DY/ jDPG/ BP/ AKE)

Time: Wednesday 16:45–18:30

Location: MA 001

Topical Talk

DY 40.1 Wed 16:45 MA 001

The Industrial Society's natural Sustainability — ●HANS G. DANIELMEYER and THOMAS MARTINETZ — Institut für Neuro- und Bioinformatik, Uni Lübeck

Human nature and industrial engineering form a predictable macro-system with six S-functional variables and biologically stabilized parameters [1]. S-functions display storing lifetimes with time shifts like Sinus functions with phase shifts. Since 18th century UK the real GDP per capita increased 100-fold; only a factor of 2.7 yields for the G7 the biologic limit of 118 years for the life expectancy.

This is orders of magnitude below all earlier predictions. The industrial society will be materially sustainable. But the present financial system is unsustainable because saturating growth and interest rates dry out saving, life insurances, and pension funds. This caused the Great Depression and the crash of 2008, not neoclassical excuses [2]. The only cure is bringing finance in line with human biology: return to the sustainable income distribution between World War II and 1980; increase retirement age; continue innovation; and defend the G7 position globally. Believing in the Neoclassical Paradigm of exponential growth is already China's problem because it wastes resources with unsustainable investments.

[1] H. G. Danielmeyer and T. Martinetz, An exact theory of the industrial evolution and national recovery, www.inb.uni-luebeck.de, 2009 pdf. [2] C. Teuling and R. Baldwin, Secular Stagnation: Facts, Causes and Cures, CEPR London 2014, www.voxeu.org/sites/default/files/Vox_secular_stagnation.pdf

DY 40.2 Wed 17:15 MA 001

The decoupling of CO2 emissions and human development — KAI KORNUBER¹, DOMINIK REUSSER¹, ●LUIS COSTA¹, JÜRGEN KROPP^{1,2}, RYBSKI DIEGO¹, and SCHELLNHUBER JOACHIM^{1,3} — ¹Potsdam Institute for Climate Impact Research, Potsdam, Germany — ²University of Potsdam, Potsdam, Germany — ³Santa Fé Institute

Evidence of a decoupling between greenhouse gas emission and socioeconomic development would benefit international climate negotiations in two ways. First, it would communicate to emerging countries that socioeconomic progress is not strictly connected with ever-growing emissions. Secondly, it informs developed economies on reduction targets that do not jeopardize progress. Using the Environmental Kuznets Curve as background and country-panel data between 1990 and 2013, a model was established to test postulated relationships between socioeconomic progress (measured using the Human Development Index (HDI)) and CO2 emissions from fossil fuels. An inverted U-curve with a time-dependent maximum moving towards higher HDI and lower per capita CO2 mission was established as the relationship delivering the lower fitting error. Extrapolating the global decoupling trend until 2050 returns global cumulative emissions of CO2 that are incompatible with meaningful with long-term climate protection targets. Individual countries presented remarkable differences in their decoupling dynamics. Further insights and implications of the analysis will be discussed, as well as future research needs.

DY 40.3 Wed 17:30 MA 001

The size distribution, scaling properties and spatial organization of urban clusters: a global and regional perspective — ●TILL FLUSCHNIK, STEFFEN KRIEWALD, ANSELMO GARCÍA CANTÚ ROS, BIN ZHOU, DOMINIK REUSSER, JÜRGEN PETER KROPP, and DIEGO RYBSKI — Potsdam Institute for Climate Impact Research (PIK)

Human development has far-reaching impacts on the surface of the globe. The transformation of natural land cover occurs in different forms and urban growth is one of the most eminent transformative processes. We analyze global land cover data and extract cities as defined by maximally connected urban clusters. The analysis of the city size distribution for all cities on the globe confirms Zipf's law.

Moreover, by investigating the percolation properties of the clustering of urban areas we assess the closeness to criticality. We study the Zipf-exponents as a function of the closeness to percolation and find a systematic decrease with increasing scale, which could be the reason for deviating exponents reported in literature.

DY 40.4 Wed 17:45 MA 001

Limits and opportunities of a regionalized food production for cities: A global analysis — ●STEFFEN KRIEWALD, ANSELMO GARCÍA CANTÚ ROS, TILL STERZEL, PRAJAL PRADHAN, and JÜRGEN P. KROPP — Potsdam Institute for Climate Impact Research, Potsdam, Germany

The massive ongoing urbanisation in the 21st century is a major challenge for societies and therefore crucial developments towards a sustainable future will take place in cities. Together with many other issues a proper food supply is essential. Today, the necessary transport of food, especially the increasing transport by plane due to the global food supply chain, leads to a significant amount of greenhouse gas emissions. A reorganisation of cities in terms of their food allocation could save a considerable amount of emissions. We provide a global overview of the potential of peri-urban agriculture based on land-use, population, yield and dietary datasets. Our analysis indicates that up to 2 billion city dwellers can be fed by local grown products. However, Climate Change will drastically decrease the possibility of a local food supply for many regions.

DY 40.5 Wed 18:00 MA 001

Food demand and supply under global change: need for sustainable agricultural intensification — ●PRAJAL PRADHAN¹, DOMINIK REUSSER¹, MATTHIAS LÜDEKE¹, and JUERGEN KROPP^{1,2} — ¹Potsdam Institute for Climate Impact Research, Potsdam — ²University of Potsdam, Dept. of Geo- and Environmental Sciences, Potsdam

Global food demand is expected to increase by 60–110% between 2005 and 2050. Meeting growing food demand along with reducing agricultural environmental impacts is a global sustainability challenge. We investigated diet shifts, emissions, livestock feed, local food, and yield gaps to address this challenge. Globally, we identified sixteen dietary patterns. Diets common in developed world, exhibit higher emissions. Currently, 40% of global crops is fed to livestock. Two billions people are self-sufficient within 5' grid, while 1 billion Asians and Africans require inter-continental trade. However, they can become self-sufficient by closing yield gaps. By 2050, the global agricultural emissions will approach 7–20 Gt CO_{2eq}/yr and feed demand may increase up to 1.3 times. The number of trade dependent people will range 1.5–6 billion which may be further increased by 4–16% due to climate change. In future, diet shifts will significantly increase crop demand, emissions, and trade. These can be reduced by technological change, consuming local food, and closing yield gaps. Sustainability of inputs and management required to close yield gaps depends on how options are chosen and implemented. Hence, a combination of sustainable intensification, expansion, trade and diet shifts is required to feed growing population.

DY 40.6 Wed 18:15 MA 001

Sustainability for a Warming Planet — ●HUMBERTO LLAVADOR^{1,2}, JOHN ROEMER³, and JOAQUIM SILVESTRE⁴ — ¹Universitat Pompeu Fabra (Barcelona) — ²Barcelona GSE — ³Yale University — ⁴University of California, Davis

A clean biosphere is a resource in jeopardy due to man-made GHG emissions. What is the fair way to share this scarce global resource across present and future generations, and across regions of the world? This study proposes that the guiding ethics should be sustainability and egalitarianism. Sustainability is interpreted as a pattern of economic activity over time that sustains a given rate of growth of human

welfare indefinitely; in doing so, the atmospheric concentration of carbon must be capped at some level not much higher than exists today.

Human welfare depends not only upon consumption, but also upon education, knowledge, and a clean biosphere. The analysis shows that we should be investing more in education and substantially more in knowledge creation than is currently the case.

International cooperation is vital in capping global greenhouse gas emissions at a sufficiently low level. We propose that solving the bar-

gaining problem between developing and developed nations requires recognizing the relationship between economic growth and the climate problem. We propose that the dates at which developing countries converge in living standards to those of developed countries should not be altered by the agreement. This principle, along with sustainability, suffices to determine how emissions should be allocated across regions and time.

DY 41: Complex Fluids and Soft Matter - Part II (joint session DY/ CPP / BP)

Time: Thursday 9:30–11:45

Location: BH-N 334

Invited Talk

DY 41.1 Thu 9:30 BH-N 334

Ultrasoft particles under out-of-equilibrium conditions — ●GERHARD KAHL — Institut für Theoretische Physik, TU Wien, Vienna, Austria

On a coarse-grained level, colloids often interact via so-called ultrasoft potentials, which assume at short interparticle distances values in the order of a few $k_B T$; thus, these particles are able to overlap at the cost of a relatively small energy penalty. Under equilibrium conditions such ultrasoft particles are able to form aggregates (clusters) of overlapping particles which can then either form a disordered or an ordered cluster phase. In the latter case, these aggregates populate the positions of a regular fcc or bcc lattice. Cluster crystals display rather unconventional properties, such as a density-independent lattice constant [1]. Also under out-of-equilibrium conditions, ultrasoft systems show unexpected features. Exposing a cluster crystal to shear leads – with increasing shear rate $\dot{\gamma}$ – to the following novel response-scenario: for small $\dot{\gamma}$ -values the crystal melts; then gradually strings parallel to the flow direction form which are arranged in a hexagonal grid in the gradient-vorticity plane. Upon further increasing $\dot{\gamma}$ this lattice eventually melts [2]. Exposing a cluster crystal to Poiseuille flow the emergence of a quantized flow pattern is observed where the height and the width of the fluid stream display well-defined plateaus, indicating a successive fluidization of crystal layers adjacent to the channel walls [3].

[1] B.M. Mladek *et al.*, Phys. Rev. Lett. **96**, 045701 (2006).

[2] A. Nikoubashman *et al.*, Phys. Rev. Lett. **107**, 068302 (2011).

[3] A. Nikoubashman *et al.*, Soft Matter **8**, 4121 (2012).

DY 41.2 Thu 10:00 BH-N 334

Dynamics of density excitations in shear-driven, confined binary mixtures — ●SASCHA GERLOFF, TARLAN A. VEZIROV, and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Understanding friction on the microscopic scale is of great interest both from a fundamental and an applicational point of view. An important topic in this context is the appearance of density heterogeneities [1].

Here we perform overdamped Brownian dynamics simulations of a thin film of charged colloidal particles with two different sizes in planar shear flow. The particles interact via a combined Yukawa- and soft-sphere-potential. The parameters are set to suit experimental data for ludox silica particles, which were previously studied. The one-component system is known to form shear-induced multi-layer configurations in confinement and to show different intra-layer structures which depend on the applied shear rate. [2]

The corresponding two-component system under shear displays density excitations, provided that mixing of the two species is prohibited. We investigate the distribution and motion of these density excitations using voronoi tessellation. The density excitations are then identified as clusters of high local density in the spirit of the Hoshen-Kopelman algorithm.

[1] T. Bohlein, J. Mikhael and C. Bechinger, Nat. Mater. **11**, 126-130 (2012).

[2] T. A. Vezirov and S. H. L. Klapp, Phys. Rev. **88**, 052307 (2013).

DY 41.3 Thu 10:15 BH-N 334

Analytical solutions for immiscible two-phase-flow in porous media — ●CHRISTOPH WOLBER and RUDOLF HILFER — Institut für Computerphysik, Universität Stuttgart, Allmandring 3, 70569 Stuttgart

A macroscopic theory for two-phase-flow in porous media that distinguishes between percolating (free-flowing) and non-percolating

(trapped, disconnected) fluid parts has been studied. The theory naturally predicts hysteresis and spatiotemporal variations of residual and irreducible saturations. The computational advantage of the generalization over the traditional theory is the strict locality in time of all processes including hysteretic processes with simultaneous drainage and imbibition. Initial and boundary value problems on semi-infinite domains with constant total flux (generalized Buckley Leverett problems) have been solved semi-analytically with and without flow reversal. Complex combinations of shock fronts and rarefaction waves have been observed as the result.

DY 41.4 Thu 10:30 BH-N 334

Saturation overshoot and hysteresis for twophase flow in porous media — ●ROUVEN STEINLE and RUDOLF HILFER — Institute for Computational Physics, University of Stuttgart, Germany

Observations of non-monotone saturation profiles (saturation overshoot) during twophase infiltration processes have recently attracted much attention because such profiles are mathematically excluded within the Richards approximation to the traditional Darcy theory. Here it is shown that a traditional Darcy theory combined with a simple hysteresis model yields non-monotone saturation profiles in the Buckley-Leverett limit. Analytical arguments and numerical simulations are reported. They agree quantitatively in predicting saturation overshoot. A simple jump-type hysteresis in the relative permeabilities suffices to yield a saturation overshoot, while hysteresis in the capillary pressure is not needed [1]. Extensive numerical simulations of the mathematical model reveal a strong dependence of the overshoot phenomenon on the initial and boundary conditions.

[1] Hilfer, R. and Steinle, R., *Saturation overshoot and hysteresis for twophase flow in porous media*, Eur.Phys.J.ST, vol. 223, pp. 2323 (2014)

DY 41.5 Thu 10:45 BH-N 334

Free energy cost of forming a solid-liquid interface — ●RONALD BENJAMIN¹ and JÜRGEN HORBACH² — ¹Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität, 40225 Düsseldorf — ²Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität, 40225 Düsseldorf

Knowledge of the solid-liquid interfacial free energy is crucial to an understanding of nucleation, crystallization, and wetting phenomena. In this talk, we present a novel simulation technique to compute this quantity directly for an interface between a crystal and its melt [1]. Our approach solves an important problem arising out of hysteresis effects which led to uncontrolled errors in previous studies. We apply our method to different interaction potentials [1, 2] and do a careful finite-size scaling analysis in each case to obtain reliable estimates of the solid-liquid interfacial free energies.

Reference:-

1.) Crystal-liquid interfacial free energy via thermodynamic integration.-R. Benjamin and J. Horbach, J. Chem. Phys. **141**, 044715 (2014).

2.) Crystal-liquid interfacial free energy of hard spheres via a novel thermodynamic integration scheme.- R. Benjamin and J. Horbach, arXiv 1410.8798 (2014).

DY 41.6 Thu 11:00 BH-N 334

Transient microrheology of viscoelastic fluids — ●JUAN RUBEN GOMEZ SOLANO^{1,2} and CLEMENS BECHINGER^{1,2} — ¹2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

Viscoelasticity is ubiquitous in soft matter ranging from biological fluids to new synthesised materials, whose mechanical response deviate from Newtonian behavior under applied stress or strain. Microrheology has proved successfully in recent years as an alternative to bulk rheology in investigating linear and steady-state flow properties of microlitre samples of such materials. More complex transient behavior, e.g. creep and strain recovery after flow startup and cessation, is far less well understood within the context of microrheology. In this work we experimentally study the transient motion of a colloidal particle actively dragged by an optical trap through different viscoelastic fluids (wormlike micelles, polymer solutions, and entangled lambda-phage DNA). We observe that, after sudden removal of the moving trap, the particle recoils due to the relaxation of the deformed fluid microstructure until its complete strain recovery. We find that the relaxational dynamics of the particle proceeds via a double exponential decay, whose relaxation times remain independent of the initial particle velocity whereas their amplitudes strongly depend on it. We show that this transient information, which has no counterpart for colloids moving in Newtonian fluids, can be exploited to determine linear and non-linear flow properties of the embedding fluid.

DY 41.7 Thu 11:15 BH-N 334

Flow properties of anisotropic fluids — ●SEBASTIAN

HEIDENREICH¹, SABINE H. L. KLAPP², and MARKUS BÄR¹ — ¹Physikalisch Technische Bundesanstalt, Berlin, Germany — ²Technische Universität Berlin, Germany

From liquid crystal polymers to suspensions of bacteria anisotropic fluids are ubiquitous in nature and technology. The flow exhibits intriguing phenomena like flow alignment, shear banding, tumbling, shear thickening/thinning, large-scale correlation and mesoscale turbulence. The emergence of such fascinating aspects is often related to the anisotropy and to the out-of-equilibrium character of the considered system. In the first part of our presentation we review selected flow phenomena of passive fluids with anisotropy. We discuss the role of the order parameter like the alignment tensor for the description of the flow properties. In particular, we introduce the relaxation equation for the alignment tensor coupled to the hydrodynamic flow and discuss the orientational dynamics in the shear flow. In the second part of the talk we focus on active fluids like dense bacterial suspensions and we introduce the governing hydrodynamic equations for self-sustained individuals that are swimming in a Newtonian fluid. We discuss the relationship to the passive counterpart and finally present recent work on mesoscale bacterial turbulence.

15 min. break

DY 42: Delay and Feedback Dynamics

Time: Thursday 9:30–11:00

Location: BH-N 128

Invited Talk DY 42.1 Thu 9:30 BH-N 128
Time-delayed feedback control of self-organized structures in dissipative systems — ●SVETLANA GUREVICH¹, FELIX TABBERT¹, and ALEXANDER KRAFT² — ¹Institut für Theoretische Physik, Universität Münster, Wilhelm-Klemm-Str.9, D-48149, Münster, Germany — ²Institut für Theoretische Physik, Technische Universität Berlin Hardenbergstr. 36 D-10623 Berlin

We are interested in the dynamical properties of periodic and localized structures in the Swift-Hohenberg equation subjected to a delayed feedback. We shall show that variation in the delay time and the feedback strength leads to the emergence of complex spatio-temporal patterns. In addition we show that the presence of spatial inhomogeneities strongly influences dynamical behavior of the system, resulting in the formation of intricate oscillatory structures.

DY 42.2 Thu 10:00 BH-N 128

Dynamics of the self-coupled FitzHugh-Nagumo system in the limit of small delays — ●LARISSA BAUER^{1,2}, LIONEL WEICKER³, THOMAS ERNEUX³, and PHILIPP HÖVEL^{1,2} — ¹Technische Universität Berlin — ²Bernstein Center for Computational Neuroscience Berlin — ³Université Libre de Bruxelles

We consider delay-induced oscillations in a paradigmatic model of neural dynamics, FitzHugh-Nagumo system, which is subject to Pyragas-type self-coupling. The uncoupled model is operated in the excitable regime close to a Hopf bifurcation, where the system exhibits a stable fixed point. We compare an analytical derivation of the period with numerical simulations. For large delays, the self-coupling sets the timescale of the oscillations. For small delays or small coupling strengths, however, an activation time has to be taken into account.

DY 42.3 Thu 10:15 BH-N 128

Feedback control of flow vorticity at low Reynolds numbers — ●MARIA ZEITZ, JENNY TRIPTOW, PETER KALLE, and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Our goal is to explore feedback control strategies to stabilize novel dynamic flow patterns in microfluidic model systems. As a first example, we investigate a Newtonian fluid in a circular geometry realizable by a long rotating cylinder. The fluid vorticity satisfies a diffusion equation. We control fluid flow via the angular velocity of the circular boundary, which we determine from the mean vorticity in the sensing area using two control strategies: feedback with hysteretic switching or with time delay.

Hysteretic feedback control generates self-regulated stable oscillations in time the frequency of which can be adjusted over several orders of magnitude by tuning the feedback parameters.

Historically time-delayed feedback was developed in order to stabilize orbits in a chaotic system. Here, we show that it can be used as well to destabilize an inherently stable system such as vortex diffusion. For large values of feedback gain we find that vorticity diverges exponentially in time. Adjusting the parameters accurately, the vorticity oscillates with a stable amplitude. Large delay times promote oscillation pulses of vorticity, resulting in a complex time periodic pattern.

In a next step we apply these control strategies to more complex fluids. We present first results on the viscoelastic two-fluid system.

DY 42.4 Thu 10:30 BH-N 128

A fundamental dichotomy for dynamical systems with variable delay — ●ANDREAS OTTO, DAVID MÜLLER, and GÜNTER RADONS — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Dynamical systems with time-varying delays can describe various phenomena in many fields such as biology, chemistry, economy, engineering and physics. We identify two fundamentally different classes of variable delays. *Conservative* delays are related to quasiperiodicity and are equivalent to constant delays. On the other hand, *contractive* delays are characterized by mode-locking and cannot be converted to constant delays.

Time-varying delays are often generated by a common transport mechanism resulting in a conservative delay. However, typical models for time-varying delays often represent both, conservative and contractive delays, depending extremely sensitive on the delay parameters. In fact, starting from a conservative delay, we show that no continuous parameter change is possible without passing a contractive delay or equivalently modeling unphysical situations.

The type of the delay affects the dynamics of the associated time delay system. For conservative delays the asymptotic scaling of the Lyapunov spectrum is logarithmic, similar to the well-known behavior for constant delays. In contrast, for contractive delays the asymptotic scaling of the Lyapunov spectrum is linear. The presented results are independent of the specific form of the attractor of the time delay system as well as independent of the specific form of the variable delay.

DY 42.5 Thu 10:45 BH-N 128

Dynamical behaviors in time-delay systems with delayed feedback and digitized coupling — ●CHIRANJIT MITRA¹, G. AMBIKA², and SOUMITRO BANERJEE^{1,3} — ¹Indian Institute of Science Education and Research, Kolkata 741246, India — ²Indian Institute of Science Education and Research, Pune 411008, India — ³King Abdulaziz University, Jeddah, Saudi Arabia

We consider a network of delay dynamical systems connected in a ring via unidirectional positive feedback with constant delay in coupling. For the specific case of Mackey-Glass systems on the ring topology, we

capture the phenomena of amplitude death, isochronous synchronization and phase-flip bifurcation as the relevant parameters are tuned. Using linear stability analysis and Master Stability Function approach, we predict the region of amplitude death and synchronized states respectively in the parameter space and study the nature of transitions between the different states. For a large number of systems in the same

dynamical configuration, we observe splay states, mixed splay states and phase locked clusters. We extend the study to the case of digitized coupling and observe that these emergent states still persist. However, the sampling and quantization reduce the regions of amplitude death and induce phase-flip bifurcation.

DY 43: Energy Systems and Power Grid (joint session DY/ AK Energy /SOE)

Time: Thursday 9:30–12:45

Location: BH-N 243

DY 43.1 Thu 9:30 BH-N 243

Decentral Smart Grid Control — ●BENJAMIN SCHÄFER¹, MORITZ MATTHIAE¹, DIRK WITTHAUT^{1,3,4}, and MARC TIMME^{1,2} — ¹Network Dynamics, Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen — ²Institute for Nonlinear Dynamics, Faculty of Physics, University of Göttingen, 37077 Göttingen — ³Forschungszentrum Jülich, Institute for Energy and Climate Research (IEK-STE), 52428 Jülich — ⁴Institute for Theoretical Physics, University of Cologne, 50937 Köln

Stable operation of complex flow and transportation networks requires balanced supply and demand. For the operation of electric power grids - due to their increasing fraction of renewable energy sources - a pressing challenge is to fit the fluctuations in decentralized supply to the distributed and temporally varying demands. Common smart grid concepts suggest to collect consumer demand data, centrally evaluate them and send price information back to customers. Besides restrictions regarding cyber security, privacy protection and large required investments, it remains unclear how such central smart grid options guarantee overall stability.

Here we propose a Decentral Smart Grid Control, where the price is directly linked to the local grid frequency at each customer. The grid frequency provides all necessary information about the current power balance such that it is sufficient to match supply and demand without the need for a centralized IT infrastructure. We analyze the performance and the dynamical stability of the power grid with such a control system and determine its stability conditions.

DY 43.2 Thu 9:45 BH-N 243

Dynamical Models of Power Grids: Identifying and Curbing Weak Links — ●MARTIN ROHDEN and HILDEGARD MEYER-ORTMANN — Jacobs University Bremen, Campus Ring 8, 28759 Bremen

The inclusion of more and more renewable energy sources into modern power grids leads inevitably to drastic changes of the topology of power grids [1]. Nevertheless it is not known to date what an optimal network topology for power transport and robustness could be. Adding simply new transmission lines can induce long-ranged alterations on the power flow [2]. Here we use the recently introduced novel criteria of redundant capacities to identify weak links in power grids. We propose new strategies to cure these critical links and show their advantages over possible alternatives. Our results may serve as a step towards optimal network topologies in real-world power grids.

[1]: M. Rohden, A. Sorge, D. Witthaut and M. Timme, *Chaos* **24**, 013123 (2014)

[2]: D. Labavic, R. Suci, H. Meyer-Ortmann and S. Kettemann, *Eur. Phys. J. Special Topics (EPJ ST)*, **223**, pp 2517-2525 (2014)

DY 43.3 Thu 10:00 BH-N 243

The induced feedback of Demand-Side Management in the German power market and grid — ●SABINE AUER^{1,2}, JOBST HEITZIG¹, and JÜRGEN KURTHS^{1,2,3,4} — ¹Potsdam Institute for Climate Impact Research, D-14412 Potsdam, Germany — ²Department of Physics, Humboldt University Berlin, D-12489 Berlin, Germany — ³Institute for Complex Systems and Mathematical Biology, University of Aberdeen, AB24 3UE Aberdeen, UK — ⁴Department of Control Theory, Nizhny Novgorod State University, Gagarin Avenue 23, 606950 Nizhny Novgorod, Russia

The integration of Variable Renewable Energy (VRE) into the German power system becomes increasingly challenging with growing wind and solar power capacities. To prevent negative energy prices and to secure future energy supply, a debate about redesigning the German power market has aroused. Two competing solutions, a capacity market and an optimized spot market, are under consideration, so far [1]. Either

using demand as negative capacities or real-time market pricing will increase the price elasticity of demand and therefore, create a feedback loop between physical loads and power pricing [2].

In our research, we study these feedbacks in regard to power market and grid, especially in terms of stability [3]. Will these new concepts increase system stability by smoothing price evolution or rather provoke highly non-linear dynamics?

[1] BMWi. Ein Strommarkt für die Energiewende (2014). [2] M. Roozbehani et. al. (2012), *IEEE*, 27(4), 1926-1940. [3] P. Menck, J. Heitzig, N. Marwan J. & Kurths (2013). *Nature Physics*, 9(2), 89-92.

DY 43.4 Thu 10:15 BH-N 243

Flow tracing in renewable electricity networks — MIRKO SCHÄFER¹, ●BO TRANBERG², and MARTIN GREINER² — ¹Frankfurt Institute for Advanced Studies — ²Aarhus University

Renewable electricity networks are defined as power grids with a large penetration of fluctuating renewable power generation. Flow tracing algorithms track the renewable power as it flows from the generation nodes through the network to the consumption nodes. This allows for fair pricing schemes of future transmission investments. A new analytical expression is presented and applied to the pan-European transmission grid.

DY 43.5 Thu 10:30 BH-N 243

Large-deviation study of the maximum-disturbance stability of power grids — ●ALEXANDER K. HARTMANN¹, TIMO DEWENTER¹, WIEBKE HEINS², and BENJAMIN WERTHER² — ¹Institut of Physics, University of Oldenburg — ²Institut für Elektrische Energietechnik, Technical University of Clausthal

We study numerically the distribution of “maximum-disturbance” stability of power grids. The model is based on networks of oscillators. Here, we consider different ensembles of random networks, like standard Erdős-Renyi and two dimensional spacial networks. To access the distribution down to very small probabilities, we use specific large deviation techniques [1]. The stability is given by a conservative estimation of an asymptotic stability boundary, which is well known in stability theory [2,3]. The starting point is the matrix \mathbf{A} defined by $\mathbf{J}^T \mathbf{A} + \mathbf{A} \mathbf{J} = \mathbf{E}$, \mathbf{J} being the Jacobean Matrix. By calculating the maximum disturbance of \mathbf{x} , which results in the quadratic form $V = \mathbf{x}^T \mathbf{A} \mathbf{x} = \epsilon(\mathbf{x})$ not being a Lyapunov-function of the system any longer, the boundaries for the stability can be found.

For comparison, for the given networks also simple stability measures based on shortest paths [4], on the eigenvalues of the Jacobi matrix and on a linearized power-flow model [5] are obtained.

[1] A.K. Hartmann, *Eur. Phys. J. B* **84**, 627-634 (2011)

[2] R. Unbehauen, *Systemtheorie* (Vol. 2), Oldenbourg, Munich (1998)

[3] E.J. Davison and E.M. Kurak, *Automatica* **7**, 627-636 (1971)

[4] A.K. Hartmann, *Eur. Phys. J. B* **87**, 114 (2014)

[5] T. Dewenter and A.K. Hartmann, preprint arXiv:1411.5233 (2014)

DY 43.6 Thu 10:45 BH-N 243

Impact of network topology on decentral frequency-based smart grid control — ●CARSTEN GRABOW¹ and JÜRGEN KURTHS² — ¹Potsdam Institute for Climate Impact Research, Potsdam, Germany — ²Potsdam Institute for Climate Impact Research, Potsdam, Germany

Replacing conventional power sources by renewables in power grids poses a big challenge nowadays. In particular, a stable operation of the power grid requires new methods and ideas in aligning the arising fluctuations in decentralised supply to the temporally varying demands. In this context, a decentral Smart Grid Control has been proposed recently in order to directly link the price information to the local grid frequency. Principally, it has been shown that this approach leads to an efficient decentralized strategy for matching supply and demand in

a dynamically stable way. However, first results are restricted to simple small and regular networks. In our talk, we will extend the local and global stability analysis of the decentral Smart Grid Control to the collective dynamics of small network motifs, in particular, star-like networks and regular grid motifs. For larger networks, we numerically investigate decentralization scenarios finding additional phenomena that have to be considered to support power grids in exhibiting a stable state.

15 min. break

DY 43.7 Thu 11:15 BH-N 243

Detours around basin stability in power networks — ●PAUL SCHULTZ^{1,2}, JOBST HEITZIG¹, and JÜRGEN KURTHS^{1,2,3,4} — ¹Potsdam Institute for Climate Impact Research, D-14412 Potsdam, Germany — ²Department of Physics, Humboldt University Berlin, D-12489 Berlin, Germany — ³Institute for Complex Systems and Mathematical Biology, University of Aberdeen, AB24 3UE Aberdeen, UK — ⁴Department of Control Theory, Nizhny Novgorod State University, Gagarin Avenue 23, 606950 Nizhny Novgorod, Russia

To analyse the relationship between stability against (large) perturbations and topological properties of a power transmission grid, we employ a statistical analysis of a large ensemble of synthetic power grids, looking for significant statistical relationships between the single-node basin stability measure and classical as well as tailor-made weighted network characteristics. Especially, we propose a strategy to directly estimate a power grid's stability - even on short time scales - to omit the need of costly simulations. The focus lies on the identification of grid nodes that appear critical for stability, using for example a version of Newman's current flow betweenness. This method enables us to predict poor values of single-node basin stability for a large extent of the nodes, offering a node-wise stability estimation at low computational cost.

Further, we analyse the particular function of certain network motifs to promote or degrade the stability of the system. Here we uncover the impact of so-called detour motifs on the appearance of nodes with a poor stability score and discuss implications for power grid design.

DY 43.8 Thu 11:30 BH-N 243

Network Measures for Power Grid Stability in Practice — ●FRANK HELLMANN — Potsdam-Institut für Klimafolgenforschung, Potsdam, Deutschland

A key challenge for the emerging future grid infrastructure is the dynamical stability of the power grid in the presence of fluctuating power sources and changing topologies.

I show how tools based on novel as well as existing network topology measures can help with identifying vulnerable points in the power grid and can guide the design of the future grid in practice.

DY 43.9 Thu 11:45 BH-N 243

Predicting critical links in complex supply networks — ●XIAOZHU ZHANG¹, DIRK WITTHAUT^{1,2,3}, MARTIN ROHDEN^{1,4,5}, SARAH HALLERBERG¹, and MARC TIMME^{1,6} — ¹Network Dynamics, Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — ²Forschungszentrum Jülich, Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE), 52428 Jülich, Germany — ³Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany — ⁴IIIrd Institute of Physics, Faculty of Physics, Georg August University, 37077 Göttingen, Germany — ⁵School of Engineering and Science, Jacobs University, 28759 Bremen, Germany — ⁶Institute for Nonlinear Dynamics, Faculty of Physics, Georg August University, 37077 Göttingen, Germany

It has been observed that most large-scale outages in power grids can be traced back to single transmission line failures [1]. Yet, identifying which infrastructures in power grids and other supply networks are critical remains an open challenge, with severe consequences for network planning and stability. In this work we propose that the critical

links can be reliably predicted from the network structure and the normal operation state prior to edge failure. Numerical simulations of a variety of flow network models confirm that the topological edge redundancy as well as renormalized linear response theory provide general key indicators for network robustness.

[1] Pourbeik et al., Power and Energy Magazine, IEEE 4.5 (2006): 22-29.

DY 43.10 Thu 12:00 BH-N 243

Modelling the Dynamical Formation of Coalitions of Power Grid Operators to Reduce Needs for Backup Capacity — ●JOBST HEITZIG¹ and SARAH BECKER² — ¹Potsdam Institute for Climate Impact Research, Potsdam, Germany — ²Frankfurt Institute for Advanced Studies, Frankfurt, Germany

Power grid operators face an increasing need for backup capacity due to a raising amount of volatile renewable energy production. This need may be decreased by extending transmission capacities between several neighbouring grids and then pooling their backup capacities. Due to the physical properties of electricity transmission grids, extending a line between two grids may however also reduce the backup capacity needs of a third connected grid, and may do so even more than when the third grid's connection were extended as well. These physical effects generate complex and interesting strategic incentives for individual grid operators to join a backup capacity sharing coalition or not. In this talk, we'll use a model of dynamic coalition formation to show which grids may form coalitions in which order, using real-world example data.

DY 43.11 Thu 12:15 BH-N 243

Short-Time Stochastic Characterization of the Offshore Wind Profile — ●CHRISTIAN BEHNKEN, PEDRO LIND, MATTHIAS WÄCHTER, and JOACHIM PEINKE — ForWind, Institute of Physics, Carl-von-Ossietzky University, 26111 Oldenburg, Germany

Currently descriptions of vertical wind profiles are mostly performed by using standard logarithmic or power law approaches. Especially for short time scales ($1s \leq t \leq 10min$) the dynamics of the profile strongly influence the load situations and the energy conversion of wind turbines. Since these short-time dynamics are not considered when using the standard techniques, a more detailed approach is presented in this work. Firstly, PDFs of spatial and temporal velocity increments, estimated from offshore wind speed data, are fitted by using a superposition of Gaussian distributions with a varying standard deviation. It is shown that the empirical PDFs follow a heavy-tailed distribution which matches the proposed theoretical distribution. Furthermore, drift and diffusion coefficients for two-dimensional systems of Langevin equations are estimated directly from wind speed data to investigate dynamic coupling along the profile. This approach gives a first insight into the dynamics of wind profiles on short time scales.

DY 43.12 Thu 12:30 BH-N 243

Intermittency and Synchronization in Wind Farm — ●MEHRNAZ ANVARI and JOACHIM PEINKE — Institute of Physics and Forwind, Carl von Ossietzky University, 26111 Oldenburg, Germany

The renewable wind and solar sources and their share in electricity production have been increased constantly in recent years. These sources have new stochastic characteristics such as intermittency and non-Gaussian behavior, which may cause instability in power grids in very short-term time scales.

In this work, we focus on wind power that influenced by atmospheric turbulence. Hence frequent extreme fluctuations in power output of wind turbines are detectable. This intermittent behavior also, is present in cumulative power of the total wind field, even for a country-wide installation. To understand the origin of such extreme events, we consider the interactions between wind turbines and for this purpose, we evaluate the phase synchronization in wind farm. We conclude that, the existence of partial phase synchronization between turbines in specific time intervals can explain the origin of extreme events in this complex system. We found that higher synchronized wind turbines will produce higher intermittent power output.

DY 44: Pattern Formation

Time: Thursday 9:30–12:15

Location: BH-N 333

DY 44.1 Thu 9:30 BH-N 333

Feedback control and semi-laning in confined colloidal suspensions — ●TARLAN A. VEZIROV, SASCHA GERLOFF, and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Colloidal particles under the combined influence of an external driving force and restricted geometry exhibit a wealth of non-linear phenomena, which are relevant in diverse fields such as directed particle transport, sorting mechanisms and friction phenomena at the nanoscale. We perform Brownian Dynamic simulations of strongly confined systems of charged colloidal particles interacting via a combined soft-sphere and Yukawa potential. Under an external shear flow such systems display a sequence of states characterised by pinning, shear-induced melting and reentrant ordering into a moving hexagonal state [1]. Here we focus on the following situations: First, we consider a crystalline bilayer. By adding a feedback equation of motion we are able to stabilise specific properties such as the degree of hexagonal ordering or the shear stress. This opens the route for a deliberate control of friction properties of the system [2]. Second, we consider an open-loop controlled trilayer system. Besides the three states already observed in the bilayer system [1] we observe a novel state, which is characterized by the separation of the middle layer into two sublayers with opposite velocities. This is enabled by the formation of microlanes.

[1] T. A. Vezirov and S. H. L. Klapp, *Phys. Rev. E* **88**, 5 (2013).
[2] T. A. Vezirov, S. Gerloff and S. H. L. Klapp, *Soft Matter* DOI: 10.1039/c4sm01414f (2014).

DY 44.2 Thu 9:45 BH-N 333

Patterns driven by combined ac and dc electric fields in nematic liquid crystals — ●ALEXEI KREKHOV¹, WERNER PESCH², NANDOR EBER³, and AGNES BUKA³ — ¹Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — ²Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany — ³Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, H-1525 Budapest, Hungary

Electroconvection and flexoelectric patterns in a nematic liquid crystal layer driven by two superimposed ac and dc voltages, where each of them would separately trigger patterns of different spatio-temporal symmetry, are investigated. An extended model of the electrohydrodynamic instabilities was used to characterize the onset of pattern formation in the two-dimensional parameter space of the magnitudes of the ac and dc voltages. It is demonstrated that depending on the type of patterns and on the ac frequency, the combined action of ac and dc fields may either enhance or suppress the formation of spatially periodic patterns. The theoretical predictions are compared with representative experiments.

DY 44.3 Thu 10:00 BH-N 333

Turning Spirals into Fingers: The Impact of Advection on Pattern-Formation in Excitable Media — ●MUNIR SALMAN, PHILIPP BAUER, and KATHARINA KRISCHER — Physik Department, Nonequilibrium Chemical Physics, TU München, James-Franck-Str. 1, 85748 Garching, Germany

Inspired by experimentally observed solitary waves with non-curling open ends in an electrochemical flow cell, we present simulations in a two dimensional excitable reaction-diffusion-advection system. Depending on the advection strength, the tip of spiral waves can be pushed toward the flow outlet, leaving a uniform system, or driven against the advective flow, resulting in a finger-shaped wave fragment. Thus, the peculiar experimental traveling 'fingers' can be explained by the presence of advective flow in the experimental system.

DY 44.4 Thu 10:15 BH-N 333

Localized states in the conserved Swift-Hohenberg equation (aka the Phase Field Crystal equation) — ●UWE THIELE¹, ANDREW J. ARCHER², MARK J. ROBBINS², HECTOR GOMEZ³, and EDGAR KNOBLOCH⁴ — ¹Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Germany — ²Department of Mathematical Sciences, Loughborough University, Loughborough, UK — ³University of A Coruna, 15192 A Coruna, Spain — ⁴Department of Physics, University of California, Berkeley, CA, USA

We consider the structure of localised states for the phase field crys-

tal (PFC) model [aka conserved Swift-Hohenberg (cSH) equation with cubic nonlinearity] that may be obtained as a local approximation of a dynamical density functional theory (DDFT) for colloidal crystallisation [1].

We determine the location of steady spatially localized structures in the temperature vs. mean order parameter plane combining numerical continuation in 1d and direct numerical simulation in 2d and 3d. The results are related to the phenomenon of slanted snaking but take the form of standard homoclinic snaking when the mean order parameter is plotted as a function of the chemical potential [2].

[1] H. Emmerich et al., *Adv. Phys.* **61**, 665 (2012). [2] U. Thiele, A. J. Archer, M. J. Robbins, H. Gomez, and E. Knobloch, *Phys. Rev. E* **87**, 042915 (2013).

DY 44.5 Thu 10:30 BH-N 333

Unveiling the Bifurcation Diagram of Pattern Formation in Surfactant Monolayer Transfer — ●MICHAEL KÖPF¹ and UWE THIELE² — ¹Departement de Physique, Ecole Normale Supérieure Paris, France — ²Institut für Theoretische Physik, WWU Münster, Germany

Spontaneous pattern formation in deposition processes at receding contact lines has become a versatile tool to coat substrates with well controlled micro- and nanostructures. As a paradigmatic example, the coating of substrates with periodically structured monolayers has in recent years been investigated by theoreticians [1,2] and experimentalists [3,4] alike. Here, we present recent progress [5], allowing for the first time to understand the intricate bifurcation diagram of the system that exhibits a snaking branch of stationary solutions. Each nose of the snake is connected to a branch of time periodic solutions. Using numerical continuation, we detect various local and global bifurcations and investigate how the solution structure depends on the system size. These results are of wide interest for the theoretical description of pattern formation in systems with nontrivial boundary conditions.

[1] Köpf, Gurevich, Friedrich, Thiele, *New J. Phys.* **14** (2012) 02316
[2] Köpf, Gurevich, Friedrich, Chi, *Langmuir* **26** (2010) 10444-10447
[3] Li, Köpf, Gurevich, Friedrich, Chi, *Small* **8** (2012) 488-503
[4] Köpf, Harder, Reiche, Santer, *Langmuir* **27** (2011) 12354-12360
[5] Köpf, Thiele, *Nonlinearity* **27** (2014) 2711-2734

DY 44.6 Thu 10:45 BH-N 333

Faraday Waves as dynamical system under time asymmetric periodic excitation — ●THOMAS JOHN^{1,2}, DIRK PIETSCHMANN², RALF STANNARIUS², and CHRISTIAN WAGNER¹ — ¹Universität des Saarlandes, 66123 Saarbrücken — ²Otto-von-Guericke-Universität Magdeburg, 39016 Magdeburg

The Faraday wave experiment is a paradigm for parametric excitable systems, in particular by periodic accelerations. We investigated the onset of the pattern formation by periodic, however time asymmetric wave form shapes in excitation. In that case a new question arises: Does the threshold amplitude of the first instability changes - if the asymmetric periodic waveform is only reversed in time. Simple wave forms like sine or square waves are identical under time reversed transformation and can't lead to an influence of the stability of the system. We present our experimental and theoretical results for the Faraday system. The linear stability analysis derived from the Navier-Stokes equations will be discussed for arbitrary periodic wave forms. In addition, a simpler analytical example system with parametric, periodic and time asymmetric driving is presented. In this example: if the shape of the excitation is exclusively time reversed (amplitude is the same) then the stability changes from unstable to stable and vice versa. The reduced complexity in the example system presents the mathematical properties more clear. Nevertheless, the linear stability analysis of the Faraday wave experiment shows a perfect agreement with our experimental obtained results. D. Pietschmann, R. Stannarius, C. Wagner and T. John, *PRL* **110**, 094503 (2013).

15 min. break

DY 44.7 Thu 11:15 BH-N 333

On the self-assembly of magnetic cubes - infinite frustration bears a sevenfold magnetic clutch — ●INGO REHBERG — Experimentalphysik V, Uni Bayreuth

The self-assembly of magnetic particles into a simple cubic lattice [1] triggers questions like: - Why do they form cuboids, rather than chains or ribbons? - What is the overall magnetization of those clusters? - How susceptible are they to external magnetic fields? - What is the arrangement of the individual magnets within those clusters?

Answers are provided by experimental investigations [1] and calculations based on dipole-dipole interaction of magnetic particles [2]. The minimal arrangement consisting of eight dipoles arranged in the corners of a cube bears a continuum of dipoles arrangements as the ground state, suggesting a seven-fold magnetic clutch operating smoothly in the flat potential valley of this goldstone mode.

[1] S. Mehdizadeh Taheri, S. Rosenfeldt, M. Michaelis, M. Drechsler, B. Förster, P. Böseke, T. Friedrich, I. Rehberg, and S. Förster, in preparation.

[2] J. Schönke, T. Schneider, and I. Rehberg, in preparation.

DY 44.8 Thu 11:30 BH-N 333

The tongue as an excitable medium — ●GABRIEL SEIDEN^{1,2} and SOFIA CURLAND² — ¹Max Planck Institute for the Physics of Complex Systems, Dresden 01187 — ²Weizmann Institute of Science, Rehovot 76100, Israel

Geographic tongue (GT) is a medical condition affecting approximately 2% of the population, whereby the papillae covering the upper part of the tongue are lost due to a slowly expanding inflammation. The resultant dynamical appearance of the tongue has striking similarities with well known out-of-equilibrium phenomena observed in excitable media, such as forest fires, cardiac dynamics and chemically driven reaction-diffusion systems. We explore the dynamics associated with GT from a dynamical systems perspective, utilizing cellular automata simulations. Our results shed light on the evolution of the inflammation and suggest a practical way to classify the severity of the condition, based on the characteristic patterns observed in GT patients.

DY 44.9 Thu 11:45 BH-N 333

Homoclinic snaking near the surface instability of a polarizable fluid — ●DAVID J.B. LLOYD¹, CHRISTIAN GOLLWITZER², INGO REHBERG², and REINHARD RICHTER² — ¹Department of Mathemat-

ics, Univ. of Surrey, Guildford, GU2 7XH, UK — ²Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany

We report on localized patches of cellular hexagons observed on the surface of a magnetic fluid in a vertical magnetic field. These patches are spontaneously generated by jumping into the neighborhood of the unstable branch of the domain covering hexagons of the Rosensweig instability. They are found to co-exist in intervals around this branch. We derive a general energy functional for the system and a corresponding Hamiltonian that provides a pattern selection principle allowing us to compute Maxwell points for general magnetic permeabilities. Using numerical continuation techniques we investigate the existence of localized hexagons in the Young-Laplace equation coupled to the Maxwell equations. We find cellular hexagons possess a Maxwell point where the energy of a single hexagon is equal to the energy of the flat state providing an energetic explanation for the multitude of measured hexagon patches. Furthermore, it is found that planar hexagon fronts and hexagon patches undergo homoclinic snaking corroborating the experimentally detected intervals.

DY 44.10 Thu 12:00 BH-N 333

Rupture dynamics of liquid crystal bubbles — ●TORSTEN TRITTEL and RALF STANNARIUS — Otto-von-Guericke Universität, Magdeburg, Germany

Several organic liquid materials are able to form stable free standing films. A famous example is the formation of soap bubbles. They are more or less stable objects, until the film is sufficiently disturbed, e.g. when it is punctured. Then, the whole structure becomes unstable and the bubble bursts. We investigate the rupture dynamics of bubbles made from different thermotropic liquid crystal materials by means of high speed imaging. In contrast to soap films, our smectic films have a complete different inherent structure. This structure allows to generate homogeneous films with very low thickness. Furthermore liquid crystal films are stable for days, without drainage or evaporation. In our study, we puncture liquid crystal bubbles with film thicknesses of between 10nm and 300 nm and diameters of about 15 mm. We focus on rupture velocities and the destabilization of the retracting rim into filaments.

DY 45: Focus: Disordered Systems, Glasses under Shear I (joint session CPP/ DY)

Time: Thursday 9:30–13:00

Location: C 243

Invited Talk

DY 45.1 Thu 9:30 C 243

Flow instabilities in soft glassy materials — ●SUZANNE FIELDING — Department of Physics, Durham University, UK

Many soft materials, including dense emulsions, microgel suspensions, star polymers, onion surfactants, and textured morphologies of liquid crystals, share underlying glassy features of structural disorder and metastability. These give rise to several notable features in the low frequency rheology of these materials: for example, the existence of a yield stress below which the material behaves like a solid, and above which it flows like a liquid. Experiments have also revealed that these materials often display a phenomenon known as shear banding, in which the flow profile across the shear cell exhibits macroscopic bands of different viscosity. Two distinct classes of yield stress fluid have been identified: those in which the shear bands apparently persist permanently (for as long as the flow is applied), and those in which banding arises only transiently during a process in which a steady flowing state is established out of an initial rest state (eg in shear startup or step stress). After surveying this motivating experimental data, we describe recent progress in addressing it theoretically, using the soft glassy rheology model and a simple fluidity model. Time permitting we shall also discuss failure modes of these "soft glassy materials" in free-surface extensional flows.

DY 45.2 Thu 10:00 C 243

Shear cessation in a Brownian-dynamics simulation for 2D hard disks — ●SEBASTIAN FRITSCHI and MATTHIAS FUCHS — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

We present results from a Brownian-dynamics computer simulation for the nonequilibrium transient dynamics in a colloidal glass former after the cessation of shear flow. In the glass, persistent residual stresses are found that depend on the flow history. The partial decay of stresses from the steady state to this residual stress is governed by the pre-

vious shear rate. Using a glassy hard-disk system, we also link this macroscale dynamics to microscopic particle motion, monitoring the transient mean-squared displacement measured during the relaxation from the steady state. A flow-induced second plateau is found in the mean-squared displacement at long times.

DY 45.3 Thu 10:15 C 243

Microrheology of a Two-Dimensional Driven Granular System — ●PEIDONG YU, BORIS EBERHARDT, SEBASTIAN PITIKARIS, and MATTHIAS SPERL — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Köln, Deutschland

We study the motion of a tracer particle pulled inside a two-dimensional granular model system, where particle movements can be controlled and precisely tracked. We put such a system on a shaking table and apply vertical agitation as thermalization. We show how well the particles are thermalized in the horizontal direction. We then drag a tracer particle through such a system with constant force or constant velocity. Effective viscosities with different parameters are measured. Different scenarios of shear thinning and shear thickening are observed. The underlying physics is discussed and compared with simulations and theories.

DY 45.4 Thu 10:30 C 243

Potential energy landscape analysis of sheared glass-forming systems — ●MARKUS BLANK-BURIAN and ANDREAS HEUER — Institut für Physikalische Chemie, WWU Münster, Deutschland

We performed molecular dynamics simulations of small binary Lennard-Jones mixtures ($65 \leq N \leq 1040$) under constant shear rates and at a very low temperature ($T = 0.01$). The shearing is achieved by applying Lees-Edwards periodic boundary conditions to the system.

In previous work on unsheared systems it was shown, that most of the physical properties of macroscopic systems are already encoded

in these small systems. The dynamics of these small systems can be described by a continuous time random walk (CTRW) between minima of the potential energy landscape (PEL). Our focus now lies on comparing these results with the constantly sheared system.

For the analysis of the sheared system, we perform energy minimization using the strain as an additional variable. We then use this information to identify inherent structures (IS) from the trajectories. These IS turn out to have zero strain. Thus, they are comparable to the unshaded system. From the resulting statistical data we hope to gain a microscopic understanding of macrorheological phenomena like the initial stress overshoot as well as the shear thinning in the plastic flow regime.

Invited Talk

DY 45.5 Thu 10:45 C 243

Dense granular flow — ●ANNETTE ZIPPELIUS — Institut für Theo. Physik, Univ. Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

In the first part of the talk I will discuss a jamming scenario of frictional particles, which can be interpreted as a nonequilibrium first order phase transition (1). Results of numerical simulations will be presented and analyzed in the framework of a simple model which can account for both, the continuous frictionless case and the discontinuous frictional case. The most important features of the frictional phase diagram are reentrant behaviour and a critical jamming point at finite stress.

The second topic to be discussed are dynamical heterogeneities and scaling in a driven granular fluid as structural arrest is approached (2). Large scale simulations of 2d bidisperse granular fluids allow us to determine spatial correlations of slow particles via the four-point structure factor. As the fluid approaches structural arrest, scaling is shown to hold. Both the dynamic susceptibility as well as the dynamic correlation, evaluated at the alpha-relaxation time, can be fitted to a power law divergence at a critical packing fraction. The measured susceptibility widely exceeds the largest one previously observed for hard sphere 3d fluids. The clusters of slow particles are neither compact nor stringlike but fractal. The cluster size distribution is shown to fall off algebraically as structural arrest is approached.

(1) M. Grob, C. Heussinger and A. Zippelius, Phys. Rev E 89, 050201 (R) (2014); (2) K. Avila, H. C. Castell, A. Fiege, K. Vollmayr-Lee and A. Zippelius, Phys. Rev. Lett. 113, 025701 (2014)

15 min. break

DY 45.6 Thu 11:30 C 243

Transient Rheology of Colloidal Suspensions - Shear Reversal — ●MIRIAM SIEBENBÜRGER¹, FABIAN FRAHSA², and MATTHIAS FUCHS² — ¹Helmholtz Zentrum Berlin, Germany — ²Universität Konstanz, Germany

At low deformations, colloidal glasses exhibit first a linear deformation, followed by a stress overshoot and the sheared steady state [1]. In this transition range from solid to fluid the reversal of the shear deformation can spend insights in the dynamics of the underlying structural transformations. Experimental investigations are performed by model suspension of thermo-sensitive colloids, consisting of a poly(styrene) core and a poly(N-isopropylacrylamide) shell. By a set of shear reversal experiments the aging effect often observed in experimental systems can be discussed separately from the structural transformations due to the shear. The height and the position of the minimum of the under-shoots in the reversed shear flow is correlated with the deformation at the start of the shear reversal. All results for different shear rates and waiting times will be compared to the Mode Coupling Theory (MCT) and simulations, which show good agreement compared to the experimental results [2].

[1] C. P. Amann, F. Weysser, M. Fuchs, M. Siebenbürger, M. Krüger and M. Ballauff, J. Rheol. 57,149 (2012).

[2] F. Frahsa, A. Bhattacharjee, J. Horbach, M. Fuchs and T. Voigtmann, J. Chem. Phys. 138, 12A513 (2013).

DY 45.7 Thu 11:45 C 243

Lattice Boltzmann Simulations of Glass Forming Liquids — ●SIMON PAPPENKORT¹ and THOMAS VOIGTMANN^{1,2} — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln — ²Heinrich-Heine-Universität Düsseldorf

The rheology of complex fluids undergoing a glass transition, such as colloidal suspensions or granular media, is highly nonlinear. The interplay between slow structural dynamics on the microscopic scale and a mesoscopic flow field gives rise to non-Newtonian flow effects. Promi-

nent examples are shear thinning, dynamic yield and residual stresses. In a confined flow geometry, the shear rates, and thereby the fluid properties, can vary considerably in space and time. Even long after the flow has stopped, the material properties are profoundly affected by residual stresses.

Starting from first principles, mode coupling theory of the glass transition is able to provide constitutive equations that describe the history effects determining the flow of glass-forming fluids. The Lattice Boltzmann method is a modern simulation scheme to solve the Navier-Stokes equations even for complex flow geometries. We introduce a new, modified LB model [1] which is able to include memory-integral effects in fluid-mechanics simulations and provides a link between both regimes.

We find the viscoelastic transient dynamics and the appearance of residual stresses after stopping the flow to depend sensitively on the chosen flow geometry.

[1] J. Chem. Phys. 140, 164507 (2014)

DY 45.8 Thu 12:00 C 243

Shear bands at the Jamming Transition: The role of Weak Attractive Interactions — ●EHSAN IRANI¹, PINAKI CHAUDHURI², and CLAUS HEUSSINGER¹ — ¹Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — ²Institute of Mathematical Sciences, Tamil Nadu, India

We study the rheology of a particulate system close to Jamming in the presence of weakly attractive interactions. Lees-Edwards boundary conditions are used to simulate a shear-controlled flow. In addition to Bagnold scaling at large shear rates, the attraction results in a finite yield stress in the limit of small shear rates. In the yield regime a fragile solid is formed and the rheology can be explained by a scaling argument that exploits the vicinity to the isostatic state. In the transition region the shear stress develops a minimum, which (in large enough systems) leads to the formation of persistent shear bands. These features are rationalized by a scenario that involves the competition between attraction-induced structure formation and its break-down because of shearing. Properties of shear bands are studied in order to reveal the physical mechanisms that underly the non-monotonic flow curve and the flow heterogeneities in the transition region. This work may help to elucidate the origin of shear bands in different materials with finite and short-ranged attractive forces.

DY 45.9 Thu 12:15 C 243

Influence of drops on particles under shear — ●LAURENT GILSON, JENNIFER WENZL, and GÜNTER AUERNHAMMER — Max Planck Institute for Polymer Research, Physics at Interfaces, Mainz

We will present shear zone formation in granulates with and without the influence of liquid droplets. 3D Laser Scanning Confocal Microscopy (LSCM) was used to image polydisperse spherical silica particles (7 μ m) during quasi-steady strain controlled shear experiments. A shear cell was formed using a fixed bottom plate and a nanoindenter tip [1]. This arrangement creates a strain-controlled shear cell without lateral walls. Samples consisted of polydisperse spherical silica particles suspended in an index matching liquid. Immiscible droplets were used as a second phase. Position and form of the droplets, as well as position and size of the particles were recorded simultaneously using a dual channel LSCM [1,2,3]. Multiple images were taken during shear. A complete record of individual particle and droplet movement during shear was extracted.

We will focus our presentation on the differences between particles attached to droplets and particles in bulk. We will discuss differences and common features, as well as compare the results to features commonly found in sheared granular matter.

[1] Wenzl, J., Seto, R., Roth, M., Butt, H.-J., Auernhammer, G., Granul. Matter, 15, 391-400 (2012). [2] Crocker, J.C., Grier, D.G, J. Colloid Interface Sci. 179(1), 298-310 (1996). [3] Roth, M., Schilde, C., Lellig, P., Kwade, A., Auernhammer, G., Eur. Phys. J. E, 35(11), 124 (2012)

DY 45.10 Thu 12:30 C 243

Shear bands in a model glass former — ●GAURAV PRAKASH SHRIVASTAV¹, PINAKI CHAUDHURI², and JÜRGEN HORBACH¹ — ¹Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Germany — ²The Institute of Mathematical Sciences, Chennai, India

We study the mechanical response of a binary Lennard-Jones mixture by shearing it below the glass transition temperature with a constant strain rate. The onset of flow is associated with an inhomogeneous flow pattern [1,2]. Highly mobile regions form a long-lived shear-band-

like structure. Although the flow curve is monotonic and stress-strain response does not show any signature of a shear band, this heterogeneity is captured very well in the mean square displacement of particles. The width of the shear band grows diffusively with time. We find that shear bands are more pronounced in the cuboid boxes than in the cubic boxes. This can be explained by the quadrupolar structure of the local strain fields. To investigate the origin of shear bands we identify the local events that lead to their formation. We observe that these initial active spots are localized to one or two particles.

[1] P. Chaudhuri, J. Horbach, Phys. Rev. E **88**, 040301(R) (2013).

[2] P. Chaudhuri, J. Horbach, Phys. Rev. E **90**, 040301(R) (2014).

DY 45.11 Thu 12:45 C 243

Creep deformation of glasses under shear stress, results from a schematic mode-coupling model — ●FABIAN FRAHSA and MATTHIAS FUCHS — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The viscoelasticity of dense colloidal dispersions causes creep deformation under constant stress. Creep provides insight in the slow structural dynamics and dissipative processes of glasses.

We present predictions for the stress-driven rheology of glass from a schematic model of the mode-coupling theory (MCT) and compare them with experiments of core-shell micro gels. The schematic model is motivated by the microscopic ITT-MCT approach to the stress response of flow-driven systems and covers incompressible and homogeneous flows neglecting hydrodynamic interactions.

DY 46: Flow-Induced Structures in Complex Fluids - Part II (joint session CPP/ DRG, Deutsche Rheologische Gesellschaft/ DY)

Time: Thursday 9:30–12:00

Location: C 264

DY 46.1 Thu 9:30 C 264

Rheology of PMMA solutions - the role of maximum stretch ratio in the nonlinear regime — ●SARA L. WINGSTRAND¹, QIAN HUAN¹, NICOLAS J. ALVARES², and OLE HASSAGER¹ — ¹Technical University of Denmark, Kgs Lyngby, Denmark — ²Drexel University, Philadelphia, USA

This work concerns linear and nonlinear rheology of poly(methyl methacrylate) (PMMA) solutions. Oligomeric methyl methacrylate is used as solvent. The concentration of polymer in solution has been adjusted, such that the maximum stretch ratio (λ_{max}) is equal to that of a polystyrene melt of 285 kg/mol (PS-285k). Accordingly, the molar mass of PMMA has been selected to obtain the same number of entanglements (Z) as the PS-285k. The solutions are characterized both in small amplitude oscillatory shear and in uniaxial extension, where the influence of λ_{max} and Z is investigated. It is found that the linear behavior of the PMMA solutions obey the tube model with a dilution exponent of 1. Consequently, as intended, the normalized dynamic moduli of the solutions overlap those of PS-285k. In the nonlinear regime the PMMA solutions exhibit a greater resemblance with PS-285k, than other polymers having same Z but significantly different values of λ_{max} . Nevertheless, the observed trend in extensional steady state viscosity vs. strain rate differs. Consequently we conclude that introducing λ_{max} in the tube model to enable application in the nonlinear regime, is not sufficient for obtaining a unifying model valid for polymer melts and solutions together.

DY 46.2 Thu 9:45 C 264

Linear and Nonlinear Rheological Behavior of Carboxymethyl Hydroxypropyl Guar Gum — ●DANIEL SZOPINSKI¹, ULRICH A. HANDGE², WERNER-MICHAEL KULICKE¹, VOLKER ABETZ^{2,3}, and GERRIT A. LUISTRA¹ — ¹Institute of Technical and Macromolecular Chemistry, University of Hamburg, Hamburg, Germany — ²Institute of Polymer Research, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ³Institute of Physical Chemistry, University of Hamburg, Hamburg, Germany

Guar gum is a natural non-ionic polysaccharide from the endosperm of the guar bean (*Cyamopsis tetragonoloba*), which primarily grows in India and Pakistan. The water-thickening property is the main driver for its industrial application, which is resulting from the high molecular weight (1000-2000 kg/mol) and the formation of superstructures. Guar gum may be chemically modified with carboxymethyl (CM) and/or hydroxypropyl (HP) entities to enhance the thermal stability and solubility in water. A comprehensive rheological characterization of carboxymethyl hydroxypropyl guar gum (CMHPG) will be presented. Material functions were determined in experiments under steady state shear flow, small amplitude oscillatory shear flow (SAOS) and extensional flow (CaBER). The flow behavior at the application relevant nonlinear viscoelastic region was mapped in large amplitude oscillatory shear (LAOS) experiments. Structure-property relationships were established for dilute and more concentrated solutions as function of concentration and molecular weight. It is a basis for a description of the superstructures that guar gum and its derivatives form in water.

DY 46.3 Thu 10:00 C 264

Relation between rheological and GPC triple detection characterization of photo-oxidated LDPE — ●VÍCTOR HUGO ROLÓN-GARRIDO, MATTHIAS KRUSE, and MANFRED H. WAGNER — Chair of Polymer Engineering/Polymer Physics Berlin Institute of Technology (TU Berlin), Fasanenstr. 90, D-10623, Berlin

Sheets of low-density polyethylene (LDPE) were subjected to photo-oxidation in the presence of air using a xenon lamp to irradiate the samples for times between 1 day and 6 weeks. The formation of long-chain branching up to 1 week of degradation and the competition between chain scission and crosslinking at longer periods of radiation were investigated by rheological characterization, Fourier transform infrared spectroscopy, and the solvent extraction method (Rolón-Garrido and Wagner. Polym Degrad Stabil 2014, 99:136, Rolón-Garrido and Wagner. J Rheol 2014, 58:199). The same samples are studied here by size exclusion chromatographic characterization using triple detection (concentration, light scattering and viscosity). The results are correlated with the model parameters (beta and f_{2max}) of the MSF model. It is confirmed that the parameter beta correlates with the gel content, while f_{2max} is found to correlate with the experimentally determined contraction factors. By comparing the data of this study with those obtained earlier for polystyrene comb melts with well defined structure, the influence of the branching frequency on f_{2max} becomes evident.

DY 46.4 Thu 10:15 C 264

Relaxation Mechanism and Molecular Structure Study of Polymer Blends by Rheological and SANS experiments — ●LUDOVICA HENGELLER¹, QIAN HUANG¹, NICOLAS J. ALVAREZ², ANDRIY DOROKHIN¹, JACOB KIRKENS GAARD³, KRISTOFFER ALMDAL¹, KELL MORTENSEN³, and OLE HASSAGER¹ — ¹Technical University of Denmark, Kgs. Lyngby, Denmark — ²Drexel University, Philadelphia, USA — ³Copenhagen University

Industrial polymers are largely polydisperse systems. One step towards understanding polydisperse polymers is the characterization of bi-disperse blends. Even though linear viscoelastic properties of bi-disperse polystyrene blends have been investigated thoroughly both theoretically and experimentally in recent years, both nonlinear shear and extensional flow properties are lacking. The purpose of the present study is to investigate the nature of interactions, namely polymer-polymer, in strong elongational flow using a bi-disperse polystyrene blend of 95 K and 545 K Mw with 50% weight ratio. We present both uniaxial extension and stress relaxation experiments to determine if orientation and extension of long PS chains induce orientation and extension in shorter chains. The extensional viscosity of systems investigated, provides only indirect evidence about the extent to which the molecules have been unraveled and stretched by the flow field. More directed information is obtained by neutron scattering on quenched liquid bridges of polystyrene. The results of such experiments will be discussed.

DY 46.5 Thu 10:30 C 264

Flow-induced crystallisation of polylactides — ●DIETMAR AUHL, NILS LEONE, YOGESH DESHMUKH, and SANJAY RASTOGI — Maastricht University, Maastricht, The Netherlands

Polylactides (PLA) obey like many biopolymers a relatively poor crystallisation behaviour and are therefore difficult to process. In addition,

tion, PLA grades may vary in D,L-enantiomer distribution and form a stereocomplex, which significantly affects the crystallisation as well as final properties or product performance. Therefore, various routes are employed to control and improve the formation of crystal domains further to optimisation of processing conditions, e.g. chain modifications, addition of plasticisers or nucleating agents [1]. In this study, the crystallisation behaviour and morphology of such different PLA grades has been investigated in detail by rheo-microscopy with polarised light imaging as well as rheo-scattering for a broad range of thermo-mechanical histories and superposed to calorimetric data from thermal analysis. The comparison of experiments and molecular theory both highlight the flow-induced effects on polymer chains of initially equilibrated Gaussian conformation that enhance the crystallisation process, for which the total deformation and rate in relation to the time scales of molecular motions are decisive. [1] Saeidlou, S.; Huneault, M. A.; Li, H.; Park, C. B. *Prog. Polym. Sci.* (2012) 1657.

15 min. break

DY 46.6 Thu 11:00 C 264

Rheological and SEC characterization of long-chain branched poly(ethylene terephthalate) — ●MATTHIAS KRUSE, VÍCTOR HUGO ROLÓN GARRIDO, and MANFRED H. WAGNER — Chair of Polymer Engineering/Polymer Physics, Berlin Institute of Technology (Berlin), Fasanenstrasse 90, D-10623 Berlin, Germany

Reactive processing is an effective and economic method to produce customized polymers fulfilling improved or additional properties. We report on reactive extrusion of poly(ethylene terephthalate) (PET) and demonstrate that linear PET can be converted into long-chain branched (LCB) PET via chain extension thereby broadening the range of possible applications. An anhydride and an epoxy based chain extender were employed, which react with the functional end groups of linear PET. Different concentrations of the two tetrafunctional coupling reagents were used to achieve different degrees of branching and to compensate for the degradation of the polymer during extrusion. The formation of LCB was proven by dynamic plate-plate rheometry and leads to a more pronounced shear thinning behavior and an increase in the complex viscosity. The increase of molecular weight and polydispersity are also confirmed by size exclusion chromatography using triple detection (concentration, light scattering and viscosity). The elongational viscosity measurements conducted with a SER device show an unexpected influence of the chain extender on the type of sample rupture at larger extensions, and give clear evidence of different levels of strain hardening with respect to the chain extender content, as quantified by the molecular stress function (MSF) model.

DY 46.7 Thu 11:15 C 264

Foaming of polystyrene-block-poly(4-vinyl pyridine) diblock copolymers: Thermal, rheological and processing properties — MARIA SCHULZE¹, ●ULRICH ALEXANDER HANDGE¹, JELENA LILLEPÄRG¹, SOFIA RANGOU¹, and VOLKER ABETZ^{1,2} — ¹Institute of Polymer Research, Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, 21502 Geesthacht, Germany — ²Institute of Physical Chemistry, University of Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Because of the high demand of polymer foams for application in the fields of lightweight construction, membrane technology, thermal and acoustic isolation the characterization of thermal and rheological properties of polymers for foam extrusion processes is of high relevance. In this study, we discuss the thermal and rheological properties of

polystyrene-b-poly(4-vinyl pyridine) diblock copolymers and processing of these diblock copolymers via batch foaming. Carbon dioxide is used as blowing agent. High pressure differential calorimetry measurements reveal that the solution of carbon dioxide in these diblock copolymers leads to a decrease of the glass transition temperature of the polystyrene and the poly(4-vinyl pyridine) blocks. Furthermore rheological experiments in the oscillatory mode were carried out in order to elucidate the influence of composition and molecular weight on the flow properties. Stress-growth experiments reveal that the steady-state viscosity is characterized by a pronounced structure viscous behavior. Batch foaming experiments show that a larger molecular weight yields a lower foam density.

DY 46.8 Thu 11:30 C 264

Combined rheology and structure analysis techniques — ●JÖRG LÄUGER — Anton Paar Germany, Ostfildern, Germany

The simultaneous use of rheological and structural analysis techniques is helpful to gain a better understanding of the dependencies between the microstructure and the mechanical properties of complex fluids. Optical techniques like Small-Angle-Light-Scattering (SALS) or microscopy measurements have been used in combination with rheology. Other techniques are Small-Angle-X-ray (SAXS) and Neutron (SANS) Scattering. The decision on which technique to choose is based on the size and type of the structure as well as on the general sample properties to be investigated. Density and orientation fluctuations within a sample, averaged over the whole scattering volume, can be well monitored by SALS. The advantage that individual structure elements are seen in microscopy can be turned into a disadvantage when combined with a rheometer. At larger shear rates or deformations the specific structure element easily moves out of the field of view and can't be followed during an experiment. A way to overcome this issue is the use of a rheometer employing two motors operating in a counter rotation or counter oscillation fashion. The aim of this paper is to give an overview over the various techniques used for structural investigations simultaneous to rheological measurements and to introduce some new techniques and methods.

DY 46.9 Thu 11:45 C 264

Combined rheo-optics and rheo-scattering study of structure evolution in biobased liquid-crystalline polymers — ●DIETMAR AUHL¹, CAROLUS WILSENS¹, ERIC STELLAMANNS², and SANJAY RASTOGI¹ — ¹Maastricht University, Maastricht, The Netherlands — ²Photon Science DESY, Hamburg, Germany

Thermotropic liquid-crystalline polymers (TLCP) are often used in high-performance applications, for which the chemical composition and flow effects on the micro- and mesoscale orientation need to be well designed. Recently developed TLCP based on p-hydroxybenzoic acid, suberic acid, and vanillic acid are partially aliphatic in contrast to commercial TLCP such as "Vectra", and they exhibit stable nematic melt morphologies up to 300°C [1,2]. In this study, we investigate the effects of temperature, shear deformation and rate on the molecular orientation and relaxation by rheo-optics as well as rheo-scattering with x-ray and small-angle light-scattering. The results show that the threaded morphology on a mesoscale breaks and orients along the flow direction under continuous flow, while also the molecules orient on a microscopic scale. The study provides detailed insights into the structure evolution of TLCP and a unique toolbox to correlate molecular parameters to properties and performance. [1] Wilsens, C., Noordover, B., Rastogi, S. *Polym.* (2014) 2432; [2] Wilsens, C., Verhoeven, J., Noordover, B., Hansen, M., Auhl, D., Rastogi, S. (2014) 3306

DY 47: Superconductivity: Higgs Modes in Condensed Matter and Quantum Gases (joint session TT/ DY/ MA/ O)

Time: Thursday 9:30–11:15

Location: H 2053

Invited Talk

DY 47.1 Thu 9:30 H 2053

A Brisk Walk through Phase Transitions in Time: Oscillating Order and the Dynamics of Topological Defects — ●DRAGAN MIHAJLOVIC — Jozef Stefan Institute, Ljubljana, Slovenia

New techniques in time-resolved optical spectroscopy allow us to investigate phase transitions under controlled, yet highly non-ergodic conditions. The measurement of the temporal evolution of not only single particle and collective excitations, but also topological excitations through the transition lead to a new insight into the emergence of functional properties under non-equilibrium conditions. Experiments on well-known rare earth and transition metal chalcogenides which I will discuss reveal some unexpected phenomena. For example, femtosecond coherent oscillations of the order parameter and the subsequent coherent creation and annihilation of topological defects leads to a transient domain structure which decays through the emission of dispersive Higgs-like amplitude waves [1,2]. Remarkably, if the conditions are right (defined by the material), the topological defects may form an ordered metastable state, which is topologically protected, opening a route to the creation of hidden states [3]. Such switching between states with different charge order occurs at unprecedented speeds and is of potential interest for ultrafast non-volatile memory technology, with either optical or electrical control.

- [1] R. Yusupov et al., *Nature Phys.* **6**, 681 (2010)
- [2] D. Mihailovic et al., *J. Phys.: Condens. Matter* **25**, 404206 (2013)
- [3] L. Stojchevska et al., *Science* **344**, 177 (2014)

DY 47.2 Thu 10:00 H 2053

Nonadiabatic dynamics and coherent control of nonequilibrium superconductors — ●ANDREAS SCHNYDER¹, HOLGER KRULL², DIRK MANSKE¹, and GÖTZ UHRIG² — ¹Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — ²Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, Otto-Hahn Straße 4, 44221 Dortmund, Germany

Inspired by recent THz pump-THz probe experiments on NbN films [1], we theoretically study the pump-probe response of nonequilibrium superconductors coupled to optical phonons. For ultrashort pump pulses a nonadiabatic regime emerges, which is characterized by amplitude oscillations of the superconducting gap [2] and by the generation of coherent phonons [3]. Using density-matrix theory as well as analytical methods, we compute the pump-probe response of the superconductor in the nonadiabatic regime and determine the signatures of the order parameter and of the phonon oscillations in the pump-probe conductivity. We find that the nonadiabatic dynamics of the superconductor reflects itself in oscillations of the pump-probe response as a function of delay time between pump and probe pulses [4]. We also consider two-band superconductors and study the interplay of the two amplitude oscillations of the two gaps.

- [1] R. Matsunaga et al., *PRL* **111**, 057002 (2013)
- [2] E. A. Yuzbashyan et al., *PRL* **96**, 097005 (2006)
- [3] A. P. Schnyder, D. Manske, and A. Avella, *PRB* **84**, 214513 (2011)
- [4] H. Krull, D. Manske, G. S. Uhrig, and A. P. Schnyder, *PRB* **90**, 014515 (2014)

DY 47.3 Thu 10:15 H 2053

THz Investigations of the Higgs Amplitude Mode in Superconducting Thin Films — ●MARTIN DRESSEL¹, UWE S. PRACHT¹, DANIEL SHERMAN², AVIAD FRYDMAN², BORIS GORSHUNOV^{1,3,4}, PRATAP RAYCHAUDHURI⁵, NANDINI TRIVEDI⁶, and ASSA AUERBACH⁷ — ¹Phys. Inst., Universität Stuttgart — ²Phys. Dept., Bar Ilan University, Ramat Gan, Israel — ³General Physics Inst, RUS, Moscow, Russia — ⁴Moscow Inst. Phys. and Techn., Dolgoprudny, Russia — ⁵Tata Inst. Fund. Res., Mumbai, India — ⁶Phys. Dept., Ohio State University, Columbus, U.S.A. — ⁷Phys. Dept., Technion, Haifa, Israel

We have measured thin superconducting films of various degrees of dis-

order by THz spectroscopy in order to investigate the optical conductivity at low temperatures. While the properties of weakly disordered superconductors, such as NbN or InO, can be well described by the BCS theory, significant deviations are observed as disorder increases towards the superconductor-insulator transition. On both sides of the transition, tunneling spectroscopy determines a finite pairing gap 2Δ . In contrast, the threshold frequency for the dynamical conductivity, which in BCS theory is associated with the gap, vanishes critically toward the superconductor insulator transition. Here we can identify an excess optical spectral weight below 2Δ as the first unambiguous evidence of a well-defined Higgs amplitude mode observed in a superconductor.

DY 47.4 Thu 10:30 H 2053

Magnon-Interactions and Higgs Mode in 2D Quantum Antiferromagnets from Raman Scattering — ●SIMON WEIDINGER and WILHELM ZWERGER — Physik-Department, Technische Universität München, 85747 Garching, Deutschland

We present a theory for Raman scattering on 2D quantum antiferromagnets. The microscopic Fleury-Loudon Hamiltonian is expressed in terms of an effective $O(3)$ - model. Well within the Neel ordered phase, the Raman spectrum contains both a two-magnon and two-Higgs contribution which are calculated diagrammatically. The spectrum is dominated by a broad two-magnon peak but it is hardly affected by the Higgs-mode of the 2D Neel ordered state. This is a consequence of the momentum dependence of the Raman vertex in the relevant B_{1g} symmetry. The resulting nontrivial spectrum, which has the antiferromagnetic exchange coupling as a single parameter, is in very good agreement with experiments on undoped cuprates.

DY 47.5 Thu 10:45 H 2053

Higgs Mechanism in Three-Dimensional Topological Superconductors and Anomalous Hall Effect in Zero Magnetic Field — ●FLAVIO NOGUEIRA and ILYA EREMIN — Theoretische Physik III, Ruhr-Universität Bochum

We discuss the peculiar nature of Higgs mechanism in an effective field theory for three-dimensional topological superconductors. The effective theory features two order parameters associated to the two chiral fermion species in the system. The resulting electrodynamics of such a topological superconductor exhibits a topological magnetoelectric effect with an axion field given by the phase difference of the order parameters. As consequence, the London regime is highly non-linear and anomalous Hall effect in the absence of an external magnetic field occurs. In this anomalous Hall effect the generated current transverse to an applied electric field changes sign with the temperature. We also discuss the scaling behavior of the penetration depth near the transition temperature, which is also shown to exhibit a scaling exponent that is crucially influenced by the axion term, varying continuously as function of the average phase difference.

DY 47.6 Thu 11:00 H 2053

Nonequilibrium dynamics of s - and d -wave superconductors — ●HOLGER KRULL², GÖTZ S. UHRIG¹, ANDREAS P. SCHNYDER², and DIRK MANSKE² — ¹TU Dortmund, Dortmund, Germany — ²Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

We study the nonequilibrium dynamics of s - and d -wave superconductors, which are induced by a ultra-short pump pulse or a quench, respectively. The dynamics is studied by use of the density matrix formalism as well as by analytical calculation. We focus on the temporal evolution of the order parameter. For s -wave superconductors the nonadiabatic evolution of the order parameter is well established in the collisionless regime. It shows a $1/\sqrt{t}$ decaying oscillation, which can be interpreted as Higgs mode in a superconductor. Here, we consider the evolution of a d -wave order parameter and compare it with the s -wave case.

DY 48: Networks: From Topology to Dynamics - Part II (joint session SOE/ DY/ BP)

Time: Thursday 12:00–13:15

Location: MA 001

DY 48.1 Thu 12:00 MA 001

Sensitivity against author name disambiguation of a motif-based success score in coauthorship networks — ●DAVID F. KLOSIK¹, STEFAN BORNHOLDT¹, and MARC-THORSTEN HÜTT² — ¹Institut für Theoretische Physik, Universität Bremen — ²School of Engineering and Science, Jacobs University Bremen

Motivated by the question whether large-scale citation datasets allow for a quantitative assessment of social influences in form of coauthorship of publications we investigate a success score [L. Krumov, C. Fretter, M. Müller-Hannemann, K. Weihe, and M.-T. Hütt, EPJ B (84), 535 (2011)] for small collaboration patterns in coauthorship networks. We find that when applied to a network compiled from aggregated citation data provided by the American Physical Society this score which is based on the scale of small induced subgraphs (as known from motif-analysis) is highly sensitive to details of the network construction from the data; especially to the inevitable disambiguation of author names (i.e., the scheme applied to group instances of author names into a vertex). We argue that these findings might not be exclusive to coauthorship networks since similar ambiguities are present in the network representations of other data [D.F. Klosik, S. Bornholdt, M.-T. Hütt, Phys. Rev. E 90, 032811 (2014)].

DY 48.2 Thu 12:15 MA 001

Random Walks on Citation Networks — ●VIMAL KISHORE and EDUARDO G. ALTMANN — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Scientific papers are the main source of communication of scientific ideas and are connected to each other through citations. The digitalization of articles allows scientists to easily trace not only the citations contained in a paper but also the citations a paper received. This motivates us to consider random walks on citation networks as models of the search of scientific information scientists perform. The spreading of the random walkers in the network provides information on the flow of scientific ideas across different publications and fields. We discuss different mechanisms leading to a sub-linear growth of the number of discovered papers as a function of random-walk steps.

DY 48.3 Thu 12:30 MA 001

Restricting the h-index to a citation time window: A case study of a timed Hirsch index — ●MICHAEL SCHREIBER — Insti-

tut für Physik, TU Chemnitz

The h-index has been shown to increase in many cases mostly because of citations to rather old publications. This inertia can be circumvented by restricting the evaluation to a citation time window. Here I report results of an empirical study analyzing the evolution of the thus defined timed h-index in dependence on the length of the citation time window.

DY 48.4 Thu 12:45 MA 001

An Interacting Network Perspective on Global Trade — ●JULIAN MALUCK and REIK V. DONNER — Potsdam Institute for Climate Impact Research, Germany

In the last years the International Trade Network (ITN) has caught rising attention among the scientific community. By decomposing countries into national industry sectors, data provided by multi-regional input-output tables allow for a more detailed investigation into the substructure of the ITN. We introduce an interacting network approach to quantify trends and extreme events in global trade patterns between 1990 and 2011. Different definitions of subgraphs exhibit different characteristic topological features of the ITN. This study compares and evaluates partitions that are defined by industry sector and by country, respectively. We assess how meaningful the notion of national economies in present-day globalized economy still is and show that the approach of interacting networks provides suitable methods to perceive important patterns in global trade.

DY 48.5 Thu 13:00 MA 001

From diffusion to evolutionary game theory on the multilayer — ●RUBÉN J. REQUEJO, NIKOS E. KOUVARIS, and ALBERT DÍAZ-GUILERA — Fundamental Physics Department, Universitat de Barcelona

I will present some results obtained within the LASAGNE project (multi-LAYer SpAtio-temporal Generalized NETworks), starting with the effect of the multiplex structure on the diffusion of particles, following with the extension of agent-based dynamics to the multiplex by means of an evolutionary game theoretical model of interacting metapopulations, which shows the effect of the multilayer structure on the replicator dynamics, and finishing with the observation of chimera states in the multiplex for a public goods game with cooperators, defectors and jokers.

DY 49: Dynamics on and of Networks (joint session SOE/ DY / BP)

Time: Thursday 12:00–13:15

Location: MA 001

DY 49.1 Thu 12:00 MA 001

Sensitivity against author name disambiguation of a motif-based success score in coauthorship networks — ●DAVID F. KLOSIK¹, STEFAN BORNHOLDT¹, and MARC-THORSTEN HÜTT² — ¹Institut für Theoretische Physik, Universität Bremen — ²School of Engineering and Science, Jacobs University Bremen

Motivated by the question whether large-scale citation datasets allow for a quantitative assessment of social influences in form of coauthorship of publications we investigate a success score [L. Krumov, C. Fretter, M. Müller-Hannemann, K. Weihe, and M.-T. Hütt, EPJ B (84), 535 (2011)] for small collaboration patterns in coauthorship networks. We find that when applied to a network compiled from aggregated citation data provided by the American Physical Society this score which is based on the scale of small induced subgraphs (as known from motif-analysis) is highly sensitive to details of the network construction from the data; especially to the inevitable disambiguation of author names (i.e., the scheme applied to group instances of author names into a vertex). We argue that these findings might not be exclusive to coauthorship networks since similar ambiguities are present in the network representations of other data [D.F. Klosik, S. Bornholdt, M.-T. Hütt, Phys. Rev. E 90, 032811 (2014)].

DY 49.2 Thu 12:15 MA 001

Random Walks on Citation Networks — ●VIMAL KISHORE and EDUARDO G. ALTMANN — Max Planck Institute for the Physics of

Complex Systems, Dresden, Germany

Scientific papers are the main source of communication of scientific ideas and are connected to each other through citations. The digitalization of articles allows scientists to easily trace not only the citations contained in a paper but also the citations a paper received. This motivates us to consider random walks on citation networks as models of the search of scientific information scientists perform. The spreading of the random walkers in the network provides information on the flow of scientific ideas across different publications and fields. We discuss different mechanisms leading to a sub-linear growth of the number of discovered papers as a function of random-walk steps.

DY 49.3 Thu 12:30 MA 001

Restricting the h-index to a citation time window: A case study of a timed Hirsch index — ●MICHAEL SCHREIBER — Institut für Physik, TU Chemnitz

The h-index has been shown to increase in many cases mostly because of citations to rather old publications. This inertia can be circumvented by restricting the evaluation to a citation time window. Here I report results of an empirical study analyzing the evolution of the thus defined timed h-index in dependence on the length of the citation time window.

DY 49.4 Thu 12:45 MA 001

An Interacting Network Perspective on Global Trade —

•JULIAN MALUCK and REIK V. DONNER — Potsdam Institute for Climate Impact Research, Germany

In the last years the International Trade Network (ITN) has caught rising attention among the scientific community. By decomposing countries into national industry sectors, data provided by multi-regional input-output tables allow for a more detailed investigation into the sub-structure of the ITN. We introduce an interacting network approach to quantify trends and extreme events in global trade patterns between 1990 and 2011. Different definitions of subgraphs exhibit different characteristic topological features of the ITN. This study compares and evaluates partitions that are defined by industry sector and by country, respectively. We assess how meaningful the notion of national economies in present-day globalized economy still is and show that the approach of interacting networks provides suitable methods to perceive important patterns in global trade.

DY 49.5 Thu 13:00 MA 001
From diffusion to evolutionary game theory on the multi-layer — •RUBÉN J. REQUEJO, NIKOS E. KOUVARIS, and ALBERT DÍAZ-GUILERA — Fundamental Physics Department, Universitat de Barcelona

I will present some results obtained within the LASAGNE project (multi-Layer Spatio-temporal Generalized Networks), starting with the effect of the multiplex structure on the diffusion of particles, following with the extension of agent-based dynamics to the multiplex by means of an evolutionary game theoretical model of interacting metapopulations, which shows the effect of the multilayer structure on the replicator dynamics, and finishing with the observation of chimera states in the multiplex for a public goods game with cooperators, defectors and jokers.

DY 50: Extreme Events (joint session DY/ SOE)

Time: Thursday 15:00–17:00

Location: BH-N 243

Invited Talk DY 50.1 Thu 15:00 BH-N 243
Branched Flows, Extreme Waves and the Random Focusing of Tsunami Waves — •RAGNAR FLEISCHMANN — Max Planck Institute for Dynamics and Self-Organization

Wave propagation in random media - this might sound abstract but is in fact very tangible and almost omnipresent in science and everyday life. Examples are surface water waves, but also light, sound, electrons, tsunamis and even earth quakes are waves that in a natural environment typically propagate through a complex medium. Due to its complexity, the medium is often best described as random, with examples including the turbulent atmosphere, complex patterns of ocean currents or a semiconductor crystal sprinkled with impurities. In recent years it has become clear that even very small fluctuations in the random medium, if they are correlated, lead to focussing of the waves in pronounced branch-like spatial structures and to extreme wave intensities. This branching has been reported for electron, micro, sound, and water waves.

I will give an overview over the progress we made in the last few years in the understanding of branched flows and the statistic of extreme waves. As an example, I will discuss the random focusing of tsunamis and its implications for the prediction of tsunami wave heights.

DY 50.2 Thu 15:30 BH-N 243

Computing the probability of rare trajectories — •JORGE C. LEITÃO¹, JOÃO M. VIANA PARENTE LOPES², and EDUARDO G. ALTMANN¹ — ¹Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — ²Department of Physics and Center of Physics, University of Minho, P-4710-057, Braga, Portugal

Estimating the probability of extreme events often requires finding rare trajectories in (high-dimensional non-linear) dynamical systems. In this talk we show how such trajectories can be efficiently sampled using importance sampling Monte Carlo methods. We argue that the applicability and efficiency of these methods depend on the sensitivity of the observed quantity (in which the extreme event is measured) to perturbations of the initial conditions (in the phase space). We show analytical results and numerical simulations for different observables in (hyperbolic and non-hyperbolic) chaotic systems.

- J. C. Leitão, J. M. Viana Parente Lopes, E. G. Altmann "Efficiency of Monte Carlo Sampling in Chaotic Systems", Phys. Rev. E 90, 052916 (2014)

- J. C. Leitão, J. M. Viana Parente Lopes, E. G. Altmann "Monte Carlo Sampling in Fractal Landscapes", Phys. Rev. Lett. 110, 220601 (2013)

DY 50.3 Thu 15:45 BH-N 243

Record statistics for complex random vector — •SHASHI C. L. SRIVASTAVA — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden Germany

In this talk, we present the analytical results for average record and average number of records in case of delta-correlated variables. These results are then compared with the numerical results for eigenfunctions of quantized standard map and found in good agreement [1]. Specifically, we will discuss the distribution of records which turns out to be a Gumbel distribution and the logarithmic dependence of average

number of records on Planck's constant.

References:

[1] Srivastava, S. C. L., Lakshminarayanan, A., and Jain, S. R. Record statistics in random vectors and quantum chaos, EPL 101, 10003 (2013).

DY 50.4 Thu 16:00 BH-N 243

Statistical analysis of extreme weather events in a changing climate — •PHILIPP MÜLLER and HOLGER KANTZ — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

It is often claimed and from the perspective of atmospheric physics also plausible, that extreme weather conditions might occur more frequently in a warmer climate. We discuss statistical approaches to the characterization of the intensity and the frequency of extreme weather conditions on moving time windows. We present analysis results from the analysis of instrumental weather data from the past 100 years in central Europe. Temperature extremes, precipitation extremes, and wind speed extremes have different properties, whereas some very destructive extremes such as hailstorms have not been sufficiently recorded. Based on these data, we are unable to prove the existence of a systematic trend in extreme weather in Germany, although there are signatures which are consistent with a trend towards warming.

DY 50.5 Thu 16:15 BH-N 243

A data-adaptive definition of extreme events in time series exhibiting seasonality — EVA K. HAUBER^{1,2,3} and •REIK V. DONNER¹ — ¹Potsdam Institute for Climate Impact Research, Potsdam, Germany — ²University of Copenhagen, Denmark — ³University of Natural Resources and Life Sciences, Vienna, Austria

Environmental time series are often characterized by strong seasonal variations. In such a case, extreme events are traditionally defined by removing the underlying seasonal component in the mean and applying a threshold-based definition of an extreme to the residuals. However, this approach is only valid if the probability distribution function (PDF) shows a seasonal modulation exclusively of its mean. In turn, real-world climatological records exhibit heteroskedasticity, implying that their variance (but often also the shape of the PDF) changes over the year as well. Here, we present a data-adaptive method that allows defining extreme events under such conditions. Our approach is based on kernel estimates of the conditional PDF of the data taking the phase during the year as a covariate, which allow estimating any given quantile of the PDF as a function of this phase. We demonstrate the capabilities of this new approach for artificial time series as well as real-world observational data. Our results indicate that even for short time series covering only a few periods, the data-adaptive method leads to a systematic reduction of false identifications of extremes in comparison to standard techniques.

DY 50.6 Thu 16:30 BH-N 243

Forecasting extreme events in high-dimensional excitable systems — •STEPHAN BIALONSKI¹, GERRIT ANSMANN^{2,3,4}, and HOLGER KANTZ¹ — ¹Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — ²Department of Epileptology, University of Bonn, Bonn, Germany — ³Helmholtz Institute for Radi-

ation and Nuclear Physics, University of Bonn, Bonn, Germany —
⁴Interdisciplinary Center for Complex Systems, University of Bonn,
 Bonn, Germany

The dynamics of many high-dimensional systems, ranging from nature to technology and society, can exhibit extreme events, i.e. large deviations from the average behaviour. Since extreme events can pose severe threats and can have implications for economy, politics, or health, a successful and reliable prediction of such events is highly desirable. We investigate extreme events in a high-dimensional deterministic system: a network of FitzHugh-Nagumo units. Mimicking field studies, we assume that the temporal evolution of only some degrees of freedom of the system is observed and that the exact equations of motion are unknown. Addressing these challenges, we present a data-driven approach to predict extreme events which is only based on the time series of some observables and on the coupling topology of the network. By iterative predictions, we are able to forecast the onset of an extreme event as well as the propagation and extinction of excitation, i.e. the full life-cycle of an extreme event.

DY 51: Complex Fluids and Soft Matter - Part III (joint session DY/ CPP / BP)

Time: Thursday 15:00–16:45

Location: BH-N 334

Invited Talk DY 51.1 Thu 15:00 BH-N 334

Melting of soft disks: From liquid-hexatic coexistence to continuous transitions — ●SEBASTIAN C. KAPFER^{1,2}, MANON MICHEL², and WERNER KRAUTH² — ¹Theoretische Physik 1, FAU Erlangen, Germany — ²LPS, Ecole normale supérieure, Paris, France

The melting transition of two-dimensional solids has been a subject of continued research for more than fifty years, with the prevalent scenarios being the KTHNY theory of defect unbinding and a conventional first-order liquid-solid transition. For hard disks, the KTHNY scenario has recently been essentially confirmed, even though the liquid-hexatic step is of first order [1]. Using a new rejection-free global-balance Monte Carlo algorithm [2], we show that this result transfers to soft interactions with inverse power-law or Yukawa potentials [3]. The order of the liquid-hexatic step can be tuned from first-order to continuous by softening the potential. We show that there is always a hexatic phase separating the liquid and solid phases, and identify two regimes of the hexatic with vastly different correlation lengths. These results rationalize a plethora of simulation results obtained in the past, and could be verified in charged-colloid experiments.

- [1] E. P. Bernard, W. Krauth, Phys. Rev. Lett. 107, 155704 (2011).
 [2] M. Michel, S. C. Kapfer and W. Krauth, JCP 140, 054116 (2014).
 [3] S. C. Kapfer, W. Krauth, preprint at arXiv:1406.7224.

DY 51.2 Thu 15:30 BH-N 334

Quasicrystalline Order and a “Crystal-Liquid” State in a Soft-Core Fluid — ●ANDREW ARCHER¹, ALASTAIR RUCKLIDGE², and EDGAR KNOBLOCH³ — ¹Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK — ²Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, UK — ³Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA

Results will be presented for a two-dimensional system of soft particles interacting via a two-length-scale potential that may be considered to be a simple model for the effective interaction between dendrimers and other such polymeric macromolecules in solution. Density functional theory and Brownian dynamics simulations reveal the system has a fluid phase and two crystalline phases with different lattice spacing. Of these the larger lattice spacing phase can form an exotic periodic state with a sizeable fraction of highly mobile particles: a “crystal liquid”. Near the transition between this phase and the smaller lattice spacing phase, quasicrystalline (QC) structures may be created by a competition between linear instability at one scale and nonlinear selection of the other. This dynamic mechanism for forming QCs is qualitatively different from mechanisms observed previously. The system first forms a small length scale crystal. Only when this phase is almost fully formed (i.e., the dynamics is far into the nonlinear regime) does the longer length scale start to appear, leading to the formation of QCs [A.J. Archer, A.M. Rucklidge, and E. Knobloch, Phys. Rev. Lett. **111**, 165501 (2013)].

DY 51.3 Thu 15:45 BH-N 334

DY 50.7 Thu 16:45 BH-N 243

The Role of Perturbation Growth in Critical Transitions and Extreme Events — ●NAHAL SHARAFI¹, SARAH HALLERBERG¹, and MARC TIMME^{1,2} — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Göttingen University, Göttingen, Germany

Extreme events and critical transitions happen in a variety of dynamical systems. Marked by their high magnitude as well as their infrequent and irregular occurrence, they can lead to disasters.

Employing quantifiers of chaos, we work towards identifying changes in the dynamical structure of complex systems before an extreme event or a critical transition happens. Next we use these changes as precursors of the events. Apart from possible practical implementations, such as predictions, we use the relation between predictor and event in order to understand the dynamical origins of the events under study.

As candidate precursors, we consider changes in different features of covariant Lyapunov vectors such as growth rate, localization or direction.

A New Particle-Based Mesoscopic Model for Nematic Liquid Crystals — ●KUANG-WU LEE and MARCO G. MAZZA — Max-Planck-Institut für Dynamik und Selbstorganisation, 37077 Göttingen, Germany

We introduce a new mesoscopic model for nematic liquid crystals (LCs). This approach combines the particle-based stochastic rotation dynamics (SRD) method and the Ericksen-Leslie formulation of nematohydrodynamics. SRD has been used to investigate hydrodynamics at the mesoscopic level because it recovers the Navier-Stokes equation. We extend the SRD scheme to anisotropic fluids, i.e. nematic liquid crystals, by including the Ericksen-Leslie equations. We verify the applicability of this hybrid model by few study-cases in LC physics, e.g. the temperature-driven isotropic-nematic phase transition and the rheology of sheared LC. Our simulation results show that this hybrid model captures many essential aspects of LC physics at the macroscopic scale, while preserving microscopic thermal fluctuations.

DY 51.4 Thu 16:00 BH-N 334

Molecular simulations of liquid crystalline ferrofluids — ●STAVROS PEROUKIDIS and SABINE KLAPP — Institute of theoretical physics, Technical University of Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We explore the phase behavior and self assembly in binary mixtures of uniaxial rod and magnetic dipolar sphere particles by means of molecular simulations. We find that the mesogenic rods support the formation of orientational ordered ferromagnetic chains which, in turn, enhance the order of the liquid crystal. This ends up to liquid crystalline ferrofluids that possess two principal directors (one for each species). The antiparallel arrangement of the ferromagnetic chains, within the mesophases, cancels out macroscopic spontaneous magnetization. Depending on the relative size of the species, the directors are on average either parallel or perpendicular to each other, giving rise to uniaxial or biaxial liquid crystalline ferrofluids including: nematic, smectic, columnar phases and phase transformations between them.

DY 51.5 Thu 16:15 BH-N 334

Density functional theory for elongated polyhedra — ●MATTHIEU MARECHAL and KLAUS MECKE — Friedrich-Alexander-Universität Erlangen-Nürnberg

Due to recent advances in synthesis of nanoparticles and colloids, many-particle system of polyhedra are readily available for experiments. This has spurred a host of many-particle simulation studies on polyhedra. Recently, the lack of theoretical tools to study these system was amended by proposing a density functional theory (DFT) for polyhedra using the frame work of fundamental measure theory.

In this contribution, the application of DFT to elongated polyhedra will be discussed. Recent advancements in the DFT of long rods allow us to consider nematic and smectic liquid crystals in addition to the isotropic phase. We will consider these phases for triangular prisms that are elongated along their rotational symmetry axes. Colloids with this shape could be synthesized using nanolithography. We

calculate the liquid crystal phase diagram and compare our results to Monte Carlo simulations.

DY 51.6 Thu 16:30 BH-N 334

Dynamical Crossover at the Liquid-Liquid Transformation of a Compressed Molten Alkali Metal — TARAS BRYK^{1,2}, SIMONE DE PANFILIS^{3,1}, FEDERICO A GORELLI^{4,5}, EUGENE GREGORYANZ⁶, MICHAEL KRISCH⁷, GIANCARLO RUOCCO^{1,5}, MARIO SANTORO⁸, TULLIO SCOPIGNO^{1,5}, and ●ARI PAAVO SEITSONEN^{9,10} — ¹Dip. Fisica, Univ. La Sapienza, Roma, Italy — ²Inst. Cond. Matter Phys. of NASU, Lviv, Ukraine — ³Centre for Life Nano Science IIT@Sapienza, Istituto Italiano di Tecnologia, Roma, Italy — ⁴Eur. Lab. for Non-Linear Spectr., Firenze, Italy — ⁵IPCF-CNR, c/o Univ. La Sapienza, Italy — ⁶Centre for Science at Extreme Conditions, Univ. Edinburgh, United Kingdom — ⁷Eur. Synchr. Res. Facility, Grenoble, France —

⁸IFAC-CNR, Sesto Fiorentino, Italy — ⁹Dept. Chemie, Univ. Zürich, Switzerland — ¹⁰Dépt. Chimie, ENS Paris, France

Density-driven phase transformations are a known phenomenon in liquids. Pressure-driven transitions from an open low-density to a higher-density close-packed structure were observed for a number of systems. Here, we show a less intuitive, inverse behavior. We investigated the electronic, atomic, and dynamic structures of liquid Rb along an isothermal line at 573 K, at 1.2-27.4 GPa, by means of ab initio molecular dynamics simulations and inelastic x-ray scattering experiments. Above 12.5 GPa, the breakdown of the nearly-free-electron model drives a transition of the pure liquid metal towards a less metallic, denser liquid, whose first coordination shell is less compact. Our study unveils the interplay between electronic, structural, and dynamic degrees of freedom along this liquid-liquid phase transition.

DY 52: Glasses and Glass transition (joint session DY/ DF/ CPP)

Time: Thursday 15:00–17:30

Location: BH-N 128

DY 52.1 Thu 15:00 BH-N 128

Binary colloidal mixtures investigated by differential dynamic microscopy — ●TATJANA SENTJABRSKAJA, MARCO LAURATI, and STEFAN U. EGELHAUF — Condensed Matter Physics Laboratory, Heinrich-Heine University, D-40225 Duesseldorf, Germany

We investigate dynamics of colloids in binary mixtures of hard spheres with large size asymmetry, using confocal differential dynamic microscopy (con-DDM). This technique allows to study wave vector dependent dynamics of particles by analysing time series of confocal microscopy images. Analysis of the Fourier spectra of image differences acquired at different delay times allows to determine the time-dependent density-density correlation functions and, from its shape and decay time, the nature and characteristic times of particles' dynamics. To benchmark con-DDM, we investigate one-component systems of colloidal particles at different volume fractions. Diffusion coefficients of particles as a function of volume fraction obtained from con-DDM measurements are found to be in good agreement with those obtained using dynamic light scattering experiments. We additionally show that con-DDM can be used to separately study the dynamics of single species in multicomponent systems using fluorescent labeling. In particular, we are able to determine the dynamics of sub-resolution tracer particles in binary colloidal mixtures with large size asymmetry, as a function of increasing volume fraction of the large particles. The motion of the tracer, small particles becomes increasingly constrained by the dense matrix of large spheres, resulting in complex, non-diffusive motion of the tracers.

DY 52.2 Thu 15:15 BH-N 128

Critical-like behaviour in non-crystalline solids caused by angular correlations — ●MARIYA RASSHCHUPKYNA^{1,2,3}, VOLODYMYR BUGAEV^{3,4}, JOHANNES ROTH⁵, GERHARD GRÜBEL^{6,1}, and PETER WOCHNER^{3,4} — ¹The Hamburg Centre for Ultrafast Imaging (CUI) — ²University of Hamburg — ³Max Planck Institute for Intelligent Systems, Stuttgart — ⁴Max Planck Institute for Solid State Research, Stuttgart — ⁵Institute for Functional Materials and Quantum Technologies, University of Stuttgart — ⁶DESY

Modern experimental techniques on the basis of coherent scattering data, such as X-ray cross-correlation analysis (XCCA) [1] allow the direct determination of angular correlations (and their modes) in molecular disordered systems. We performed molecular dynamics (MD) simulations for model systems with Dzugutov-type [2] interaction adjusted for the creation of glassy-type quasi-equilibrium states. XCCA applied to the simulated coherent scattering patterns of the MD samples reveals a four-point dodecahedral dominant mode responsible for the formation of non-commensurate structures, as found in glasses and quasicrystals. Strikingly, this mode exhibits a pronounced temperature-dependence indicating a critical-type behavior in the vicinity of the glassy-type transition.

References

1. P. Wochner, C. Gutt, T. Autenrieth, T. Demmer, V.N. Bugaev, A. D. Ortiz, A. Duri, F. Zontone, G. Grübel, H. Dosch, Proc. Natl. Acad. Sci. USA 106, 11511 (2009).
2. M. Dzugutov, Phys. Rev. Lett. 70, 2924 (1993).

DY 52.3 Thu 15:30 BH-N 128

Nonaffine deformations, glass transition, and yielding in disordered solids — ●ALESSIO ZACCONE — Physics-Department, Technische Universität München

A new approach to the glass transition has been recently developed from the angle of nonaffine elasticity. Due to structural disorder, the particle motions in glasses under shear do not merely follow the imposed affine pathways prescribed by the strain tensor of standard continuum linear elasticity, but deviate significantly to undergo additional nonaffine displacements. Importantly, these nearest-neighbour forces would exactly cancel out mutually in any ordered lattice with local center-inversion symmetry. The concept of nonaffine free energy of deformation can be applied to molecular and atomic glasses. The resulting scheme has been implemented to predict the T-dependence of the shear modulus of polymer glasses and its vanishing at the glass transition. The main effect leading to vanishing of rigidity can be identified with the decrease of the average effective intermolecular connectivity as the material expands upon increasing T. In turn, this makes the negative nonaffine contribution to free energy become increasingly more important as T rises, until the free energy of deformation vanishes at a critical temperature for mechanical instability, which is very close to the calorimetric glass transition. Besides nonaffinity, an important role is played by anharmonic interactions which control the thermal expansion coefficient of the glass, which in turn controls how connectivity decreases with increasing T.

DY 52.4 Thu 15:45 BH-N 128

The Potential Energy Landscape of microrheologically driven supercooled liquids — ●CARSTEN F. E. SCHROER^{1,2} and ANDREAS HEUER^{1,2} — ¹Westfälische Wilhelms-Universität, Münster, Germany — ²NRW Graduate School of Chemistry, Münster, Germany

We perform computer simulations of a fragile model glass-former in which a single particle is driven by an external force through the liquid. Thereby, we track the path the system takes through its underlying Potential Energy Landscape (PEL) and aim for understanding how this is altered by the external field^[1,2] and how the altering is related to the nonlinear responses of dynamic quantities.

In the PEL approach, the dynamics of undriven (strong and fragile) glass formers have found to be very well described in terms of an improved trap model, the Gaussian Glass Former (GGF)^[3]. In this talk we want to demonstrate, how the GGF can be extended to driven supercooled liquids. This enables one to predict typical nonlinear responses like the nonlinear decay of the local friction coefficient as well as highly nontrivial effects like the occurrence of effective temperatures. Within this framework we can quantitatively predict the numerically observed effective temperatures in terms of the kinetics of the force-dependent hopping processes in the PEL. This establishes an intimate relation between the thermodynamics and the kinetics also in the highly non-equilibrium regime.

- [1] C. F. E. Schroer, A. Heuer, *J. Chem. Phys.* **138**, 12A518 (2013)
- [2] C. F. E. Schroer, A. Heuer, *Phys. Rev. Lett.* **110**, 067801 (2013)
- [3] A. Heuer, *J. Phys.: Condens. Matter* **20**, 373101 (2008)

DY 52.5 Thu 16:00 BH-N 128

Physical mechanisms of nonlinear conductivity: A model analysis — ●ANDREAS HEUER and LARS LÜHNING — Institute for

Physical Chemistry, University of Münster, Germany

Nonlinear effects are omnipresent in thin films of ion conducting materials showing up as a significant increase of the conductivity upon increasing electric field. For a disordered hopping model general physical mechanisms are identified giving rise to the occurrence of positive or negative nonlinear effects, respectively. Analytical results are obtained in the limit of high but finite dimensions [1]. They are compared with the numerical results for 3D up to 6D systems. A very good agreement can be found. The results can also be used to rationalize previous numerical simulations. The implications for the interpretation of nonlinear conductivity experiments on inorganic ion conductors are discussed.

[1] A. Heuer, L. Lühning, *J. Chem. Phys.* 140, 094508 (2014).

15 min. break

DY 52.6 Thu 16:30 BH-N 128

Where to go in a rough free-energy landscape? — ●STEFAN SCHNABEL and WOLFHARD JANKE — Universität Leipzig

Frustrated spin systems like the Edwards-Anderson spin glass are notorious for disorder-induced frustration. Sampling their rough free-energy landscape is very challenging and only small systems can be investigated. Over the years great efforts have been made to improve both hardware and implementation, yet the basic method for the investigation of 3d spin glasses is and has been parallel tempering [1]. Here, we explore the possibility of using additional information obtained by a local minimization procedure similar to the basin-hopping algorithm [2]. Altering the statistical weight of conformations according to the depth of nearby local minima can reduce autocorrelation time. We investigate whether this improvement outweighs the additional computational cost.

[1] K. Hukushima and K. Nemoto, *J. Phys. Soc. Japan* 65 (1996) 1604. [2] D. J. Wales, *J. Phys. Chem. A* 101 (1997) 5111.

DY 52.7 Thu 16:45 BH-N 128

Evidence for a Novel Relaxation Mechanism in Glasses at Very Low Temperatures — ●MARIUS HEMPEL, ANDREAS REISER, ANDREAS FLEISCHMANN, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The acoustic and dielectric properties of amorphous solids at low temperatures are governed by two level tunneling systems and can be described in similar ways. One difference is however, that electric fields couple only to tunneling systems carrying an electric dipole moment, whereas acoustic measurements couple to all tunneling systems. Thus, the two methods complement each other and can therefore lead to a better understanding of the underlying processes.

Low frequency measurements of the dielectric properties of the two multicomponent glasses N-KZFS11 and HY-1, containing significant amounts of tantalum and holmium respectively, have recently shown unexpected behavior, which cannot be understood in terms of the so called standard tunneling model. This behavior has been attributed to the very large nuclear electric quadrupole moments of ^{181}Ta and ^{165}Ho .

We present the first measurements of the acoustic properties of N-KZFS11 and HY-1 in the kHz range down to 10 mK. The results of these measurements underpin the observations seen in dielectric experiments and provide further evidence for a novel relaxation mechanism in such glasses.

DY 52.8 Thu 17:00 BH-N 128

Non-Universal Dielectric Properties of Glasses at Very Low Temperatures — ●ANNINA LUCK, ANDREAS REISER, ANDREAS FLEISCHMANN, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The universal behaviour of amorphous solids at low temperatures, governed by two level tunneling systems and described by the standard tunneling model, has long been a generally accepted fact. In the last years, however, measurements of dielectric two-pulse polarization echoes have revealed that nuclear electric quadrupole moments involved in atomic tunneling systems can cause specific material-dependent effects in magnetic fields.

We show measurements of dielectric properties of the two multicomponent glasses N-KZFS11 and HY-1, containing significant amounts of tantalum and holmium respectively. As ^{181}Ta and ^{165}Ho both carry very large nuclear electric quadrupole moments, these glasses are ideal candidates to determine the influence of these moments on the physical properties of glasses down to very low temperatures.

Our measurements not only show unique dielectric behaviour in both glasses, but also differ significantly from various predictions of the standard tunneling model.

DY 52.9 Thu 17:15 BH-N 128

Thermography on Luminescent Barium Borate Glass for White-LED Applications — ●FLORIAN WAGNER¹, PETER NOLTE², and STEFAN SCHWEIZER^{1,2} — ¹South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — ²Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Mechanics of Materials IWM, Lübecker Ring 2, 59494 Soest

White light-emitting diodes (W-LEDs) represent one of the most promising lighting technologies for the future. Primarily used in many lighting applications is a blue LED combined with a yellow phosphor. The phosphor powder is usually embedded in an organic polymer and coated onto the LED chip. Heat-induced degradation of the organic encapsulate, however, results in an efficiency decrease and color temperature change. Luminescent glasses or glass ceramics are an interesting alternative due to their higher thermal and chemical stability. This work focuses on the thermal behaviour of luminescent barium borate glasses under intense excitation with ultraviolet/blue light. The glasses are doped with rare-earth ions for optical activation. Upon absorbing the ultraviolet/blue light, the rare-earth ions show their typical emission in the visible spectral range. Here, not all of the absorbed light is frequency-downshifted, but a significant part is released in the form of heat. Contact-free infrared thermography enables an analysis of the heat development in these materials. An algorithm based on the partial differential heat equation is developed to calculate the heat source density of the optical excitation from the surface temperature distribution.

DY 53: Focus: Disordered Systems/Glasses under Shear (joint session CPP/ DY)

Time: Thursday 15:30–17:00

Location: C 243

Invited Talk

DY 53.1 Thu 15:30 C 243

Microscopic flows of complex suspensions — ●ANKE LINDNER — PMMH-ESPCI, Paris

The flow of complex suspensions is ubiquitous in nature and industrial applications. Their non-Newtonian character is due to flow-induced orientation, rearrangement, or deformation of microscopic objects suspended in simple fluids. These objects can be isotropic or anisotropic, rigid or deformable, active or passive. Linking the microstructure on the particle level to the macroscopic response under flow is one of the fundamental scientific challenges of soft matter physics. Recent micro-fabrication techniques lead to a precise control of even complex particle properties and new microfluidic rheometers show high resolution. Using these new approaches, we present two examples of flows of complex suspensions in chosen microfluidic geometries which allow this link to be established. First, we use a solution of flexible polymers, where

normal stresses are known to arise when the polymers are stretched under flow and characterize the onset of elastic flow instability in a serpentine channel as a function of its curvature. The calibrated serpentine channel can then be used as a sensitive rheometer to detect even small normal stresses in unknown suspensions. Second, we employ a Y-channel, a powerful rheometer for measuring shear viscosities, to study the viscosity of active suspensions of e-coli bacteria. In this way we link the activity of the bacteria to the measured non-Newtonian effective viscosity.

DY 53.2 Thu 16:00 C 243

Thinning and Thickening in Active Microrheology — ●TING WANG and MATTHIAS SPERL — Institut für Materialphysik im Weltraum, DLR, Köln, Germany

When pulling a probe particle in a driven granular system with con-

stant velocity, one can characterize the probe by a velocity-dependent friction coefficient. With increasing control velocity, the friction of the probe keeps constant in the small-velocity regime (linear response), decreases in the moderate-velocity regime (thinning), and then increases in the large-velocity regime (thickening).

There are three distinct processes behind those phenomena: diffusion, damping and direct collision; the magnitude of the pulling velocity determines which process dominates, resulting in thinning or thickening behavior. We confirm this physics picture by stochastic simulation.

DY 53.3 Thu 16:15 C 243

Transition to flow of binary glasses under applied stress or strain rate — ●MARCO LAURATI¹, TATJANA SENTJABRSKAJA¹, JAN HENDRICKS¹, ALAN R. JACOBS², GEORGE PETEKIDIS², and STEFAN U. EGELHAAF¹ — ¹Condensed Matter Physics Laboratory, Heinrich-Heine University Düsseldorf — ²IESL-FORTH, University of Crete

We investigate and compare the transition to flow of glasses composed by two species of colloidal hard spheres presenting large size asymmetry, upon application of a constant stress or constant shear rate. The transition to flow of the binary glasses is affected by the composition of the mixture, and reflects changes in the prevailing caging mechanism, i.e. transitions between different glass states [1]. Furthermore, the timescales characterising the onset of flow significantly differ depending on the nature of the applied field, i.e. stress or strain. The relaxation of the accumulated stress after removal of the applied field demonstrates the presence of residual stresses that can be tuned through the mixture's composition. The recovery of strain after creep reveals a non monotonic dependence of the recovery time as a function of the previously applied stress, with a maximum recovery time observed in correspondence to the yield stress of the glass. [1] T. Sentjabrskaja et al. (2014), *Soft Matter*, 10, 6546-6555.

DY 53.4 Thu 16:30 C 243

Yielding in concentrated colloidal dispersions: relation between stress overshoot and microscopic structure and dynamics — MARCO LAURATI, KEVIN MUTCH, and ●STEFAN EGELHAAF — Condensed Matter Physics Laboratory, Heinrich Heine University, 40225 Düsseldorf, Germany

The microscopic structure and dynamics of concentrated colloidal dispersions at different times after application of shear is determined using confocal microscopy. When the stress overshoot occurs in the rheological response, we observe super-diffusion and a maximally deformed cage, i.e. maximum structural anisotropy [1,2]. The anisotropy is not only characterized by a quadrupolar (angular momentum $l = 2$) distortion expected by continuum elasticity theory, but also a higher order hexadecupolar ($l = 4$) mode which marks the transition from reversible elastic to irreversible plastic deformation [3]. This mode suggests that yielding of local cages proceeds through the rearrangement of particles in the first neighbour shells, which switch from the compressional to the extensional axis. Also in the steady-state of shear, cage-breaking events are found to persist. In addition to the anisotropic cage deformation, yielding is also accompanied by a strong rise in the isotropic ($l = 0$) distortion, which corresponds to a pressure increase.

- [1] N. Koumakis et al. (2012) *Phys. Rev. Lett.* 108, 098303.
 [2] K.J. Mutch et al. (2013) *Eur. Phys. J. - Special Topics* 222, 2803.
 [3] C.P. Amann et al. (2013) arxiv:1302.2030.

DY 53.5 Thu 16:45 C 243

Continuum Mechanics Simulations in Glass Forming Liquids — ●HELIANA CARDENAS and THOMAS VOIGTMANN — Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany

Amorphous glassy materials show complex flow features when they are formed by solidification of dense liquids. An important feature of such systems is the non-linear nature of the flow rule relating stresses and strains when they are perturbed by external forces. The transition itself is characterized by slow dynamics where the intrinsic relaxation time plays a determining role on describing this behavior.

Schematically, the interaction of non-linear rheology and slow relaxation can be captured by so-called “fluidity” models, where the (spatially local) structural relaxation rate is a function of flow rate. The spatial dynamics of fluidity is controlled by a diffusion coefficient related to a cooperativity length scale.

We use finite volume method (FVM) to combine the resulting constitutive equation with the Navier-Stokes equations to effectively describe the flow behavior of glass-forming systems in various geometries and for different time-dependent protocols.

DY 54: Microswimmers, Active Liquids - Part II (joint session CPP/ BP/ DY)

Time: Thursday 15:45–18:00

Location: PC 203

Invited Talk

DY 54.1 Thu 15:45 PC 203

Flagellar synchronisation through direct hydrodynamic interactions — ●MARCO POLIN¹, DOUGLAS BRUMLEY², KIRSTY WAN³, and RAYMOND GOLDSTEIN³ — ¹University of Warwick, Coventry, UK — ²MIT, Boston, MA, US — ³University of Cambridge, Cambridge, UK

Microscale fluid flows generated by ensembles of beating eukaryotic flagella are crucial to fundamental processes such as development, motility and sensing. Despite significant experimental and theoretical progress, the underlying physical mechanisms behind this striking coordination remain unclear. We describe a novel series of experiments in which the flagellar dynamics of two micropipette-held somatic cells of *Volvox carter*, with measurably different intrinsic beating frequencies, are studied by high-speed imaging as a function of their mutual separation and orientation. From analysis of beating time series, we find that the interflagellar coupling, which is constrained by the lack of chemical and mechanical connections between the cells to be purely hydrodynamical, exhibits a spatial dependence that is consistent with theoretical predictions. At close spacings it produces robust synchrony which can prevail for thousands of flagellar beats, while at increasing separations this synchrony is systematically degraded by stochastic processes. Through dynamic flagellar tracking we quantify the associated waveforms and show that they are significantly different in the synchronised state. This study unequivocally reveals that flagella coupled only through a fluid medium are capable of exhibiting robust synchrony despite significant differences in their intrinsic properties.

Invited Talk

DY 54.2 Thu 16:15 PC 203

Active motion: From single microswimmers to their emergent collective behavior — ●HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Active motion of artificial and biological microswimmers is relevant in microfluidics and biological applications but also poses fundamental questions in nonequilibrium statistical physics. Mechanisms of single microswimmers need to be understood and a detailed modeling of microorganisms helps to explore their complex cell design and their behavior. The collective motion of microswimmers generates appealing dynamic patterns.

In this talk I review some of our work modeling biological microswimmers such as *E. coli* [1] and the African trypanosome [2], the causative agent of the sleeping sickness, in order to contribute to their better understanding. Using simpler model microswimmers such as active Brownian particles, I will demonstrate their emerging collective behavior. Hydrodynamic interactions lead to a clustering transition dependent on swimmer type [3] or to the formation of fluid pumps in 3D harmonic traps [4]. Self-phoretic active colloids show biomimetic autochemotactic behavior, which can induce dynamic clustering, oscillating clusters, or a chemotactic collapse [5].

- [1] R. Vogel and H. Stark, *Phys. Rev. Lett.* **110**, 158104 (2013).
 [2] D. Alizadehrad et al., to be published in *PLoS Comp. Biol.*
 [3] A. Zöttl and H. Stark, *Phys. Rev. Lett.* **112**, 118101 (2014).
 [4] M. Hennes et al., *Phys. Rev. Lett.* **112**, 238104 (2014).
 [5] O. Pohl and H. Stark, *Phys. Rev. Lett.* **112**, 238303 (2014).

DY 54.3 Thu 16:45 PC 203

Collective behavior and clustering of self-propelled rod shaped catalytic motors: A theoretical study — ●DAVOUD POULADSAZ¹ and ZAHRA ESKANDARI² — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Max Planck Institute for Intelligent Systems, Stuttgart, Germany

In the last few years, catalytic micro-motors have attracted considerable attention and different experiments have performed in order to

investigate their applicability in biology, e.g. colloidal cargo transportation. The collective behaviour of these micro-engines and their dynamic self-organization have recently been studied in experiments. In our study, we did Brownian dynamics simulation of rigid rods as a model for the interaction of catalytic motors, in a framework of stochastic processes which explain the force generating chemical reactions, and theoretically investigated the effect of spatial geometry of these active rods in the pattern formation of their clusters.

DY 54.4 Thu 17:00 PC 203

Vortex pattern formation of curved active polymers — ●LORENZ HUBER, JONAS DENK, EMANUEL REITHMANN, and ERWIN FREY — Ludwig-Maximilians-Universität, München, Deutschland

During bacterial cytokinesis FtsZ filaments assemble into a ring-like structure. Recent experiments with reconstituted FtsA-dependent recruitment of FtsZ filaments to supported membranes have observed self-organization into vortex patterns. Accounting for the treadmilling dynamics of curved FtsZ on the membrane, we propose a model for systems of polymers with equal length and curvature that undergo effective propulsion. The FtsZ filaments are assumed to sterically repel each other. Employing Brownian dynamics simulations and a kinetic Boltzmann ansatz to study these systems on microscopic and mesoscopic length scales, respectively, we identify activity, intrinsic curvature, and steric repulsion as sufficient to control the stability of vortex patterns. In our microscopic approach we modeled the FtsZ membrane dynamics as a two-dimensional system of propelled elastic polymers and find a parameter regime of dense and stable vortices. Furthermore, we employed a mesoscale description in terms of a kinetic Boltzmann approach to investigate general effects of intrinsic curvature on collective behavior in active systems. We obtain a phase diagram featuring a confined parameter region of steady dense swirls. Our results provide a generic and robust mechanism for pattern formation in actual biological systems of curved filaments.

DY 54.5 Thu 17:15 PC 203

The many faces of drag in micro-swimming — ●JAYANT PANDE¹, LAURA MERCHANT^{1,2}, JENS HARTING³, and ANA-S. SMITH^{1,4} — ¹Inst. for Theo. Phys., Friedrich-Alexander Univ., Erlangen, Germany — ²School of Phys. and Astronomy, Univ. of St. Andrews, Scotland — ³Dept. of Appl. Phys., Eindhoven Univ. of Technology, Eindhoven, the Netherlands — ⁴Ruder Bošković Inst., Zagreb, Croatia

Although the theoretical study of micro-swimming is becoming increasingly important, the role of the drag force faced by swimmers—clearly one of the cornerstones of micro-locomotion—remains inadequately understood. We shed light in this talk on some of the fundamental ways in which this force affects micro-swimming, using a very simple yet versatile model of a bead-spring swimmer, based on the three-sphere design of Najafi and Golestanian. The drag force on these swimmers enters in various guises—through the influence of the mean bead shape, through any induced transitory shape changes during the swimming cycle if the beads are non-rigid, and through the fluid viscosity. We consider the effect of each contribution separately by letting the beads be of any shape as well as of rigid or flexible material, and by analyzing the various forces on them in fluid. We show that in general an increase in the drag force can have a net positive or a negative impact on the velocity, and it is the swimmer elasticity which decides this. Depending on the latter, we present precise expressions for the

parameter ranges where the drag has opposing effects. We support the theory using lattice Boltzmann method-based simulations, and discuss the parts of the theoretical parameter space which are accessible to the simulations.

DY 54.6 Thu 17:30 PC 203

Formation, compression and surface melting of colloidal clusters by active particles — ●FELIX KÜMMEL¹, PARMIDA SHABESTARI¹, and CLEMENS BECHINGER^{1,2} — ¹Physikalisches Institut, Universität Stuttgart, D-70569 Stuttgart, Germany — ²Max-Planck-Institut für Intelligente Systeme, D-70569 Stuttgart, Germany

Artificial active swimmers, i.e. Janus particles, suspended in a critical binary mixture, are capable of a self-diffusiophoretic motion upon illumination [1][2]. In previous experiments, the dynamics of such swimmers close to walls and periodic arrays of rigid obstacles has been investigated [1]. Here, we experimentally examine the structural changes in a mixture of passive and a small number of active colloidal particles of equal diameters in a two-dimensional system. With increasing passive particle area fraction, we observe the formation of clusters with passive particles in the interior and active particles at their boundaries. Further increase of the passive area fraction leads to the merging and compression of such clusters and eventually to local melting of crystalline regions by enclosed microswimmers. Our results demonstrate that the addition of only a small amount of active particles largely changes the structure and the dynamics of colloidal suspensions.

[1] VOLPE G, BUTTINONI I, VOGT D, KÜMMERER H J AND BECHINGER C 2011 MICROSWMIMERS IN PATTERNED ENVIRONMENTS SOFT MATTER 7, 8810 (2011) [2] B. TEN HAGEN, F. KÜMMEL, R. WITTKOWSKI, D. TAKAGI, H. LÖWEN, AND C. BECHINGER, NATURE COMMUNICATIONS 5 (2014)

DY 54.7 Thu 17:45 PC 203

Detention times of microswimmers close to surfaces — ●ANDREAS ZÖTTL¹, KONSTANTIN SCHAAR^{1,2,3}, and HOLGER STARK¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin — ²Robert Koch-Institut, D-13353 Berlin — ³Institut für Theoretische Biologie, Humboldt Universität Berlin, D-10115 Berlin

The locomotion of biological microswimmers such as bacteria in aqueous environments is determined by low-Reynolds-number hydrodynamics and influenced by thermal and intrinsic biological noise. In many relevant environments such as in the human body or in the ocean microorganisms swim in the presence of soft or solid boundaries. When bacteria approach surfaces they accumulate there and form aggregates such as biofilms. A key ingredient for the observed near-wall accumulation are the relatively large times the microswimmers reside at a surface before leaving the surface. Recently, the role of noise compared to hydrodynamic interaction with the surface for the dynamics of microswimmers at a surface has been discussed controversially.

In our work we study theoretically the collision of microswimmers with surfaces by including both hydrodynamic interactions and noise. We introduce a general framework to calculate their wall detention time distribution, i.e., the time they stay at the surface. We map the escape of the microswimmer from the surface to a mean-first passage problem and apply our theory to different swimmer models (pusher, puller, source-dipole swimmer). While source dipole swimmers have a reduced and pullers an increased detention time compared to a simple active Brownian particle, pushers can have both.

DY 55: Poster – Quantum Systems

Time: Thursday 16:00–18:00

Location: Poster A

DY 55.1 Thu 16:00 Poster A

Reappearance of Localization in Open Chaotic Systems with a Partial Barrier — ●MARTIN KÖRBER¹, ARND BÄCKER^{1,2}, and ROLAND KETZMERICK^{1,2} — ¹TU Dresden, Institut für Theoretische Physik, Dresden — ²MPI für Physik komplexer Systeme, Dresden

The chaotic dynamics of generic Hamiltonian systems is governed by partial barriers. They also strongly influence the system's quantum-mechanical properties and lead to a localization of eigenstates on either side of a partial barrier. If the classical flux across a partial barrier is larger than the Planck cell, eigenstates delocalize in closed systems. In open systems, however, we observe that the resonance states localize again if the escape rate through the opening is sufficiently large.

Here, we present a model which predicts the localization transition of a resonance state based on its decay rate.

DY 55.2 Thu 16:00 Poster A

Global structure of regular tori in a generic 4D symplectic map — ●STEFFEN LANGE¹, FRANZISKA ONKEN¹, ARND BÄCKER^{1,2}, and ROLAND KETZMERICK^{1,2} — ¹TU Dresden, Institut für Theoretische Physik, Dresden — ²MPI für Physik komplexer Systeme, Dresden

The dynamics of Hamiltonian systems (e.g., planetary motion) can be investigated by symplectic maps. While the phase-space structures of 2D symplectic maps are well established, much less is known for higher dimensions.

Using 3d phase-space slices[1] and frequency analysis we investigate

the global organization of regular tori of a generic 4D symplectic map with a mixed phase space[2]. We show how all of the regular 2D-tori are organized around a skeleton of elliptic 1D-tori in the 4D phase space. The 1D-tori occur in two types of one-parameter families: The first type are Lyapunov families attached to elliptic-elliptic periodic orbits. We explain how the second type originates from remnants of broken resonant 2D-tori. In combination these results allow for describing the self-similar hierarchy of regular tori in the 4D phase space analogous to the island-around-island hierarchy in 2D maps.

[1] M. Richter, S. Lange, A. Bäcker, and R. Ketzmerick, *Visualization and comparison of classical structures and quantum states of four-dimensional maps*, Phys. Rev. E **89**, 022902 (2014)

[2] S. Lange, M. Richter, F. Onken, A. Bäcker and R. Ketzmerick, *Global structure of regular tori in a generic 4D symplectic map*, Chaos **24**, 024409 (2014)

DY 55.3 Thu 16:00 Poster A

Structure of eigenstates of four-dimensional quantum maps — ●FLORIAN IDE¹, SHASHI C. L. SRIVASTAVA², ARND BÄCKER^{1,2}, and ROLAND KETZMERICK^{1,2} — ¹TU Dresden, Institut für Theoretische Physik, Dresden — ²MPI für Physik komplexer Systeme, Dresden

We investigate the structure of eigenstates of quantized 4D maps whose classical dynamics has a mixed phase space in which regions of regular and chaotic motion coexist. One of the challenges is the strong increase in computing time of the matrix diagonalization in the semiclassical limit, which can be minimized by a symmetry reduction. Furthermore, a direct visualization of eigenstates in 4D phase-space is not possible. By applying the method of 3D phase-space slices [1] we visualize Husimi functions of eigenstates and compare them with the classical phase-space structures. This allows for identifying regular states, chaotic states and also scarred states concentrating around hyperbolic periodic orbits.

[1] M. Richter, S. Lange, A. Bäcker, and R. Ketzmerick, *Visualization and comparison of classical structures and quantum states of four-dimensional maps*, Phys. Rev. E **89**, 022902 (2014)

DY 55.4 Thu 16:00 Poster A

Coupling of microcavities — ●JAKOB KREISMANN — TU Ilmenau, FG Theoretische Physik II, Postfach 10 05 65, 98684 Ilmenau

Microcavity lasers made of dielectric disk-shaped resonators with sizes in the micrometer range have gained a lot of interest in recent years. A drawback of pure disk resonators for microlaser applications is their isotropic light output. To overcome this problem, deformed cavities were proposed such as limaçon-shaped resonators which display direc-

tional light emission attractive for microcavity lasers.

In this work the coupling of a disk resonator to a limaçon-shaped cavity is studied using three dimensional FDTD calculations. For this purpose a limaçon resonator is placed on top of a disk resonator, a whispering gallery mode with high Q-factor is excited inside the disk resonator and its coupling into the limaçon cavity is analyzed for different geometric configurations.

DY 55.5 Thu 16:00 Poster A

Is the fractal Weyl law valid in partially absorbing systems? — ●MORITZ SCHÖNWETTER and EDUARDO G. ALTMANN — Max-Planck-Institut für Physik komplexer Systeme, Dresden

The fractal Weyl law is a prominent showcase for the nontrivial effect of classical dynamics in a quantum systems. It states that in a chaotic system with an opening the number of long-living quantum states grows with the system size as a power law with a fractional exponent. The exponent is the fractal dimension of the classical invariant set. We study systems in which the opening partially reflects classical trajectories. In this case the fractal dimension of the classical invariant set is equal to the phase-space dimension. Yet, we observe that the number of long-living resonances still scales with a nontrivial exponent. We explain this observation using a statistical procedure that estimates an effective volume available for the resonances. This procedure suggests that in the semiclassical limit the fractal Weyl law is valid with a modified fractal dimension, which cannot be recovered directly from the classical invariant set and its measures.

DY 55.6 Thu 16:00 Poster A

Dynamics of dissipative quantum lattice systems with interaction — ●STEFAN WOLFF and CORINNA KOLLATH — Helmholtz-Institut für Strahlen- und Kernphysik, Bonn, Germany

Most experimental systems are subjected to environmental influences. Typically the coupling to such an environment is one of the main problems for the realization of quantum devices, since it leads to an exponential fast decoherence. However, the interplay of dissipation and interaction can lead to fascinating effects such as unconventional non-exponential behavior. For example in interacting bosonic quantum-many-body systems coupled to a Markovian environment, quantum coherence decays algebraically.

In our studies we apply the Lindblad master equation for an interacting lattice system. We present results obtained using stochastic wave function sampling with time-dependent DMRG-methods to investigate the relevant system dynamics.

DY 56: Poster - Statistical Physics

Statistical Physics (general); Statistical Physics far from Thermal Equilibrium; Statistical Physics in Biological Systems; critical phenomena

Time: Thursday 16:00–18:00

Location: Poster A

DY 56.1 Thu 16:00 Poster A

From classical to quantum and back: Hamiltonian coupling of classical and Path Integral models of atoms — KARSTEN KREIS^{1,2}, DAVIDE DONADIO¹, KURT KREMER¹, and ●RAFFAELLO POTESTIO¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Graduate School Materials Science in Mainz, Mainz, Germany

Quantum delocalization of atomic nuclei affects the physical properties not only of low temperature systems, such as superfluid helium, but also of room temperature molecules containing light atoms. An accurate modeling of these effects can be achieved making use of the Path Integral formulation of Quantum Mechanics, which is however computationally very demanding. By restricting this numerically expensive description to a small region of space, while modeling the remaining atoms as classical particles, the amount of computational resources required for a simulation can be significantly reduced. In the present work we derive a Hamiltonian formulation for a bottom-up, theoretically solid coupling between a classical model and a Path Integral description of the same system. The validity of this approach is demonstrated by means of simulations of low temperature parahydrogen.

DY 56.2 Thu 16:00 Poster A

The symmetric Anderson impurity model in a continuum limit of the Hubbard model — ●YAHYA ÖZ and ANDREAS KLÜMPER — Bergische Universität Wuppertal

Starting from a generalization of the Hubbard model by use of Shastry's R -matrix with two independent spectral parameters an integrable lattice model can be constructed, which yields the symmetric Anderson impurity model in the continuum with all interaction parameters. We use the continuum limit for the derivation of the thermodynamic equations of the symmetric Anderson impurity model from those of the Hubbard model. We consider two alternative formulations and obtain the infinite set of TBA equations, but also a finite set of nonlinear integral equations which allows a much more efficient numerical treatment.

DY 56.3 Thu 16:00 Poster A

Large deviations in Taylor diffusion — ●MARCEL KAHLEN and ANDREAS ENGEL — Institut für Physik, Universität Oldenburg, Deutschland

Diffusion of particles in streaming liquids is ubiquitous. Taylor diffusion addresses the dispersion of particles in shear flow.

Using a large-deviation principle, we approximate the time dependent particle distribution for large times in a Taylor diffusion setting

with N layers. The stochastic transitions of the particles between the layers is modelled as a Markovian jump process. Applying the contraction principle to the rate function for the empirical density of this process as given by Donsker and Varadhan, we obtain a set of non-linear equations for the lateral particle distribution at large times. For the simplest case of $N = 2$ layers the contraction can be performed analytically and reproduces known results. In the general case a linearisation yields an approximate solution which we compare with simulation results.

DY 56.4 Thu 16:00 Poster A

Transverse correlation functions in the Ising antiferromagnet on the anisotropic kagome lattice — ●WALTER APEL¹ and HANS-ULRICH EVERTS² — ¹PTB Braunschweig, PSt4, 38116 Braunschweig — ²LUH, Inst. f. Theoret.Physik, 30167 Hannover

We study the anisotropic kagome Ising antiferromagnet, i.e. a model in which the coupling along one of the three directions differs from the couplings along the other two directions.

In previous work [J of Statistical Mechanics: Theory and Experiment 2011], we calculated rigorously the correlation function parallel to the chains. Now, we devise a method to calculate rigorously the correlation functions transverse to the chains. The phase diagram and first results for the correlation functions are given.

DY 56.5 Thu 16:00 Poster A

Poly(3-hexylthiophene) (P3HT) Molecules Interacting with Au(001) Substrates — ●MOMCHIL IVANOV, JONATHAN GROSS, and WOLFHARD JANKE — Institut für Theoretische Physik, Universität Leipzig

One of the main objectives of this project is to gain, with the help of computer simulations, a better understanding of adsorption properties and recognition of surface patterns of macromolecules such as polymers and proteins when interacting with material surfaces and nanoparticles (external constraints), and of the interplay of these phenomena with polymer collapse, crystallization, aggregation and folding (internal constraints). This study reports on an approach to combine the experimental observation of polymer chain conformations adsorbed on a metal surface with coarse-grained Monte Carlo simulations. P3HT chains with a maximum length of 60 monomers were simulated in contact with an Au(001) surface and the end-to-end distance as well as the radius of gyration of the molecules were determined.

DY 56.6 Thu 16:00 Poster A

Computer Simulations of Semiflexible Polymers in Disordered Environments — ●JOHANNES BOCK and WOLFHARD JANKE — ITP Leipzig

We report computational studies of the behavior of semi-flexible polymers in disordered media. An off-lattice chain growth algorithm based on the Monte Carlo method is used to examine configurational properties of the polymers such as the end-to-end distance and tangent-tangent correlation. Particular attention is paid to the comparison of the occurring phenomena in two and three dimensions.

DY 56.7 Thu 16:00 Poster A

Comparability of microcanonical data sampled by Molecular Dynamics and Monte Carlo simulations — ●PHILIPP SCHIERZ, JOHANNES ZIERENBERG, and WOLFHARD JANKE — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

In this work we performed microcanonical simulations with statistical Monte Carlo (MC) sampling [1,2,3] and dynamical Molecular dynamics (MD) integrations. Our aim was to get both methods into agreement which needed a careful consideration of the conservation laws we encountered in MD simulations [4,5]. We applied a time series reweighting technique to transform the MD sampling to the full NVE ensemble without conservation laws. For a higher number of degrees of freedom the differences between the simulation techniques diminished as expected. We adapted the known multi histogram reweighting technique WHAM to use it for microcanonical MD simulation data. Therefore we got an estimate of the density of states from MD simulations. For this procedure we needed an accurate knowledge of the sampled ensembles.

[1] J. R. Ray, Phys. Rev. A 44 (1991) 4061.

[2] B.A. Berg and T. Neuhaus, Phys. Lett. B 267 (1991) 249; Phys. Rev. Lett. 68 (1992) 9;

[3] W. Janke, Int. J. Mod. Phys. C 03 (1992) 1137; Physica A 254 (1998) 164.

[4] R. Lustig, J. Chem. Phys 100 (1994) 3048.

[5] F. Calvo, J.P. Neirotti, D.L. Freeman, and J.D. Doll, J. Chem. Phys 112 (2000) 10350.

DY 56.8 Thu 16:00 Poster A

crumpling of plastic wires in spherical cavities — ALI FARNUDI¹, JAVAD NAJAFI², M REZA SHAEBANI³, and ●MEHDI HABIBI^{1,4} — ¹Department of Physics, Institute for Advanced Studies in Basic Sciences, Zanjan, Iran — ²Department of Experimental Physics, Saarland University, Saarbrücken, Germany — ³Department of Theoretical Physics, Saarland University, Saarbrücken, Germany — ⁴Van der Waals-Zeeman Institute, University of Amsterdam, Amsterdam, The Netherlands

We study the morphology of crumpled plastic wires irreversibly packed into spherical cavities. The total length of the injected wire follows a power-law dependence on the relative system size, that is the ratio of sphere and wire radii. The exponent (or, equivalently, the mass-size fractal dimension) depends on the friction coefficient between the wire and the cavity walls, reflecting friction-dependent structural differences. While ordered coil formation is partially observed at low frictions, highly disordered structures emerge at large friction limit, where the number of folds exhibits a power-law scaling in the relative system size. The probability distribution of the fold-size broadens and becomes more asymmetric for relatively larger spheres. We present a self-avoiding random walk model for the injection of the plastic wire at high friction regime, which provides a new insight into the underlying mechanism and remarkably reproduces the experimental results.

DY 56.9 Thu 16:00 Poster A

Infinitesimal Monte Carlo Algorithms — ●MANON MICHEL¹, SEBASTIAN C. KAPFER², and WERNER KRAUTH¹ — ¹Laboratoire de Physique Statistique, 24 rue Lhomond 75005 Paris France — ²Institut für Theoretische Physik 1 Staudtstr. 7 91058 Erlangen Germany

Monte Carlo methods, most notably the Metropolis algorithm, are a powerful tool in statistical physics. But local random walks induce a high rate of rejections, making any simulations around a phase transition point too expensive. To address this problem, we reformulate the Metropolis algorithm at the most fundamental level, upgrading the diffusive dynamics to a convective one. We therefore construct a new framework for Monte Carlo algorithms, based on a new factorization of the Metropolis acceptance probability. It leads to a class of rejection-free Markov chain Monte Carlo algorithms for sampling general multidimensional probability distributions, without introducing discretizations in time or in space [1]. These algorithm break detailed balance yet satisfy global balance. They generalize the recent and successful hard-sphere event-chain Monte Carlo method and were recently used in bidimensional melting with soft interactions. Finally, this new framework allows direct access to quantities as pressure and stress in multiparticle systems. Generally, it leads also to new insights on elastic constants derivation from first principles, yielding a precise determination of existence of hexatic phase[2].

[1] M. Michel, S. C. Kapfer, W. Krauth, Journal of Chemical Physics 140 54116 (2014)

[2] M. Michel, S. K. Kapfer, W. Krauth, manuscript in preparation

DY 56.10 Thu 16:00 Poster A

Deriving elasticity theory for non-ideal crystals: application to cluster crystals — ●JOHANNES HÄRING, MATTHIAS FÜCHS, and CHRISTOF WALZ — Universität Konstanz, 78457 Konstanz

For non-ideal crystals density fluctuations can be expressed by deformations of the underlying lattice structure plus changes in the occupancy of the single lattice sites. In our approach these density variations from a equilibrium density play the role of the displacement from the equilibrium position in normal elasticity theory.

Through classical density functional theory it is possible to obtain the hydrodynamic equations of motion, a wave equation, expressions for the constants of elasticity and the isothermal compressibility.

A well-known model for cluster crystals, the so called generalized exponential model is used to demonstrate the capability of the theory because its big differences in occupancy of each lattice site (e.g. fluctuations from 12 to 15 particles per lattice site) lead to a significant deviation from the ideal crystal.

DY 56.11 Thu 16:00 Poster A

Stiff Directed Lines in Random Media — ●HORST-HOLGER BOLTZ and JAN KIERFELD — TU Dortmund, Dortmund, Germany

We investigate the behaviour of stiff directed lines with bending energy in a random medium. We show that a stiff directed line in 1+d dimensions undergoes a localization transition with increasing disorder for $d > 2/3$. We demonstrate that this transition is accessible by numerical transfer matrix calculations in 1+1 dimensions and analyze the properties of the disorder-dominated phase. On the basis of the two-replica problem, we propose a relation between the localization of stiff directed lines in 1+d dimensions and of directed lines under tension in 1+3d dimensions, which is strongly supported by identical free energy distributions. This shows that pair interactions in the replicated Hamiltonian determine the nature of directed line localization transitions with consequences for the critical behavior of the Kardar-Parisi-Zhang (KPZ) equation. Furthermore, we quantify how the persistence length of the stiff directed line is reduced by disorder. Additionally, we study the depinning of stiff directed lines. Their equation of motion is the (quenched) Herring-Mullins equation, which also describes surface growth governed by surface diffusion. We employ analytical arguments and numerical simulations to determine the critical exponents and compare our findings with previous works and functional renormalization group results, which we extend to the different line elasticity. We see evidence for two distinct correlation length exponents.

DY 56.12 Thu 16:00 Poster A

Second law-like inequality for periodic, feedback-driven quantum engines — ●MICHAEL BAUER, KAY BRANDNER, MICHAEL SCHMID, and UDO SEIFERT — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

A genuine feature of projective quantum measurements is that they inevitably alter the mean energy of the observed system if the measured quantity does not commute with the Hamiltonian of the observed system. Compared to the classical case, Jacobs proved that this additional energetic cost leads to a stronger bound on the work extractable after a single measurement from a system initially in thermal equilibrium [Phys. Rev. A 80, 012322 (2009)]. Here, we show that the same bound holds for a large class of feedback-driven quantum engines operating periodically and in finite time. The bound thus implies a natural definition for the efficiency of information to work conversion in such devices.

For a simple model consisting of a laser-driven two level system, we maximize the efficiency with respect to the observable whose measurement is used to control the feedback protocol. We find that the optimal observable typically does not commute with the Hamiltonian and hence would not be available in a classical two level system. This result reveals that periodic feedback engines operating in the quantum realm can exploit quantum coherences to reach high efficiency.

DY 56.13 Thu 16:00 Poster A

Brownian motion with external force: investigation of validity of the Jarzynski equality — ●NINA MEGIER and WALTER T. STRUNZ — Institut für Theoretische Physik, TU Dresden

We examine a harmonic oscillator coupled linearly to a harmonic bath. Initially our system of interest is in equilibrium, at later times it is driven far away from equilibrium by a time dependent force. We investigate both, the classical and the quantum case for the validity of the Jarzynski equality, also in strong coupling limit. Our analysis is based on the Gaussian statistics of the stochastic force acting on the harmonic oscillator in the Langevin picture.

DY 56.14 Thu 16:00 Poster A

Fluctuating efficiency for a microscopic Carnot engine — ●JOHANNES HOPPENAU — Carl-von-Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Recently the probability density function of the efficiency of microscopic heat engines gained particular interest. In [1,2] G. Verley et al. analyze the distribution of efficiencies by using large deviation techniques. We propose a simple model of a microscopic Carnot engine to illustrate their results. In addition, we analyze the efficiency distribution in the limiting case of slow driving. Even in this case we find strong fluctuations of work and heat not compatible with a normal distribution of these quantities.

[1] G. Verley, M. Esposito, T. Willaert, and C. Van den Broeck, Nat. Commun. 5, 4721 (2014).

[2] G. Verley, T. Willaert, C. Van den Broeck, and M. Esposito, Phys. Rev. E 90, 052145 (2014).

DY 56.15 Thu 16:00 Poster A

A minimalistic but realistic evolutionary food web model — ●TOBIAS ROGGE, BARBARA DROSSEL, and KORINNA T. ALLHOFF — TU Darmstadt, Germany

We present an evolutionary food web model that includes no population dynamics but is nevertheless able to generate a large variety of complex, multi-trophic networks with an ongoing turnover of species. The nodes represent species, which are characterized by three traits, namely body mass, feeding center and feeding range. These traits also define the links to other species in the network representing feeding and competition interactions.

The evolutionary algorithm starts with a simple initial network. At each iteration step, a new species is added to the system as a modification of a randomly chosen parent species. This "mutant" changes the environment for those species that now have a new predator, prey or competitor species. Some species are therefore removed from the system, if they no longer fulfill a survival criterion that depends on the interactions of the species. Subsequently, the next "mutant" is introduced. In contrast to many other evolutionary food web models, population dynamics is not explicitly taken into account. However, its effects are captured in the survival criterion. Thus, realistic network structures emerge and evolve with little computational effort. The model is therefore a valuable tool to evaluate statistical properties over long timescales, over a large parameter space, and for larger communities of coupled networks. We present selected results obtained from our simulations of the model.

DY 56.16 Thu 16:00 Poster A

Markov state modeling of polymers in shear flow — ●FABIAN KNOCH and THOMAS SPECK — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

The dynamical properties of polymers driven by shear flow have been investigated intensively. In shear flows, polymers show a coil to globular transition. This switch-like dynamics is not only relevant in the context of biology (proteins flowing through blood vessels are also exposed to shear flows) but also from the point of non-equilibrium statistical dynamics. We study numerically a generic polymer model [1]. Instead of performing constant shear rate simulations, we investigate the dynamics subjected to constant interparticle stress σ_{const} . Similar to the constant shear rate case, the constant stress simulations also show a switch-like dynamics depending on σ_{const} . Using stochastic thermodynamics, we develop a new method to construct dynamical Markov state models [2] for polymers in shear flow.

[1] Alexander-Katz, A. and Schneider, M. F. and Schneider, S. W. and Wixforth, A. and Netz, R. R., PRL 97(13), 2006

[2] Noé, F. and Horenko, I. and Schütte, C. and Smith, J. C., J. Chem. Phys. 126(15), 2007

DY 56.17 Thu 16:00 Poster A

Markov State Model with reweighting: application to small molecules with perturbed potential — LUCA DONATI and ●BETTINA KELLER — Freie Universität Berlin, Berlin, Germany

We have studied the effect of small perturbations in the potential energy surface of molecular systems by performing numerical simulations and constructing Markov State Model of the trajectories. The Markov State Models are a valid tool to analyze the large amounts of data generated by Molecular Dynamics simulations and to extract information on the timescales. In general, it is necessary to perform a new simulation after having changed the potential to construct the Markov State Model of the perturbed molecule. However, if we consider small perturbations of the system, we can use reweighting methods [1] to construct a Markov State Model that does not need a new simulation, but that uses the trajectory of the initial not-perturbed molecule. Our method is based on the Girsanov theorem [2], that has been already tested successfully for diffusive processes (e.g. a double well potential perturbed by an external force). We applied it on small molecules subjected to alchemical transformations. We studied the effect of varying the charges and the van der Waals radii on the conformational dynamics. The approach is relevant to force-field optimization, but it could eventually also be used to study mutations in proteins.

[1] Jan-Hendrik Prinz et.al., The Journal of Chemical Physics, **134**, 2011

[2] Schütte Christof et.al., Molecular Physics, **00**, 2014

DY 56.18 Thu 16:00 Poster A

Vortex arrays and mesoscale turbulence of self-propelled par-

ticles — ●ROBERT GROSSMANN¹, PAWEŁ ROMANCZUK², MARKUS BÄR¹, and LUTZ SCHIMANSKY-GEIER³ — ¹Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin, Germany — ²Princeton University, Princeton, New Jersey 08543, USA — ³Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany

We present a self-propelled particle model with Turing-like interactions: short-range alignment and anti-alignment at larger distances. The model is able to produce polarly ordered states, periodic vortex patterns and mesoscale turbulence, which resembles observations in dense suspensions of swimming bacteria. The model allows a systematic derivation and analysis of a kinetic theory as well as hydrodynamic equations for density and momentum fields. A phase diagram with regions of pattern formation as well as orientational order is obtained from a linear stability analysis of these continuum equations. Microscopic Langevin simulations of self-propelled particles are in agreement with these findings.

DY 56.19 Thu 16:00 Poster A

Emergent large-scale structures of Boolean networks optimized for criticality — MARCO MÖLLER¹ and ●TIAGO P. PEIXOTO² — ¹Institut für Festkörperphysik, Technische Universität Darmstadt — ²Institut für Theoretische Physik, Universität Bremen

We construct statistical ensembles of modular Boolean networks which are constrained to lie at the critical line between frozen and chaotic dynamic regimes. The ensembles are maximally random given the imposed constraints, and thus represent null models of critical networks. The structures of the ensembles undergo several phase transitions from a fully random structure to several ordered ones, including a prominent core-periphery structure, and an "attenuated" two-group structure, where the network is divided in two groups of nodes, and one of them has Boolean functions with very low sensitivity. This shows that such simple large-scale structures are the most likely to occur when optimizing for criticality, in the absence of any other constraint or competing optimization criteria.

DY 56.20 Thu 16:00 Poster A

Characterization of K-Complexes and Slow Wave Activity in a Neural Mass Model — ARNE WEIGENAND¹, ●MICHAEL SCHELLENBERGER COSTA¹, HONG-VIET VICTOR NGO^{1,2}, JENS CHRISTIAN CLAUSSEN^{3,1}, and THOMAS MARTINETZ¹ — ¹Institut für Neuro- und Bioinformatik, Univ. Lübeck — ²Institut für Medical Psychology and Behavioral Neurobiology, Univ. Tübingen — ³Computational Systems Biology Lab, Jacobs Univ. Bremen

NREM sleep is characterized by two hallmarks, namely K-complexes (KCs) during sleep stage N2 and cortical slow oscillations (SOs) during sleep stage N3. While the underlying dynamics on the neuronal level is well known and can be easily measured, the resulting behavior on the macroscopic population level remains unclear. On the basis of an extended neural mass model of the cortex, we suggest a new interpretation of the mechanisms responsible for the generation of KCs and SOs [1]. As the cortex transitions from wake to deep sleep, in our model it approaches an oscillatory regime via a Hopf bifurcation. Importantly, there is a canard phenomenon arising from a homoclinic bifurcation, whose orbit determines the shape of large amplitude SOs. A KC corresponds to a single excursion along the homoclinic orbit, while SOs are noise-driven oscillations around a stable focus. The model generates both time series and spectra that strikingly resemble real electroencephalogram data and points out possible differences between the different stages of natural sleep.

[1] A. Weigenand, M. Schellenberger Costa, H-VV Ngo, JC Claussen, T. Martinetz, PLoS Comput Biol 10, e1003923 (2014)

DY 56.21 Thu 16:00 Poster A

Wilson-Cowan oscillators as minimal bifurcation models of Non-REM sleep — ●ANNIKA REINKE¹, ARNE WEIGENAND¹, and JENS CHRISTIAN CLAUSSEN^{2,1} — ¹Institut für Neuro- und Bioinformatik, Univ. Lübeck — ²Computational Systems Biology Lab, Jacobs Univ. Bremen

When sleep deepens to sleep stages N2 and N3, specific oscillations emerge, namely sleep spindles in N2, and slow oscillations and K complexes in N3. While several models, after sufficient fit of parameters, can be made to reproduce experimental data, often several parameter sets or even slightly different models yield similar match with data. This calls for a simplification of the models. Here we adopt standard models of neural oscillators that are generic for a normal form of the same bifurcation phenomenology, and compare them to EEG time series. We conclude that a simple Wilson-Cowan oscillator can be adapted to exhibit the essential bifurcations when transiting to N2 and N3, including the canard phenomenon associated with the onset of the anharmonic sleep oscillations.

DY 56.22 Thu 16:00 Poster A

On the effect of the drive on self-organized criticality — MARCO WINKLER¹, ●JOHANNES FALK², and WOLFGANG KINZEL¹ — ¹Institute of Theoretical Physics, University of Würzburg, 97074 Würzburg, Germany — ²Institute for Condensed Matter Physics, Technical University of Darmstadt, 64289 Darmstadt, Germany

The well known Sandpile model of self-organized criticality generates avalanches of all length and time scales, without tuning any parameters. In the original models the external drive selects sites randomly. We analyse a drive which depends on the present state of the system, namely the effect of favouring sites with a certain height in the deposition process. We investigate, that the system stays in a critical state, if sites of height three are favoured. Our numerical results indicate the same universality class as the original model with random deposition, although the stationary state is approached very differently. In contrast, when favouring sites of height two, only avalanches which cover the entire system occur. Furthermore, we study the distributions of sites with a certain height, as well as the transient processes of the different variants of the external drive.

DY 56.23 Thu 16:00 Poster A

Multifractal analysis of states in Voronoi-Delaunay lattices — ●MARTIN PUSCHMANN, PHILIPP CAIN, and MICHAEL SCHREIBER — Institute of Physics, Technische Universität Chemnitz, Chemnitz

The Voronoi-Delaunay lattice (VDL) is a set of nearest-neighbor connections between randomly positioned sites. It is a simple model for amorphous solids and foams. We consider the transport of non-interacting electrons in this lattice and assume that all connections have the same strength. Consequently, the VDL is topologically disordered by connectivity only. Whether this form of disorder is sufficient to obtain localized states in two- and three-dimensional lattices was studied by the multifractal analysis of electronic wave functions and the finite-size scaling approach. We observe localized states in both dimensionalities with energies very close to the band edges. A localization-delocalization transition was found only in the three-dimensional lattice, in accordance with the localization theory. The corresponding critical exponent of localization is equal to the exponent of the orthogonal Wigner-Dyson class. Furthermore, we analyzed the case of additional random on-site potentials in the three-dimensional lattice. We obtain a phase diagram by varying the disorder strength of these potentials. The mixing of these different disorders does not affect the critical exponent.

DY 57: Poster - Diffusion

Brownian Motion and Transport; Reaction-Diffusion Systems; Anomalous Diffusion; Brownian Motion and Transport; Microswimmers

Time: Thursday 16:00–18:00

Location: Poster A

DY 57.1 Thu 16:00 Poster A

Mobility of colloids driven through a permeable corrugated channel — ●KONSTANTIN ZAK, ROBERT GERNERT, and SABINE H. L. KLAPP — Institut für theoretische Physik, Technische Universität Berlin

Nonequilibrium transport of colloidal suspensions is an active field of research – even for the paradigmatic model of effectively one-dimensional flow through a channel with a corrugated confinement. Here we consider a non-perfect confinement where the particles may escape from the system and enter to it. This permeable confinement is modelled via a high energetic barrier between the channel and a particle bath with constant density. For the theoretical description of the overdamped, effectively one-dimensional flow of hard spheres through the channel we employ the Dynamical Density Functional Theory (DDFT). The influence of the system-bath interaction is studied in terms of mobility and density distribution of the colloids in flow direction. We also present first results concerning the generalisation of the system towards two dimensions.

DY 57.2 Thu 16:00 Poster A

A Lattice Monte Carlo Battery Model — ●OLIVER RUBNER, VOLKER LESCH, LINUS SCHOLZ, and ANDREAS HEUER — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster

The theoretical simulation of Li-Ion batteries is an essential tool for the understanding of the complex processes that take place in electrodes as well as in electrolytes. Many models exist that focus on molecular details involving quantum chemical, molecular dynamics or continuum Monte Carlo calculations on the one hand and continuum models that treat a battery cell as a whole system on the other hand. We want to bridge the gap between these approaches by presenting a lattice Monte Carlo model that uses molecular and macroscopic parameters provided by experiments or these aforementioned techniques. We show how the influence of molecular parameters like interaction energies on cell properties like voltage and capacity can be determined in this simplified model and how it can be used to understand some of the basic principles of Li-batteries.

DY 57.3 Thu 16:00 Poster A

Thermal conductivity and self-diffusion coefficients for the TIP4P/2005 water model over a wide range of thermodynamic conditions — ●SVEN ENGELMANN and REINHARD HENTSCHEKE — Bergische Universität, 42279 Wuppertal, Germany

Using the Molecular Dynamics simulation technique we compute thermal conductivity and self-diffusion coefficients for the TIP4P/2005 water model together with a number of other thermodynamic quantities. The transport coefficients are obtained using the attendant Green-Kubo relations applied to equilibrium trajectories. The thermodynamic conditions include the saturation line in the temperature range from 273K to 373K. In addition we obtain results along two isotherms at 300K and 400K for pressures ranging from about 10 bar to 10 kbar and along an isobar at 1 bar covering again the above temperature range. The simulation data are compared to experimental measurements as well as to previous simulation results obtained with a number of other methods including also other water models. We present a critical evaluation of all simulation results in relation to the different thermodynamic conditions.

DY 57.4 Thu 16:00 Poster A

A coupled Molecular Dynamics / kinetic Monte Carlo Approach for Protonation Dynamics in Extended Systems — ●GABRIEL KABBE¹, CHRISTIAN DRESSLER¹, CHRISTOPH WEHMEYER², and DANIEL SEBASTIANI¹ — ¹Department of Chemistry, Martin-Luther Universität, Halle-Wittenberg, von-Danckelmann-Platz 4, 06120 Halle/Saale, Germany — ²Institute of Mathematics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We propose a multi-scale simulation scheme that combines first-principles Molecular Dynamics (MD) and kinetic Monte Carlo (kMC) simulations to describe ion transport processes. On the one hand, the molecular dynamics trajectory provides an accurate atomistic struc-

ture and its temporal evolution, and on the other hand, the Monte Carlo part models the long-time motion of the acidic protons. Our hybrid approach defines a coupling scheme between the MD and kMC simulations that allows the kMC topology to adapt continuously to the propagating atomistic microstructure of the system. We exemplify the performance of our MD/kMC model on the basis of various proton conducting molecular systems.

DY 57.5 Thu 16:00 Poster A

Excited State Proton Transfer in Aqueous Media: Ab-Initio Molecular Dynamics Simulation of Photoacids — ●GÜL BEKCIÖGLÜ, FELIX HOFFMANN, and DANIEL SEBASTIANI — Martin-Luther-Universität Halle-Wittenberg, Institut für Chemie - Theoretische Chemie

Photoacids are molecules which undergo a decrease in pKa value upon photoexcitation.[1,2] Since their acidity can be controlled in a very defined manner they are important model system for the investigation of proton transport in aqueous media. However, many details of the proton transfer from the photoacid to water remain elusive, for example, the structure and stability of the contact ion pair between the photoacid and the hydrated proton. A particular drastic drop in pKa value is exhibited by the "super" photoacid N-methyl-6-hydroxyquinolinium (HMQ). [3] Here, we present a microscopic study of the role water plays in mediating excited state proton transfer of HMQ in aqueous solution. The central question addressed here is the determination of elementary steps that lead to a full dissociation of the proton. In this regard, we computed IR spectra from Wannier center calculations to elucidate spectroscopic fingerprints of specific intermediates during the acid dissociation. [3]

[1] G. Bekcioglu, C. Allolio, M. Ekimova, E. T. J. Nibbering, and D. Sebastiani, Phys. Chem. Chem. Phys.,16, 13047-13051, (2014)

[2] G. Bekcioglu, C. Allolio, and D. Sebastiani, Phys. Chem. Chem. Phys., Submitted, (2014)

[3] G. Bekcioglu, F. Hoffmann, and D. Sebastiani, in preparation.

DY 57.6 Thu 16:00 Poster A

Bifurcations in two-dimensional oscillator arrays: numerical study — ●CLAUDIA LENK and J. MICHAEL KÖHLER — Institut für Chemie und Biotechnologie, TU Ilmenau, Ilmenau, Deutschland

In the range of critical coupling strength bifurcations arise in arrays of locally coupled nonlinear oscillators. Thereby, interesting effects as amplitude modulations, multiperiodic oscillations and burst patterns occur, which are similar to patterns observed in neuronal networks or in the heart. We study the occurrence of bifurcations and special patterns by calculations of the Fitzhugh-Nagumo equations of a catalyst distribution in form of a micro spot pattern. Its dependence on spot size, spot distance, spot shape and parameter variations will be discussed. The importance of gradients of spot distance or spot size for the appearance of bifurcations will be shown. Furthermore, we study the influence of the dimensionality of the oscillator arrays and the introduction of defects in the oscillator arrays for arising of burst and other special patterns.

DY 57.7 Thu 16:00 Poster A

From integrated Brownian motion to Lévy walks — ●TONY ALBERS and GÜNTER RADONS — Technische Universität Chemnitz, Germany

In a recent publication [1], we investigated the weakly nonergodic behavior of integrated Brownian motion. In this contribution, we will show how integrated Brownian motion can be mapped to a continuous time random walk with a spatiotemporal coupling of the form $\psi(x, t) \propto \delta(|x| - t^{3/2})t^{-3/2}$, where $\psi(x, t)$ describes the probability for the occurrence of a waiting time of duration t followed by a jump of length x . We investigate the nonergodic behavior of this Lévy walk by contrasting the time dependence of the ensemble-averaged and the time-averaged mean-squared displacement (MSD) and analyzing the random nature of the latter. Moreover, all quantities are studied in dependence on the ageing time which is the elapsed time between the beginning of the process and the beginning of the measurement. We

compare our findings with the results obtained for integrated Brownian motion and discuss the similarities and differences.

[1] Tony Albers and Günter Radons, Phys. Rev. Lett. **113**, 184101 (2014)

DY 57.8 Thu 16:00 Poster A

Non-adiabatic quantum pumping by a randomly moving potential barrier — STANISLAV DERVYANKO¹ and DANIEL WALTNER² — ¹Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel — ²Fakultät für Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

We look at random AC fluctuations of the electrical charge in an open 1D quantum system where the potential barrier experiences random lateral motion in time. Our treatment is essentially non-adiabatic. Both diffusive and ballistic (Lévy) regimes are considered. For a finite size system the probability current as well as the net accumulated electric charge experience random fluctuations over the static background. We show that in the large-time limit $t \rightarrow \infty$ the wavefunction is naturally separated into the Berry-phase component (resulting from the singular part of the wave amplitude in the co-moving frame) and the non-adiabatic correction (arising from fast oscillating, slow decaying tails of the same amplitude). In the special limit of delta-correlated continuous Gaussian random walk we obtain a closed analytical expressions for the ensemble averaged amplitude in the co-moving frame and demonstrate that the main contribution to the average wavefunction and probability current comes from the Berry-phase component.

DY 57.9 Thu 16:00 Poster A

Simulation of Anomalous Transport in Model Crowded Media — MARKUS SPANNER¹, FELIX HÖFLING², GERD E. SCHRÖDER-TURK¹, and THOMAS FRANOSCH³ — ¹Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — ²MPI für komplexe Systeme and IV. Institut für Theoretische Physik, Universität Stuttgart, Germany — ³Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Austria

We study large-scale computer simulations of particles in 2d and 3d dense-packed porous systems. Subdiffusive dynamics $\delta r^2(t) \sim t^{2/z}$, $z > 2$ can be observed at a critical obstacle density, when the tracer particle can barely squeeze through between the host structure.

Starting from the Lorentz model, which simply consists of a point-like tracer moving through an array of random overlapping spheres, we modify a number of simulation details (tracer dynamics, obstacle distribution, introduction of an external force) one at a time – from most simple towards more realistic porous systems. By extracting critical exponents of the dynamics in these systems, we gain a better understanding of the universal or non-universal nature of the observed exponents.

DY 57.10 Thu 16:00 Poster A

Active Brownian micro-swimmers in viscoelastic media — JUAN RUBEN GOMEZ SOLANO^{1,2} and CLEMENS BECHINGER^{1,2} — ^{1,2}Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

The motion of many natural micro-swimmers, such as bacteria and spermatozoa, commonly takes place in viscoelastic fluids or in complex crowded environments. The understanding of their swimming mechanisms has triggered a lot of experimental and theoretical work in recent years as well as the development of artificial self-propelled macro- and micro-swimmers. Although the motion of artificial swimmers in Newtonian fluids has been extensively studied, only few works have focused on active swimmers in viscoelastic media. In this work, we experimentally investigate the motion of spherical Janus particles in a critical binary viscoelastic fluid. The particles are self-propelled by local demixing of the fluid induced by laser illumination. We find that, unlike active Brownian motion in a Newtonian fluid, the rotational diffusion coefficient of a particle moving in a viscoelastic fluid dramatically increases with increasing particle velocity. This gives rise to a significant increase of the effective translational diffusion coefficient of the active particles with increasing laser illumination compared to the Newtonian case, which can be interpreted as an enhanced micro-swimming mechanism.

DY 57.11 Thu 16:00 Poster A

Lane formation in a two dimensional system with Lennard-Jones like interactions — CHRISTOPHER WÄCHTLER, FLORIAN KOGLER, and SABINE H. L. KLAPP — Institut für Theoretische

Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Using Brownian Dynamics simulations we investigate a prototype model system undergoing lane formation. The latter is a non-equilibrium transition in binary mixtures of oppositely driven particle species. In contrast to previous studies of repulsively interacting particles, which form perfect lanes only at infinitely large driving forces [1], we here examine this transition in a system involving attractive Lennard-Jones like interactions. We present new findings on how parameters such as system size, driving force and interaction strength influence lane formation in this system.

[1] T. Glanz, H. Löwen, J. Phys. Condens. Matter 24, 464114 (2012)

DY 57.12 Thu 16:00 Poster A

Numerical investigation of droplets driven by Marangoni flow — LAURA STRICKER, JUERGEN VOLLMER, and STEPHAN HERMINGHAUS — Max Planck Institute for Dynamics and Self-Organization (MPI-DS), Goettingen, Germany

The motion of artificial microswimmers can strikingly resemble collective motion in biological systems even though it only involves physical and chemical processes. A detailed understanding of their emergent swarming properties may therefore help to distinguish merely physics-related from biology-related aspects of motion in biological systems. In the present work, we focus on modelling a new type of artificial microswimmers, where propulsion is achieved by Marangoni flow. In particular, we characterize the parametric dependence of the motion and we address the propulsion mechanism. In order to do so, we developed a flexible CFD model based on a level set method, easily adaptable to different kinds of swimmers. We derived the flow field inside and outside individual droplets, and took into account the two-way coupling of the swimmers motion and the external flow. This allowed us to explore the dependence of propulsion on experimentally tunable parameters, like the droplet size and surfactant concentration. Future extensions of the present work will include the interactions between small numbers of swimmers, and the collective behavior of large assemblies, in the framework of a full multiscale approach

DY 57.13 Thu 16:00 Poster A

Active particles in inhomogeneous environments

— KEVIN SCHRÖER, MARTIN P. MAGIERA, and LOTHAR BRENDL — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, D-47047 Duisburg, Germany

Recent molecular dynamics simulations of dense suspensions of self-propelled Brownian spheres show the appearance of self-organized patterns, large-scale collective motion and phase separation via particle agglomeration [1].

In addition to that we follow the idea of an environment-dependent propulsion mechanism by introducing "passivity"-areas in which the propulsion of the particles is suppressed. Accumulation-effects are observed in and around these areas which serve as accumulation-nuclei. The swimmers are modeled in 2D and 3D via Langevin-Dynamics in order to include inertial effects and to reevaluate the latter's importance for the accumulation process. Further investigations focus on the question to which extent hydrodynamic interactions play a role in the particle interplay and the collective behavior.

References:

[1] A. Wysocki, R.G. Winkler, G. Gompper, EPL 105, 48004 (2014)

DY 57.14 Thu 16:00 Poster A

Active microrheology of dense microswimmer suspensions — ALEXANDER LILUASHVILI and THOMAS VOIGTMANN — DLR, Köln, Deutschland

The dynamics of self-propelled particles like microswimmers in dense environments are studied using the mode coupling theory of the glass transition. The theory is developed to investigate the glassy dynamics of active suspensions out-of-equilibrium, violating the fluctuation-dissipation-theorem relations.

As a starting point of mathematical calculations the Mori-Zwanzig equations with orientational degrees of freedom in two dimensions are used. The final equations for the density two-point function and the friction coefficient in the time domain are solved numerically in a schematic model including the orientational degrees of freedom, but neglecting the spatial fluctuations.

DY 57.15 Thu 16:00 Poster A

Soft Elastic Capsules in Axisymmetric Linearized Viscous Flow — ●HORST-HOLGER BOLTZ and JAN KIERFELD — TU Dortmund, Dortmund, Germany

We present an iterative solution scheme to find the stationary shape of a deformable axisymmetric elastic surface moving at very low Reynolds numbers. We use this to study the sedimentation of soft elastic capsules with Hookean stretching and bending energies.

DY 57.16 Thu 16:00 Poster A

How fast is a magnetic snail creeping down a hill? — ●ANITA FREUNDORFER, STEFAN HARTUNG, INGO REHBERG, and REINHARD RICHTER — Experimentalphysik 5, Universität Bayreuth, D-95440 Bayreuth, Germany

We investigate a permanent magnet floating on a drop of ferrofluid, which is positioned at the upper most end of an inclined plane of per-spex. Releasing a trigger the magnet travels down the ramp leaving a

trace of ferrofluid behind. For different angles of inclination α of the plane we record the time dependent position $x_\alpha(t)$ of the magnet and determine its velocity $v_\alpha(t) = dx_\alpha(t)/dt$. The latter depends on the thickness $h_\alpha(t)$ of the ferrofluidic film which is measured by means of light absorption. For a specific time we plot the layer thickness $h_\alpha(t)$ versus the capillary number $Ca = \frac{\eta v}{\sigma}$ where η denotes the viscosity and σ the surface tension. In the regime $Ca < 0.01$ we find $h \propto Ca^{2/3}$, whereas for $Ca > 0.01$ the scaling $h \propto a \cdot Ca^{1/2}$ is confirmed. These scaling laws for the film thickness are in accordance with those found for a vertical plate pulled out of a liquid [1]. After the magnet arrives at the bottom of the plane the latter is switched to $\alpha = 0$. The magnet creeps back on its trace, up to the end, like an inverse snail absorbing its own slime, which is also investigated quantitatively.

[1] S. Weinstein, K. Ruschak, *Annu. Rev. Fluid. Mech.* vol.76, 066301 (2004).

DY 58: Poster - Fluids

Fluid Dynamics and Turbulence Complex Fluids and Soft Matter

Time: Thursday 16:00–18:00

Location: Poster A

DY 58.1 Thu 16:00 Poster A

Optimal Mixing in Thin Liquid Films — ●MICHAEL WINKLER and MARKUS ABEL — Statistical Physics and Chaos Theory, Department of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Films are nanoscopic elements of foams, emulsions and suspensions, and form a paradigm for nanochannel transport that eventually tests the limits of hydrodynamic descriptions. The complex interplay of thermal convection, interface and gravitational forces yields optimal turbulent mixing and transport.

Our experimental setup allows to capture thin film interference patterns under controlled surface and atmospheric conditions. The convection is realized by placing a cooled copper rod in the center of the film. The temperature gradient between the rod and the liquid film at ambient temperature results in a density gradient, so that the varying buoyancy induces turbulent motion.

Here we present the statistical analysis of a stable two eddy convection pattern by calculating the entropy and Lyapunov exponents and compare to the maximally possible mixing efficiency. Additionally, conditional probabilities for the center jet deflection are analyzed to look for deterministic components.

DY 58.2 Thu 16:00 Poster A

Markov processes linking stochastic thermodynamics and turbulent cascades — ●DANIEL NICKELSEN — Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, Germany

An elementary example of a Markov process (MP) is Brownian motion. The work done and the entropy produced for single trajectories of the Brownian particles are random quantities. Statistical properties of such fluctuating quantities are central in the field of stochastic thermodynamics. Prominent results of stochastic thermodynamics are so-called fluctuation theorems (FTs). FTs express the balance between production and consumption of entropy.

Turbulent cascades of eddies are assumed to be the predominant mechanism of turbulence generation fixing the statistical properties of developed turbulent flows. An intriguing phenomenon of developed turbulence, known as small-scale intermittency, are violent small-scale fluctuations in flow velocity that exceed any Gaussian prediction.

In analogy to Brownian motion, we show how the assumption of the Markov property leads to a MP for the turbulent cascade that is equivalent to the seminal K62 model. In addition to the K62 model, we demonstrate how many other models of turbulence can be written as a MP, including scaling laws, multiplicative cascades, multifractal models and field-theoretic approaches. Based on the various MPs, we discuss the production of entropy and the corresponding FTs. In particular, an experimental analysis indicates that entropy consumption is linked to small-scale intermittency, and a connection between entropy consumption and inverse cascades is suggestive.

DY 58.3 Thu 16:00 Poster A

Bernoulli bond percolation on random recursive trees —

●RÜDIGER KÜRSTEN — Institut für Theoretische Physik, Universität Leipzig, Brüderstr. 16 D-04103 Leipzig

Random recursive trees are obtained from a root node by repeatedly attaching nodes randomly to one of the existing nodes. We use a stochastic coupling to obtain some exact results for Bernoulli bond percolation on random recursive trees of fixed size. We obtain among other things the expectation value of the root cluster size, of the number of nodes in the n -th generation clusters and the number of clusters of size one. Some combined limits of system size and percolation probability are considered and compared to previous work.

DY 58.4 Thu 16:00 Poster A

From low-dimensional chaos to complex behaviour in transitional pipe flow — ●PAUL RITTER — Lehrstuhl für Strömungsmechanik, Cauerstraße 4 91058 Erlangen

Turbulent pipe flow so far escapes an analytical explanation. The common approach of applying bifurcation theory to the linearized equations fails in this case because the transition occurs via finite amplitude perturbations and is characterized by localized turbulent spots surrounded by laminar flow (so-called “puffs”). A recent proposition to explain the origin of puffs postulates that, in analogy to low dimensional chaotic systems, turbulence is organized around invariant solutions of the governing equations, glimpses of which can be observed experimentally as coherent structures.

The work presented here tries to link some of the theory of low-dimensional chaotic systems to the infinite-dimensional spatio-temporal complexity of the Navier-Stokes equations. I present a mechanism, which elucidates how mildly chaotic transients acquire more complexity with respect to size, speed and kinematic properties and hence approach the properties of actually observed turbulence. This mechanism consists of the interaction and merging of chaotic saddles with distinct dynamical characteristics. The link between the saddles suggests that invariant solutions with a varying degree of internal wavelengths, possibly created in a snaking-like mechanism, might be responsible for the creation of the saddles. Finally, results from a search for these elementary building blocks of turbulence will be presented in several symmetry subspaces.

DY 58.5 Thu 16:00 Poster A

Sedimentation stacking diagram of colloidal mixtures under gravity — ●DANIEL DE LAS HERAS and MATTHIAS SCHMIDT — Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

The observation of stacks of distinct layers in a colloidal or liquid mixture in sedimentation–diffusion–equilibrium is a striking consequence of bulk phase separation. Drawing quantitative conclusions about the phase diagram is, however, very delicate. Here we present a general theory to obtain a unique stacking diagram of all possible stacks under gravity. Simple bulk phase diagrams generically lead to complex stacking diagrams. We also extend the Gibbs phase rule to determine the maximum number of sedimented layers under gravity.

References:

- [1] D. de las Heras, and M. Schmidt, *Soft Matter*, 9, 8636, (2013)
 [2] D. de las Heras, and M. Schmidt, Accepted in *J. Phys.: Condens. Matter*, (2014)

DY 58.6 Thu 16:00 Poster A

Photonic Bands of Colloidal Quasicrystals — ●RICARDO ATAHUALPA SOLORZANO KRAEMER and SCHMIEDEBERG MICHAEL — Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Quasicrystals are structures with long-range positional order but no translational symmetry. These structures lie between periodic and disordered structures but still show sharp diffraction patterns that confirm the long-range order. They possess several interesting properties that differ from those of periodic crystals or glasses. This may lead to an important role for new photonic applications.

Determining photonic bands of quasiperiodic systems represents a challenge. In this work we study the paths of photons in quasiperiodic Lorentz gas models in order to calculate the photonic bands. The models can be extended to achieve more realistic results. For example, in order to consider the effects of refraction, we employ Fresnel's equations. In order to include diffraction, we use Mie scattering. We calculate the band structures for three different geometries: periodic square lattices, the quasiperiodic Penrose tiling, as well as for a quasicrystal with 8-fold rotational symmetry.

DY 58.7 Thu 16:00 Poster A

Photonic Bands of Colloidal Quasicrystals — ●RICARDO ATAHUALPA SOLORZANO KRAEMER and MICHAEL SCHMIEDEBERG — Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

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DY 58.8 Thu 16:00 Poster A

Excitation of defects in colloidal quasicrystals close to the melting transition — ●MIRIAM MARTINSONS and MICHAEL SCHMIEDEBERG — Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine Universität Düsseldorf, 40204 Düsseldorf, Germany

Quasicrystals are structures with long range order but no translational symmetry. They can have any rotational symmetry including those that are not allowed in periodic crystals. In quasicrystals there are phononic modes as well as additional hydrodynamic modes called phasons. Such phasons correspond to correlated rearrangements of the particles and arise as a consequence of the additional degrees of freedom that do not exist in periodic crystals.

We study how local and global excitations or defects develop in quasicrystals close to the melting transition. Local excitations termed phasonic flips only occur in quasiperiodic systems. Other defects, e.g. dislocations and disclinations, cause the melting of the quasicrystal as predicted by the KTHNY theory. We analyze the positional and bond-orientational correlation functions during the melting process. Our studies reveal the similarities and differences of the melting mechanism of quasicrystals as compared to the melting of periodic crystals.

DY 58.9 Thu 16:00 Poster A

Effects of temperature on spinodal decomposition in liquid-vapor systems — ●MARTIN PÜTZ and PETER NIELABA — University of Konstanz, Germany

We use the "Smoothed Particle Hydrodynamics" (SPH) simulation method to investigate the dynamics and thermal evolution of spinodal decomposition of instantaneously temperature-quenched liquid-vapor systems. The numerical approach follows a modern formulation of SPH

with a van der Waals equation of state, thermal conduction and a simple scaling thermostat that allows thermal fluctuations at a constant predicted mean temperature. The results are in excellent agreement with theoretical predictions for all time regimes from the initial growth of "homophase fluctuations" up to the inertial hydrodynamics regime. We find that the initial stage spinodal decomposition is strongly affected by the temperature field. The domain growth in the late stage of demixing is found to be rather unaffected by thermal fluctuations. However, the crossover between these stages is found to occur earlier in time for higher initial temperatures. We explain this dependency with the phase interfaces that become diffuse and hence overlap when the predicted temperature becomes closer to the critical point.

DY 58.10 Thu 16:00 Poster A

Lateral migration of soft microparticles in wavy microchannels — ●MATTHIAS LAUMANN¹, BADR KAOU¹, ALEXANDER FARUTIN², ANDREAS KÖNIG¹, DIEGO KIENLE¹, CHAOUQI MISBAH², and WALTER ZIMMERMANN¹ — ¹Theoretische Physik, Universität Bayreuth, Bayreuth — ²Laboratoire Interdisciplinaire de Physique, CNRS-Université Joseph Fourier / UMR 5588, BP 87, F-28402 Saint-Martin d'Herès Cedex, France

We study the cross-streamline migration (CSM) of deformable particles in the limit of vanishing Reynolds number in 2D and 3D Poiseuille channel flow, which boundaries are spatially modulated. Using 1D dumbbells, 2D ring polymers, and 3D tetrahedrons (all of which may be symmetric or asymmetric), we demonstrate how the CSM can be modified when the waviness of the micro-channel is varied. Starting with the case of flat boundaries (zero modulation), these particles perform a CSM that is always directed towards the channel center[1]. In the case of wavy boundaries, this centric motion may be reversed once the modulation amplitude exceeds a lower threshold, in which case the particles migrate off-center and approach a stationary, non-curved trajectory, located between the walls and the center of the channel. The distance between such a trajectory and channel center can be increased by turning up the modulation amplitude, but depends also on other parameters such as the particle elasticity, for example. The results shown are obtained via a perturbation calculation of the wavy Poiseuille flow in the limit of small modulation amplitudes, and compared with those from Stokesian particle dynamics for arbitrary modulation amplitudes, showing good agreement. Our study suggests that the flow generated between wavy boundaries may be exploited for the separation of particles with varying properties in microfluidic channels.

[1]B. Kaoui, G. H. Ristow, I. Cantat, C. Misbah, W. Zimmermann, *Phys. Rev. E* 77, 021903 (2008)

DY 58.11 Thu 16:00 Poster A

Cross-streamline migration of soft and asymmetric particles in oscillatory shear flow — ●MATTHIAS LAUMANN¹, PAUL BAUKNECHT², ANDRE FÖRTSCH¹, STEPHAN GEKLE², DIEGO KIENLE¹, and WALTER ZIMMERMANN¹ — ¹Theoretische Physik, Universität Bayreuth, 95440 Bayreuth, Germany — ²Biofluid Simulation, Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

We investigate the dynamics and cross-streamline migration (CSM) of asymmetric, soft particles in oscillatory, linear shear flow. Using 1D dumbbells, 2D ring polymers, and 3D capsules as elementary representatives of such particles, we show that these may indeed migrate within the shear plane only if they have an intrinsic material asymmetry and if the shear gradient varies with time. The CSM exists over a wide range of parameters and, importantly, is a generic property, i.e., it does neither depend on the dimensionality of the particle nor on the details how the particle asymmetry is realized. The migration velocity can be tuned by various parameters, including the frequency and amplitude of the time-dependent, linear shear flow as well as the elastic properties of the particle. Besides the fundamental importance of this phenomenon, the ability to tune the migration process externally has promising applications in microrheology such as particle separation.

DY 58.12 Thu 16:00 Poster A

A Theoretical Investigation of Patterned Depositions from Thin Films of Evaporating Solutions — ●WALTER TEWES, SVETLANA GUREVICH, and UWE THIELE — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 9 48149 Münster, Germany

We aim at a theoretical description of patterned deposition of solute from an evaporating thin film of solution on a substrate.

For this purpose we formulate a system of coupled partial differential equations for thin solution layers, describing phase separation within the solution as well as dewetting and evaporation of the solvent.

The deposition process is investigated in the case of a contact line of the solution film which recedes due to pulling of the substrate (dip-coating) and/or evaporation.

The deposition patterns obtained by direct numerical simulations comprise stripes and patterns of hexagonal type. Central control parameters defining the properties of the occurring patterns are the velocity of the receding contact line and the initial concentration of the solution.

DY 58.13 Thu 16:00 Poster A

The shapes of simple comb polymers — ●CHRISTIAN VON FERBER¹, MARVIN BISHOP², THOMAS FORZAGLIA², COOPER REID², and GREGORY ZAJAC² — ¹Coventry University, UK — ²Manhattan College

This paper proposes an innovative approach towards the determination of shapes of branched polymers in the long chain limit. The method proposed develops an earlier suggestion by G. Wei which however in its evaluation is limited to specific regular structures. Here, we show that

by numerically evaluating and extrapolating the corresponding sums and integrals this approach is very powerful and will e.g. allow to determine in the same spirit the shapes of irregular branched structures. The carefully performed simulations including two different simulation schemes fully support the results of the semi-analytic approach. We demonstrate the method and compare the results with two different carefully performed MC simulation methods which favorably support the analytical results.

DY 58.14 Thu 16:00 Poster A

Differential Dynamic Microscopy of fluid microstructures in eutectic systems — ●CHRISTOPHER WITTENBERG — Universität Mainz, Mainz, Rheinland-Pfalz

The Differential Dynamic Microscopy (DDM) is a novel light microscopy technique to gain dynamic information of mesoscopic systems via real space imaging. DDM excels if the probed system is inhomogeneous in nature. In this case the advantage of microscopy comes into effect by sampling a specified location in the system. Using DDM the dynamics of various microstructures in a eutectic system has been analysed. We observed much smaller dynamic changes of such a structure over time compared to the variation between different microstructures.

DY 59: Poster - networks

Time: Thursday 16:00–18:00

Location: Poster A

DY 59.1 Thu 16:00 Poster A

Topological Phenotypes in Complex Leaf Venation Networks — ●HENRIK RONELLENFITSCH¹, JANA LASSER¹, DOUGLAS DALY², and ELENI KATIFORI¹ — ¹Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — ²New York Botanical Garden, Bronx, NY, USA

The leaves of vascular plants contain highly complex venation networks consisting of recursively nested, hierarchically organized loops. We analyze the topology of the venation of leaves from ca. 200 species belonging to ca. 10 families, defining topological metrics that quantify the hierarchical nestedness of the network cycles. We find that most of the venation variability can be described by a two dimensional phenotypic space, where one dimension consists of a linear combination of geometrical metrics and the other dimension of topological, previously uncharacterized metrics. We show how this new topological dimension in the phenotypic space significantly improves identification of leaves from fragments, by calculating a “leaf fingerprint” from the topology and geometry of the higher order veins. Further, we present a simple model suggesting that the topological phenotypic traits can be explained by noise effects and variations in the timing of higher order vein developmental events. This work opens the path to (a) new quantitative identification techniques for leaves which go beyond simple geometric traits such as vein density and (b) topological quantification of other planar or almost planar networks such as arterial vasculature in the neocortex and lung tissue.

DY 59.2 Thu 16:00 Poster A

Complex Network Based Role Attribution in International and Intersectoral Trade — ●JULIAN MALUCK and REIK V. DONNER — Potsdam Institute for Climate Impact Research, Germany

Supply chains in contemporary economy result in a complex network of trade relationships with a highly non-trivial topology. Multi-regional input-output tables summarize the monetary flows between industry sectors and can be meaningfully interpreted as a weighted and directed network of interacting subgraphs. We show that complex network theory provides sophisticated methods to attribute characteristic roles to industry sectors and countries. Specifically, in a directed network different patterns of clustering coefficients are attributed to different roles in the supply chain. In order to evaluate the robustness of trade relationships we introduce a generalization of the Hamming distance to weighted networks. In addition, we discuss how further standard network measures can be adapted on an economically meaningful way for studying the network properties of global trade.

DY 59.3 Thu 16:00 Poster A

Controllability of bipartite networks — ●CHIRANJIT MITRA and REIK DONNER — Potsdam Institute for Climate Impact Research, P.O. Box 60 12 03, 14412 Potsdam, Germany

We investigate the controllability of bipartite networks using the established concept of maximum matching as well as the more recently explored minimum dominating set approach. We consider random undirected bipartite networks consisting of two sets of N_1 and N_2 nodes, respectively, where every possible edge occurs independently with probability p . Under such settings, we find that for any given value of p , the number of unmatched nodes increases with $N_1 - N_2$. Likewise, for low values of p , although the domination number increases with $N_1 - N_2$ the change is not so sharp as compared to the change in the number of unmatched nodes obtained in a similar setting. However, for higher values of p , the domination number is almost independent of $N_1 - N_2$. For any given value of $N_1 - N_2$, the number of unmatched nodes is found to be mostly independent of p . On the other hand, for any given value of $N_1 - N_2$, the domination number decreases with increasing p . Moreover, we observe that at given values of $N_1 - N_2$ and p , the number of unmatched nodes is generally greater than or equal to the domination number.

DY 59.4 Thu 16:00 Poster A

Significance tests for topological characteristics of spatially embedded networks — ●MARC WIEDERMANN^{1,2}, JONATHAN F. DONGES^{1,3}, REIK V. DONNER¹, and JÜRGEN KURTHS^{1,2} — ¹Potsdam Institute for Climate Impact Research, Germany — ²Humboldt University, Berlin, Germany — ³Stockholm Resilience Centre, Stockholm University, Sweden

Spatially embedded complex networks, i.e., networks where the nodes are embedded in some metric space, have attracted increasing attention in many fields of science. In such systems, it is of particular interest to study which network properties can solely be explained by the spatial embedding of the nodes and which are unique to the system under study with respect to a predefined null hypothesis. For this purpose, we introduce a set of random null models for spatially embedded networks, which are constrained by the spatial embedding of the nodes to different extents. These surrogate networks are generated by randomly shuffling edges in the original network but preserving spatial properties such as the edge length distribution or the average length of edges emerging from each node. For three different real world systems, we use our framework to evaluate to what extent measurable network characteristics can be explained by the spatial embedding of the system alone. The proposed random network models serve to generally evaluate the significance of links and network characteristics in general spatially embedded networks and are applicable also to functional networks, where links represent significant similarities between different localized areas or monitoring points in the system under study.

DY 59.5 Thu 16:00 Poster A

Symmetry-based coarse-graining of regular evolved networks — ●STEFFEN KARALUS and JOACHIM KRUG — Institut für Theoretische Physik, Universität zu Köln

Virtually all empirical network structures are adjusted to their functional requirements by some evolutionary process adapting the topology for the specific needs. In most cases the functionality of a network is associated with the global behavior of dynamical processes based on the network. Many important processes are governed by the graph Laplacian. Its spectrum determines the overall behavior of such dynamics on a network. The strategy of evolutionary optimization can be successfully applied to find networks with a specific spectral dimension (power-law in the Laplacian spectrum) such that a non-trivial (subdiffusive) dynamical behavior emerges [1].

Networks evolved under the additional constraint of k -regularity exhibit an abundance of certain symmetric motifs. This can be exploited to construct quotient networks as systematic coarse-graining based on network symmetry [2]. This coarse-graining removes redundancies but retains the overall network structure. In this way we obtain a significant simplification of the evolved networks while the power-law spectrum and spectral dimension are preserved.

[1] S. Karalus and M. Porto, EPL 99, 38002 (2012).

[2] B. D. MacArthur and R. J. Sánchez-García, Phys. Rev. E 80, 026117 (2009).

DY 59.6 Thu 16:00 Poster A

Self-organized alternating chimera states in oscillatory media — ●SINDRE W. HAUGLAND, LENNART SCHMIDT, and KATHARINA KRISCHER — Physik-Department, Nonequilibrium Chemical Physics, Technische Universität München, James-Frank-Str. 1, D-85748 Garching, Germany

Oscillatory media can exhibit the coexistence of synchronized and desynchronized regions, so-called chimera states, for uniform parameters and symmetrical coupling. In a phase-balanced chimera state, where the totals of synchronized and desynchronized regions, respectively, are of the same size, the symmetry of the system predicts that interchanging both phases still gives a solution to the underlying equations. Through simulations of an oscillatory medium gov-

erned by a complex Ginzburg-Landau equation with nonlinear global coupling, we observe this kind of interchange as a self-emergent phenomenon, occurring repeatedly for an apparently indefinite amount of time. Simulations also corroborate the hypothesis that a steady expansion of the turbulent phase is favoured, whereas a global constraint restricts its overall size. In contrast to the case of the non-alternating chimera states also found in our model system, the phase balanced state is not stable for alternating chimera states, leading to diffusional growth slightly beyond phase balance and a subsequent interchange of phases. The existence of self-emergent, self-sustaining alternating chimera states broadens the scope of future research into chimera states in general, and may help improve our understanding of chimera-like phenomena observed in biology.

DY 59.7 Thu 16:00 Poster A

Topological and geometrical properties of mitochondrial networks — ●ANDREAS VERES, SVEN BAUERNEFELD, and MATTHIAS WEISS — University of Bayreuth, Bayreuth, Germany

Mitochondria typically form extended networks in eukaryotic cells which span throughout the cytoplasm. It is commonly believed that network formation correlates with the cells energy demand, yet the basic physico-chemical self-organization processes that govern network formation and maintenance are poorly understood. Using live-cell imaging and quantitative image analysis we have studied topological and geometrical properties of mitochondrial networks in untreated cells and in cells lacking microtubules. In particular, we have quantified the network efficiency via the "node betweenness" and we have used a number-and-brightness analysis and quantitative bleaching experiments to estimate the local flux within mitochondrial tubes. In response to drug treatment, we observed gross changes in the organization of mitochondria. Based on our experimental data, we have formulated a quantitative simulation model that rationalizes the observed transition.

DY 60: Poster - complex systems and data analysis

Time: Thursday 16:00–18:00

Location: Poster A

DY 60.1 Thu 16:00 Poster A

Modelling and prediction using symbolic regression by genetic programming — ●MARKUS QUADE, MARKUS ABEL, and RUGGERO VASILE — Ambrosys GmbH, Potsdam, Deutschland

Machine learning assisted modelling is used successfully in a broad variety of systems. However, the models are often not physically interpretable. Symbolic regression, in contrast, yields formulas as results, which can be analyzed by means of dynamical systems methods.

Specifically, we use evolutionary principles to explore possible models to forecast the production of green energy by genetic programming. In order to find suitable models in acceptable time, we extend the standard genetic programming method.

One advantage of this approach is that it is in principle not biased by human perception. Of course, prior knowledge about the system investigated should be used by providing building blocks and a goodness of fit measure. Finding a model means searching for a best fit in function and/or parameter space.

We illustrate our ideas in detail with real measurements and the corresponding prediction.

DY 60.2 Thu 16:00 Poster A

Complex Systems Approaches to Detecting Tipping Behavior in Paleoclimate Time Series — ●JASPER G. FRANKE and REIK V. DONNER — Potsdam Institute for Climate Impact Research, Potsdam, Germany

In the last years the existence of tipping elements in the Earth's climate system has gained increased attention. Here, tipping behavior refers to dynamical transitions of some subsystem leading to a qualitatively different state. In the light of the recent debate on possible regime shifts due to global climate change it is necessary to understand if, when and where such transitions have occurred in the past in order to assess possible future risks.

As tipping of climate elements should be accompanied by changes in the nonlinear dynamics (e.g., due to bifurcations or noise-induced transitions), methods from nonlinear time series analysis can lead to addi-

tional insights regarding the existence of past transitions. In this work, we study the capabilities of several recently developed methods like recurrence network analysis or visibility graphs as well as spatio-temporal methods to reveal complex signatures of past nonlinear regime shifts. The potentials and limitations of these novel approaches are systematically compared with those of classical early warning indicators like increasing autocorrelation, variance, etc. We illustrate the performance of the different methods for synthetic time series exhibiting tipping point behavior as well as different paleoclimate time series.

DY 60.3 Thu 16:00 Poster A

(How) Can we trust in Lyapunov exponents estimated from time series? — ●ULRICH PARLITZ — Max Planck Institute for Dynamics and Selforganization, Göttingen, Germany — Institute for Non-linear Dynamics, Georg-August-Universität Göttingen, Germany

Lyapunov exponents are fundamental for quantifying sensitive dependence on initial conditions and chaos. While their computation using dynamical evolution equations is quite straight forward (even for high dimensions and extended systems) estimating Lyapunov exponents from time series remains a challenge. We shall discuss and illustrate problems and pitfalls using time series generated by different chaotic systems. In particular we shall consider a six dimensional Lorenz-96 model that possesses a chaotic attractor (Kaplan-Yorke dimension $D=4.18$) with a single positive Lyapunov exponent. For this example estimation of the (largest) Lyapunov exponent(s) turns to be quite difficult and requires very long time series indicating practical limits of purely data based estimation methods.

DY 60.4 Thu 16:00 Poster A

Inhomogeneous shear-induced alignment of anisotropic binary mixtures — ●HENNING REINKEN, RODRIGO LUGO-FRIAS, and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Due to their presence in a wide variety of biological contexts and technological applications, the study of homogenous [1] and inhomogeneous mixtures of anisotropic particles has increased considerably in recent

years. One important question in that context is how their rheological properties change when they are driven out of equilibrium by means of a steady flow.

In the present work we develop an inhomogeneous equation for the shear-induced alignment of anisotropic binary mixtures in the scope of irreversible thermodynamics [2,3]. To this end, we calculate the entropy production that accounts for flow velocity, pressure and alignment. To guarantee a positive value, we establish the appropriate linear relations between the thermodynamic fluxes and forces.

- [1] R. Lugo-Frias and S. H. L. Klapp, in preparation (2015).
 [2] S. R. de Groot, P. Mazur, *Non-Equilibrium Thermodynamics*, Ed. Dover (1984).
 [3] S. Hess, I. Pardowitz, *Z.Naturforsch. A* **36a**, 554 (1981).

DY 60.5 Thu 16:00 Poster A

Finding optimal solutions for the delacorte numbers problem by using a hybrid optimization approach — ●JAN JURCZYK and ALEXANDER ECKROT — University of Regensburg, Regensburg, Germany

The delacorte numbers problem was proposed by Al Zimmermann in his computational contests. The goal is to find the maximum and minimum groundstate, where an interaction was defined by the greatest denominator times the euclidean distance in a square matrix containing the numbers from 1 to n^2 . Our approach is similar to the well known TSP-Problems, where finding backbones within the solution is critical in generating possible groundstates.

DY 60.6 Thu 16:00 Poster A

Markovian approximation and perturbation theory of transport processes in geophysical flows — NAOYA FUJIWARA¹, KATHRIN KIRCHEN^{2,3}, JONATHAN F. DONGES^{3,4}, ●REIK V. DONNER³, JÜRGEN KURTHS^{3,5}, and KAZUYUKI AIHARA¹ — ¹University of Tokyo, Japan — ²University of Bonn, Germany — ³Potsdam Institute for Climate Impact Research, Germany — ⁴Stockholm Resilience Centre, Sweden — ⁵Humboldt University, Berlin, Germany

We propose a Markov chain-based framework for analyzing passive transport in geophysical flows. For this purpose, the available space is coarse-grained, and transition probabilities between different boxes are estimated. The stochastic transition matrix becomes time-dependent if the underlying flow exhibits changes with time. In order to analytically treat this case, we introduce a first-order perturbation theory that allows evaluating the corresponding changes in terms of the largest eigenvalue and associated eigenvector of the perturbed transition matrix. Specifically, three different problem classes are studied that are potentially relevant for geophysical applications: point-wise absorption of particles, absorption in the presence of a constant input of particles, and changes in the steady state in the case of mass conservation. For some simple 2D flow model exhibiting Lagrangian turbulence, we demonstrate numerically that the absorption rates provided by first-order perturbation theory describe the actual dynamics of the system very well.

DY 60.7 Thu 16:00 Poster A

Non-global coupling in two- and three-state systems — ●SIMON CHRIST, BERNARD SONNENSCHNIG, and LUTZ SCHIMANSKY-GEIER — Humboldt-Universität zu Berlin, Institut für Physik, Deutschland

Two- and three-state renewal models with non-exponential waiting

time densities have been used to mimic noisy excitable and oscillatory systems to describe various processes like chemical reactions or neural networks. In this work effects of non-global coupling on steady and oscillatory states in random binary networks with exhibitory coupling or with indirect coupling as an active medium are investigated. In order to study global oscillations and bistable behaviour with respect to noise intensity and coupling strength or delayed feedback, direct numerical simulations are performed as well as an approximate mean field model is proposed for complex networks. It allows solution for the steady states supplemented with their stability analysis. Transition states and multistability were observed if varying the network structure.

DY 60.8 Thu 16:00 Poster A

Long-range response in AC and DC electricity grids — ●DANIEL JUNG and STEFAN KETTEMANN — School of Engineering and Science, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany

Local changes in the topology of electricity grids can cause overloads far away from the disturbance [1], making the prediction of the robustness against power outages a challenging task. The impact of single-line additions on the long-range response of DC electricity grids has recently been studied [2]. With this work, we extend the investigation to the case of alternating currents. Therefore, we study electricity grids with a random distribution of complex impedances on the edges of a regular 2D grid. By determining the resonance frequencies of the circuit, we are able to forecast consequences for the conditions for stable grid operation. Further, we analyse the spatial distribution of the voltage amplitudes.

- [1] D Witthaut, M Timme, *Eur. Phys. J. B* **86**, 377 (2013).
 [2] D Labavic, R Suci, H Meyer-Ortmanns, S Kettmann, *Eur. Phys. J. Spec. Top.* (2014).

DY 60.9 Thu 16:00 Poster A

The Coincidence Skill Score - a new approach to quantify event simultaneity in climate applications — ●JONATAN F. SIEGMUND and REIK V. DONNER — Potsdam Institut für Klimafolgenforschung, Postfach 601203, 14412 Potsdam

Besides gradual changes of the mean behaviour of climate variables, global climate change results in higher frequencies and intensities of extreme events like heat waves, droughts or intense rain events. The impacts of these events on terrestrial ecosystems are hardly known.

In this study, we develop an extension of the Coincidence Analysis, a method to detect non-random simultaneous appearances of extreme events in two time series. For this purpose, we consider a Non-Reaction-Rate, complementing the formerly studied Coincidence Rate, to define a Coincidence Skill Score, related to the Peirce Skill Score which is widely used in meteorological applications. The new method has the advantage of distinguishing between different cases of simultaneous and non-simultaneous events and therefore provides an alternative for the comparison of time series with different numbers of extreme events.

We apply this approach to investigate the influence of climatic extreme events on wildlife plant flowering phenology for Germany. Our results underline formerly found relationships and additionally highlight long-term-dependencies between extremely high temperatures and very early plant flowering with a time-lag of almost one year. These results support hypotheses, that more and stronger climate extreme events might sustainably disturb domestic ecosystems.

DY 61: Poster - Glasses

Time: Thursday 16:00–18:00

Location: Poster A

DY 61.1 Thu 16:00 Poster A

Molecular dynamics simulation of Two-Dimensional silica using multi-body potentials. — ●PROJESH KUMAR ROY¹ and ANDREAS HEUER² — ¹Institute of Physical Chemistry, University of Muenster. — ²Institute of Physical Chemistry, University of Muenster.

The discovery of a new material called "Two-dimensional silica bilayer"[1][2]; has created a great excitement among the glass scientists. Using STM and SPM method it was revealed that the material consists of only two atomic layers of silica. It behaves like a 2-D system due to a very remarkable symmetry present between the layers. Under different reaction condition both crystalline and amorphous form was produced separately and sometimes both in the same layer. The nature of the amorphous form is very similar to the Zacharisen's 2D silica glass model. Earlier a "Soft-Core Yukawa"[3] type potential was used to a 2-D model of silica bilayer to describe this structure formation in amorphous state by energy minimization method of the "Inherent Structures"[4]. For a stable 3D model; a continuous surface potential, a gravitational field, and a multi-body potential; such as Stillinger-Weber type three body potential [5]; was used. The system was simulated in various temperatures in NVT. Thermodynamic and kinetic properties of the system were studied and a crystal amorphous transition was characterized.[1]Heyde M. et al,Chem.Phys.Lett. 550,1(2012).[2]HuangP.Y. et al,Nano Lett.,12,1081(2012) [3]Mendez-Maldonado et al.,J.Chem.Phys.137,054711(2012).[4]Stillinger F. et al,Phys.Rev.A 25,2,978(1982). [5]Feuston B.P. et al,J.Chem.Phys,89,9(1988).

DY 61.2 Thu 16:00 Poster A

Influence of Atomic Tunneling Systems carrying a Large Nuclear Quadrupole Moment on the Dielectric Properties of Glasses at Very Low Temperatures — ●ANNINA LUCK, NILS HAUFF, ANNE ZEISSNER, ANDREAS FLEISCHMANN, ANDREAS REISER, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

Glasses containing significant amounts of isotopes carrying large nuclear electric quadrupole moments show very surprising effects that are not explained by the standard tunneling model. These effects appear in dielectric measurements, both in the low frequency and the microwave regime.

The nucleus of ¹⁶⁵Ho carries a very large electric quadrupole and therefore appears to be a good candidate to investigate the influence of atomic tunneling systems carrying a large nuclear quadrupole moment on the dielectric properties of glasses down to very low temperatures. Here, we present measurements of dielectric properties of the multi-component glass HY-1, containing several percent of holmium. These measurements have been performed in a wide frequency range from 60 Hz to 1 GHz and at temperatures between 7 mK and several Kelvin.

Our measurements show surprising temperature, frequency and electric field strength dependent effects that indicate a non-phonon based thermal relaxation process.

DY 61.3 Thu 16:00 Poster A

Effects of Confinement on the Dynamics of Aqueous Mixtures — ●MATTHIAS SATTIG and MICHAEL VOGEL — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt

The dynamical behavior of aqueous mixtures in bulk and in confinement is a topic of great interest. For example, a water concentration dependent behavior of the glass transition temperature was found in PG-water and in PGME-water mixtures, which is very different for the two cases [1]. This was attributed to different possibilities of both molecules to form H-bonds in the bulk and different mechanisms of H-bonding in the presence of additional water. The forming of H-bonds can be disturbed by introducing a geometrical confinement, whose surface interacts with the guest molecules and spatially restricts the bond network. We present rotational correlation times τ of both above mentioned mixtures in bulk and in mesoporous silica MCM-41 at several water concentrations, obtained from ²H-NMR. In the high temperature regime spin-lattice-relaxation experiments show similar results for both mixtures in bulk and in confinement. At lower temperatures they hint at the occurrence of a phase separation, assisting the interpretation from Elamin et al. [2]. They propose the idea of water clustering at the surface. Our results are compared with results from dielectric spectroscopy of the mixtures in bulk and confinement. Similarities with water confined in MCM-41 are discussed, where the observable relaxation at low temperatures was attributed to surface layer of water[3].

[1] Sjöström et al., PCCP, 12, 10452, 2010 [2]; Elamin et al., to be published; [3] Sattig et al., PCCP,16, 19229, 2014

DY 61.4 Thu 16:00 Poster A

Theory of heterogeneous viscoelasticity — ●WALTER SCHIRMACHER^{1,2,3}, GIANCARLO RUOCCO³, and VALERIO MAZZONE³ — ¹Universität Innsbruck — ²Universität Mainz — ³Università "La Sapienza" Roma

We present a new theory of viscoelasticity of a glass-forming viscous liquid near and below the glass transition. In our model we assume that each point in the material has a specific viscosity, which varies randomly in space according to a fluctuating activation free energy. We include a Maxwellian elastic term and assume that the corresponding shear modulus fluctuates as well with a similar distribution as that of the activation barriers. The model can be mapped to an effective heterogeneous elasticity theory, which is solved in coherent-potential approximation (CPA). The theory predicts an Arrhenius-type temperature dependence of the viscosity in the vanishing-frequency limit, independent of the distribution of the activation energies. It is shown that this activation energy is generally different from that of a diffusing particle with the same barrier-height distribution. At finite, but low frequencies the theory describes low-temperature alpha relaxation together with the beta wing. Good agreement with data on metallic glasses is obtained. At high frequencies the theory reduces to heterogeneous elasticity theory, which explains the occurrence of the boson peak and related vibrational anomalies.

DY 62: Poster - Dynamics

Nonlinear Dynamics, Synchronization and Chaos; Delay and Feedback Dynamics; Pattern Formation
Modelling of non-linear dynamics in biological movement; Granular Matter /Contact Dynamics

Time: Thursday 16:00–18:00

Location: Poster A

DY 62.1 Thu 16:00 Poster A

Ergodicity criterion for small Hamiltonian systems — ●PATRICK PIETZONKA and UDO SEIFERT — II. Institut für Theoretische Physik, Universität Stuttgart

We study the long-time behavior of Hamiltonian systems in the context of a formalism developed by H. Mori, R. Zwanzig and M. H. Lee (MZL) [1]. This formalism leads to the representation of autocorrelation functions of dynamical observables as infinite continued fractions. From the convergence properties and the analysis of these mathematical constructs we derive a simple formulation of an ergodicity criterion.

We illustrate this criterion by applying it to non-linear oscillators and short chains of non-linearly coupled particles. These examples require the numerical computation of a large number of continued fraction coefficients.

Our approach reveals some general limits of the MZL formalism for certain classes of correlation functions. To overcome these limits we suggest a generalization that may lead to better approximations of correlation functions and entail a refined ergodicity criterion.

[1] M. H. Lee, Phys. Rev. Lett. **49**, 1072 (1982)

DY 62.2 Thu 16:00 Poster A

A prototype dynamical system with a generalized mechanical potential — ●BULCSÚ SÁNDOR and CLAUDIUS GROS — Institut für Theoretische Physik, Goethe Universität, Frankfurt am Main, Germany

In dynamical systems theory, prototype systems are often used to investigate different bifurcation scenarios or certain dynamical behaviours. Systems, like the van der Pol oscillator, the Takens-Bogdanov system, or the Rössler system, are considered to be prototypical examples for the birth of limit cycles, homoclinic and period doubling bifurcations respectively, but leave little or no possibility to be reshaped for exploratory purposes while keeping their major dynamical features unchanged. Thus, one would sometimes like to design simple systems with predefined properties to understand the bifurcations of systems with higher complexity.

In this work a new class of prototype systems is proposed, which provides a mechanistic understanding for many different dynamical behaviours, including the previously mentioned bifurcations. We introduce a generalized mechanical potential which allows the local minima to be placed at arbitrary locations. Together with a velocity dependent force term one can easily control the flow through the parameters, by changing the balance between energy uptake and dissipation along the trajectory. Increasing the dimensionality of the system a whole cascade of limit cycle bifurcations is revealed, culminating in a period-doubling route to chaos.

DY 62.3 Thu 16:00 Poster A

Transient dynamics reveal network connectivity — ●JOSE CASADIEGO^{1,3} and MARC TIMME^{1,2,3} — ¹Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — ²Institute for Nonlinear Dynamics, Faculty of Physics, University of Göttingen, 37077 Göttingen, Germany — ³IMPRS Physics of Biological and Complex Systems, Göttingen Graduate School for Neurosciences, Biophysics and Molecular Biosciences, 37077 Göttingen, Germany

Determining the physical structure of interactions within a network poses a great challenge to date. Still, current methods are mostly designed to deal with long recordings of network dynamics, which (sometimes) may be infeasible. Thus, developing methods that rely only on short recordings will fill an important gap. Here we demonstrate that transient-responses of networks to dynamical perturbations reveal its structure. By applying external driving signals to units, we track how networks transiently respond to signals for short periods of time (~10 measurements). We explicitly demonstrate the direct relation between these transient responses and network connectivity. As examples, we retrieve full connectivity of networks of coupled Kuramoto-like oscillators exhibiting complex non-periodic dynamics. Assuming sparseness, we safely recover network connectivity even if the number of different transient dynamics is much smaller than the number of units in the network. Our approach is model independent and does not rely on particular features of specific systems (e.g. fixed points or limit cycles).

DY 62.4 Thu 16:00 Poster A

Slow points and adiabatic fixed points in small neural networks — ●HENDRIK WERNECKE and CLAUDIUS GROS — Institut für Theoretische Physik, Goethe-Universität, Max-von-Laue-Str. 1, Frankfurt am Main, Germany

Fixed points and limit cycles play an important role for the dynamics of neural networks. However, in the present work we examine the influence of slow points on the flow and motion in phase space.

A special kind of slow points, so-called attractor remnants, come into existence when adding a slowly varying dimension to a (faster) system. At the fixed points of the faster system the flow does no longer necessarily vanish, but these points are still present in the network as slow points. In order to examine the influence of the slow points on the compound system, the concept of adiabatic fixed points is introduced and the effect on small neural networks is discussed.

It turns out that with the help of these remnants one can describe a mechanism that spans limit cycles and determines the dynamical behaviour of the system. To analyze and compare systems of different dimensionality measures such as the system's speed in phase space or the distance of the trajectory to the adiabatic fixed points are defined and their properties are examined.

DY 62.5 Thu 16:00 Poster A

Delay-Induced Dynamics of Localized Structures in Systems

with Spatial Inhomogeneities — ●FELIX TABBERT and SVETLANA GUREVICH — Institut für Theoretische Physik, Münster

We are interested in the control of localized structures in spatially extended dissipative systems by time-delayed feedback. We show that changes in the delay time and the delay strength lead to various dynamical solutions including the formation of traveling waves, the annihilation of the localized solutions as well as drifting localized structures. We provide a linear stability analysis of the delayed system and obtain an analytical expression for the delay-induced instability threshold. Numerical simulations are also carried out, showing good agreement with the predicted instability-thresholds.

We also consider the effects of spatial inhomogeneities and defects, which are inevitable in any experimental setup. These inhomogeneities break symmetries of the system under consideration and therefore affect the critical modes of a localized solution. The competing effects of destabilizing delay and stabilizing defects are studied both numerically and in terms of a linear stability analysis.

DY 62.6 Thu 16:00 Poster A

Bifurcations in a minimal model of predator-swarm interactions — ●LUKAS OPHAUS and UWE THIELE — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Germany

We analyse a minimal model of predator-swarm interactions, that was first introduced by Y. Chen and T. Kolokolnikov. It was found that depending on the employed parameters and model details different dynamics occur. The complex shapes of the swarm are similar to observations in nature [1].

Here, we investigate in particular the bifurcations between static and dynamical states. We focus on the predator strength. Different outcomes are e.g. a stable ring of the prey with the predator at its centre, periodic chasing dynamics and solutions with irregular dynamics.

[1] Chen Y., Kolokolnikov T., J. R. Soc. Interface 11: 20131208 (2014).

DY 62.7 Thu 16:00 Poster A

Sound absorption of granular materials — ●TAMARA ZÜHLSDORFF¹, ANNA-MARIA DAXLBERGER¹, and THOMAS GRILLENBECK^{1,2} — ¹Ignaz-Günther-Gymnasium Rosenheim — ²Fakultät für angewandte Natur- und Geisteswissenschaften, Fachhochschule Rosenheim

We examine the sound absorption coefficient of granules. We are especially interested in how the sound absorption depends on the state and the history of the material. Our experiment is implemented with variant of "Kundt's pipe" which sends an acoustic noise to granules and appraises the results. With these data we can calculate the sound absorption coefficient.

DY 62.8 Thu 16:00 Poster A

A Computer Simulation and Experiments to explain the phenomenon of convection rolls in rotating boxes — ●ANN-KATHRIN RAAB^{1,2}, ADRIAN EBERT², and THOMAS GRILLENBECK² — ¹Technische Universität München D-85748, Germany — ²Ignaz-Günther-Gymnasium Rosenheim D-83026, Germany

In an investigation of self-organized pattern formation in rotating packings, several experiments showed a phenomenon which no one can explain yet: In 2D packings sometimes there are convection rolls and sometimes not, whereas in 3D packings the patterns appear every time. A computer simulation should help to find out, whether the pattern building in 2D packings appears spontaneously or if there are any undiscovered circumstances which might lead to convection rolls. By using simple experiments with self constructed packings we will determine possible connections between the 2D simulation and the previous 2D and 3D experiments.

DY 62.9 Thu 16:00 Poster A

Controlling electrical charges in granular matter — ●ANDRÉ SCHELLA, MATTHIAS SCHRÖTER, and STEPHAN HERMINGHAUS — Max-Planck Institut für Dynamik und Selbstorganisation (MPIDS), Am Faßberg 17, 37077 Göttingen

It is known since ancient times that two bodies rubbed together acquire electrostatic charges. Even though such charges can have a tremendous impact on e. g. industrial powder manufacturing and dust storms, the physical basis behind this process called contact electrification is still on open debate [1], [2]. Recently, Liao et al. [3] examined the influence of the shaking conditions on the electrostatic charge of identical beads in a container. There, it was argued that contact electrification

is mainly due to a contact potential difference between the beads and the container walls, whereas other authors found electrification even in same materials [4]. In this contribution, we present charge measurements of identical beads that were vertically shaken in a container. We will work out if material properties of the beads resp. the container, the shaking conditions and the environmental conditions affect the charge gained via contact electrification. [1] L. McCarty and G. Whitesides; *Angew. Chem. Int. Ed.* 47 (2008) 2188 [2] D. Lacks and R. Sankaran; *J. Phys. D: Appl. Phys.* 44 (2011) 453001 [3] Liao et al.; *Powder Technology* 208 (2011) 1-6 [4] S. Waitukaitis et al.; *Phys. Rev. Letters* 112 (2014) 218001

DY 62.10 Thu 16:00 Poster A

Simulation of the Chain Fountain — ●LUKAS ZWIRNER, VOLKER BECKER, and KLAUS KASSNER — Otto-von-Guericke Universität Magdeburg, Institut für Theoretische Physik/Computerorientierte Theoretische Physik

Although chain dynamics is a subject of investigation since the 17th century, chains exhibit various counterintuitive behaviors, e.g. the end of a chain falls faster than g , due to tension (Hamm, Geminard: *Am. J. Phys.*, Vol 78, No. 8. Aug. 2010).

Another spectacular example — the chain fountain — was investigated by Biggins et al. (*Proc. R. Soc. A* 470, 2014) inspired by a famous youtube video, which was made by Steve Mould and scored ~ 1.5 million views. Such a chain fountain can be established by pulling an appropriate chain, resting in a beaker, over the rim. Then, it 'flows' out due to gravity. However, instead of just sliding on the rim the chain forms a fountain. Biggins et al. argued that the origin of the chain fountain should be a pushing reaction force from the beaker during pickup process.

Our aim is to simulate these phenomena. Therefore a two-dimensional DEM simulation for granular matter was altered to allow links between polygonal particles, represented by damped springs. This allows us to study the behavior of different 2D chains with little restrictions (the chain elements need to be convex polygons) and to get detailed insight into the forces and tensions acting in the chain and thus into the origin of the fountain formation.

DY 62.11 Thu 16:00 Poster A

Feuchtetransport in granularen Medien — ●YANNICK WEIS¹ und THOMAS GRILLENBECK² — ¹Ignaz-Günther-Gymnasium, Rosenheim — ²Fakultät für angewandte Natur- und Geisteswissenschaften, Fachhochschule Rosenheim

Herrscht ein Konzentrationsunterschied, so wandern Teilchen auch bei ruhiger Umgebung vom Ort höherer Konzentration zum Ort niedrigerer Konzentration. Liegt dieser Unterschied im Dampfdruckgehalt vor, so wandert Feuchte vom Ort höheren Drucks zum Ort niedrigeren Drucks. Dies kann auch durch eine Trennwand geschehen (Feuchtediffusion).

Wir untersuchen experimentell den Feuchtetransport durch granuläre Packungen. Proben, welche ein Glas, gefüllt mit Trockenmittel (dry-cup) oder Wasser (wet-cup), abdichten (Holz im Vergleich zu Porenbeton), werden in den Klimaschrank bei 20 Grad Celsius und 50 % relativer Luftfeuchte gestellt. Die Proben bilden die Trennwand zwischen zwei Klimata mit unterschiedlich konstantem Dampfdruck bei konstanter Temperatur. Durch das Dampfdruckgefälle diffundiert Wasserdampf durch die Probe in den trockeneren Raum und erhöht dort die Wassermasse. Im feuchteren Raum wird die Wassermasse geringer. Diese Veränderung der Masse kann durch Wägung bestimmt werden.

DY 62.12 Thu 16:00 Poster A

Mechanical properties of sheared wet granular piles — ●ANNALENA HIPPLER¹, MARC SCHABER¹, SOMNATH KARMAKAR¹, MARIO SCHEEL³, MARCO DI MICHIEL³, MARTIN BRINKMANN², and RALF SEEMANN^{1,2} — ¹Experimental Physics, Saarland University, 66041 Saarbrücken, Germany — ²MPI for Dynamics and Self-Organization, Am Faßberg 17, 37077 Goettingen, Germany — ³European Synchrotron Radiation Facility, 6 rue Jules Horowitz, 38000 Grenoble, France

The mechanical properties of dry and wet bead packs are explored when being sheared with a parabolic profile at constant shear volume. The dissipated energy can be determined from the measured differential pressure and increases about linearly with external pressure for both dry and wet bead packs. However, the dissipated energy for wet beads has a finite value for vanishing external pressure and increases slower with external pressure compared to dry beads.

Using a downsized version of the shear cell the reorganization of

beads and liquid is imaged using ultrafast x-ray micro-tomography. The movement of each bead can be tracked during the shear process. The relative movement of the beads causes the breakup of liquid capillary bridges and the liquid that was stored in the liquid bridges is redistributing within the bead pack. The contribution of the breaking capillary bridges to the dissipated energy can be quantified by directly detecting individual rupture events and by analyzing the bead-to-bead-distances.

DY 62.13 Thu 16:00 Poster A

Mesoscale Modelling of Aeolian Sand Transport — ●ANNE MEIWALD, MARC LÄMMELE, and KLAUS KROY — Institute of Theoretical Physics, Leipzig, Germany

When driven by wind, sand in the desert or at the beach generates an impressive zoo of structures ranging from delicate ripples to wavy sand seas spanning orders of magnitude in their size. To understand how these structures emerge, it is essential to thoroughly describe of the underlying, seemingly chaotic, hopping motion of the sand grains. In order to make the complex grain scale physics more amenable to analytical studies, a coarse-graining approach was proposed that maps the ensemble of grain trajectories onto two populations representing fast salting and slow reptating grains [1,2]. On this basis, we now analyse the mesoscale structure of aeolian sand transport. We find the predicted mesoscopic observables like the mean hop length or height and particle velocity to be in a remarkable agreement with experimental data gained from various field and wind tunnel experiments. Since the physics on the mesoscopic scale is apparently insensitive to a higher resolution of the grains movement, we argue that our coarse-grained model offers a suitable starting point for the efficient numerical mesoscale modelling of aeolian sand transport and structure formation.

[1] Andreotti, B., *J. Fluid Mech.* 510, 47-70 (2004)

[2] Lämmel, M., Rings, D., Kroy, K., *NJP* 14, 093037 (2012)

DY 62.14 Thu 16:00 Poster A

Clustering and melting of a driven wet granular monolayer — PHILIPP RAMMING, INGO REHBERG, and ●KAI HUANG — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany

Due to the cohesion arising from the capillary interactions, partially wet granular matter exhibits dramatically different mechanical properties in comparison to its dry counterpart. Focusing on agitated wet spherical particles in a quasi-two-dimensional configuration, we investigate experimentally how the cohesion influences the collective behavior of wet granular matter and discuss possible links to the mobility of individual particles. As the agitation strength increases, a clustering into a wet granular crystal followed by a gradual melting arises. We characterize both transitions with the bond orientational order parameters and the mean kinetic energy of the particles through particle tracking. Moreover, the influence from the liquid content and the filling fraction will also be presented.

DY 62.15 Thu 16:00 Poster A

Thermal conductivity and geometric cohesion in aspherical granular materials — ●KATHARINA STAUDT¹, FELIX TRISKA¹, and THOMAS GRILLENBECK^{1,2} — ¹Ignaz-Günther-Gymnasium Rosenheim — ²Fachhochschule Rosenheim

It is well known that the thermal conductivity of a granular material depends on the volume of granules per unit volume (packing fraction): The more intense the packing of thermo-conductive granules in a less conductive medium, the higher the thermal conductivity of the composite material. Most experiments and theoretical considerations use spherical granules; much less is known about the thermal conductivity of aspherical granular materials. Here, we use standard U-shaped staples as radically aspherical granules. Due to their peculiarity to show geometric cohesion (i.e., cohesion due to particle geometry), we hypothesize that their thermal conductivity at low packing fractions is higher than for comparable spherical granular materials.

In our experiments, we will systematically vary the packing fraction of the staples (in air) by different perturbations (like vibrating) or different manual stacking procedures and determine the thermal conductivity afterwards.

DY 62.16 Thu 16:00 Poster A

Contact angle hysteresis of a capillary bridge - control with inkjet printing — ●SIMEON VÖLKELE, INGO REHBERG, and KAI HUANG — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

When walking on the beach, one can notice a stripe of particularly firm ground splitting the dry sand and the sea. The stiffness of partially wet granular matter, particularly in the so called pendular regime, arises from the cohesion conveyed by the capillary bridges between adjacent granular particles. Existing models describing such a cohesive force typically include a constant contact angle between the wetting liquid and the particle as a parameter. In practical situations, e.g. wet sand at the beach, an equilibrium contact angle should not be taken as granted due to environmental changes such as raining or draining.

In order to address experimentally such an influence, we control the volume of a single capillary bridge between two spherical particles with nanoliter resolution using an ink jet printer and employ evaporation for volume withdrawal. Using this technique we can drive our system into a limit cycle, which in turn allows precise measurement of the contact angle hysteresis via image analysis.

DY 62.17 Thu 16:00 Poster A

3D contact force measurement in a granular packing — ●JUNAID MASUD LASKAR¹, STEPHAN HERMINGHAUS¹, MATTHIAS SCHRÖTER¹, and KAREN E. DANIELS² — ¹Dynamics of Complex Fluids, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Department of Physics, North Carolina State University, Raleigh, USA

Knowing the contact forces and their statistical distributions inside a granular packing is a central question in granular physics. Measurement of contact force distributions and force chains till now have been possible only in 2D [1,2]. However, the physics is expected to be different inside 3D granular packings.

Towards this end, we have implemented a two photon spectroscopy technique, by harnessing the pressure dependent fluorescence property of ruby [3]. The technical challenges, introduced by the high refractive index ($RI \sim 1.76$) of ruby, are solved by designing a high numerical aperture ($NA \sim 1.4$) objective lens and finding a RI matched light scattering free immersion liquid solution. The first proof of concept experimental results will be discussed.

References: [1] T. S. Majumdar and R. P. Behringer, *Nature* 453, 1079 (2005) [2] Karen E. Daniels and Nicholas W. Hayman, *J. of Geophys. Res.* 113, B11411 (2008) [3] Y. Chen et al., *J. Appl. Phys.* 101, 084908 (2007)

DY 62.18 Thu 16:00 Poster A

Friction with your neighbors? Think locally! — ●MATTHIAS SCHRÖTER¹, MAX NEUDECKER¹, CYPRIAN LEWANDOWSKI², PASCAL WIELAND², CLAUD HEUSSINGER², FABIAN SCHALLER³, and GERD SCHRÖDER-TURK³ — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen — ²Georg-August University of Göttingen — ³Friedrich-Alexander-Universität Erlangen-Nürnberg

Understanding how the number of contacts Z in a packing of particles depends on the global volume fraction ϕ is a fundamental questions in soft matter physics. If the particles under consideration are soft and frictionless spheres, such as emulsions and foams, assuming $Z(\phi)$ is reasonable because additional contacts are formed by the globally isotropic compression of the particles which also increases ϕ . However, in frictional granular media the control of ϕ is not achieved by compression but by changing the geometric structure of the sample; if we want to fill more grains into a container we do not compress them with a piston, but we tap the container a couple of times on the table.

But if Z and ϕ are not simultaneously controlled by a globally defined parameter such as pressure, the idea of a function $Z(\phi)$ runs into an epistemological problem. Contacts are now formed at the scale of individual particles and their neighbors, a scale where ϕ is undefined. What is therefore needed for the theoretical description of frictional particles is an ansatz which explains Z using only locally defined parameters. This poster reviews recent progress towards such a theory based on experimental results obtained by X-ray tomography of packings of spheres, ellipsoids, cylinders and tetrahedra.

DY 62.19 Thu 16:00 Poster A

Coarse-grained Simulations of Dune Field Evolution — ●MEIKE WILL, SVEN AUSCHRA, MARC LÄMMEL, and KLAUS KROY — Institut für Theoretische Physik, Universität Leipzig, Germany

Crescent-shaped sand dunes, so-called barchans, are among the most impressive structures observed in arid regions on Earth and on Mars. Well established dune models [1] suggest that isolated barchans are unstable when fed by constant sand flux – they either shrink until they vanish or grow forever. As barchans commonly arrange in large and homogeneous fields, the existence of these assemblies indicates that

interactions among adjacent dunes can stabilise them [2].

To investigate the underlying mechanism, we start from an approximate analytical parametrization of the shape and mass evolution of individual barchans [3] and develop a coarse-grained model that explicitly accounts for the wind-driven mass exchange between consecutive dunes. Sand supplied by the horns of upwind followers to a barchan initiates a complex response of its shape and mass. A numerical implementation of the derived model relations is used to simulate large barchan fields. Preliminary results indicate that the dune field, as it advances downwind, converges towards a steady state that is characterized by a fixed point that closely controls dune size and density, thereby reproducing field observations.

[1] Kroy, K. et al., *Phys. Rev. Lett.* 88, 054301 (2002)

[2] Durán, O. et al., *Nonlin. Processes Geophys.* 18, 455-467 (2011)

[3] Fischer, S. et al., *Phys. Rev. E* 77, 031302 (2008)

DY 62.20 Thu 16:00 Poster A

Traveling waves: orientational and reflection effects induced by sudden control parameter changes — ●FABIAN BERGMANN and WALTER ZIMMERMANN — Theoretische Physik, Universität Bayreuth, Bayreuth

Traveling wave (TW) patterns are observed in many nonequilibrium systems, including chemical reactions [1, 2] or biological systems. In light-sensitive chemical reaction-diffusion systems or in certain biological systems [3] the respective control parameter can be suddenly changed from beyond to below critical.

We reveal some generic phenomena induced by such control parameter steps in one and two dimensions. In 2d we find an orientational effect of the step on TWs, where the waves orientate with their propagation direction perpendicular to the step. This behavior has also been found in a recent experiment.

If we restrict our system to one spatial dimension, a sudden control parameter drop from beyond to below threshold has consequences similar to suppressing boundary conditions [4]. Depending on the length scale of the control parameter change or on the group velocity of the TWs we can switch between TWs in the supercritical range to so-called blinking states, where the envelope of TWs changes as a function of time.

[1] M. Dolnik, A. R. Rovinsky, A. M. Zhabotinsky, I. R. Epstein, *J. Phys. Chem. A* 103, 38 (1999) [2] V. Vanag and I. R. Epstein, *Phys. Rev. Lett.* 87, 228301 (2001) [3] J. Schweizer, M. Loose, M. Bonny, K. Kruse, I. Münch, P. Schwille, *PNAS* 109, 15382 (2012) [4] M. C. Cross, *Phys. Rev. A* 38, 3593 (1988)

DY 62.21 Thu 16:00 Poster A

Influence of spatio-temporal modulations on the orientation of stripe patterns — ●LISA RAPP, VANESSA WEITH, ALEXEI KREKHOV, and WALTER ZIMMERMANN — Theoretische Physik, Universität Bayreuth, Bayreuth

Labyrinth-like stripe patterns occur in a variety of isotropic systems from chemical reactions, thermal convection and vegetation patterns to diblock copolymers. For a deeper understanding of the dynamics of patterns as well as for many technical applications, however, the control of the stripe patterns is important. We show that spatiotemporal modulations are an effective mechanism to control the pattern morphology. Using traveling, large modulation wavelengths compared to the intrinsic periodicity of the pattern, labyrinth-like patterns can be straightened in favor of regular stripe patterns. The orientation of the stripes can be controlled and selected by varying the velocity of the traveling modulation. In systems with broken symmetries long-wavelength modulations can be used to suppress other patterns such as hexagons or squares in favor of stripe patterns. To support the results obtained from linear stability analysis, we quantitatively analyze simulations of the two-dimensional Swift-Hohenberg model with regard to the distributions of local orientation angles of the stripes.

DY 62.22 Thu 16:00 Poster A

Non-Equilibrium Heating Dynamics of Interacting Luttinger Liquids — ●SEBASTIAN HUBER^{1,2}, MICHAEL BUCHHOLD^{1,2}, and SEBASTIAN DIEHL^{1,2} — ¹Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden, Germany — ²Institute of Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria

Thermalization dynamics of one dimensional bosonic systems have recently attracted strong attention. As a generic example of a non-integrable model, we investigate the dynamics of an interacting Luttinger Liquid driven out of equilibrium by persistent heating. In order to find signatures of thermalization and determine the non-equilibrium

dynamics of this system, we derive the kinetic equation for the time dependent phonon density and self-energy in a Keldysh non-equilibrium framework.

The resulting dynamics of the time dependent phonon density can be separated into two distinct momentum regimes. For large momenta, an effective thermalization process sets in, spreading continuously to lower momenta. In contrast, at low momenta, the system is described by a non-equilibrium distribution, growing linear in the momentum variable. This linear increase is protected by the structure of the three-phonon scattering vertex.

In the non-equilibrium regime, the scaling form of the phonon lifetimes is modified compared to the known equilibrium result, resulting in a new universal exponent. We show that both the structure of the phonon density and the scaling of the phonon lifetimes can be experimentally detected by means of Bragg spectroscopy.

DY 62.23 Thu 16:00 Poster A

Synchronization and Phase Separation of Motile Oscillators — ●SEBASTIAN MILSTER and LUTZ SCHIMANSKY-GEIER — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr.15, 12489 Berlin

We present a model of noisy interacting Kuramoto phase oscillators with unimodal and bimodal frequency distributions. The oscillators have also the ability to move in two spatial dimensions as noisy self-propelled particles. Within a small sensing radius, these moving oscillators are locally coupled. The motility facilitates a rearrangement of the oscillators. It changes locally the network structure while maintaining the global degree distribution.

This complex temporal network of non-identical phase oscillators exhibits various behaviors ranging from completely disordered over transient waves to globally synchronized states. In this work we study the influence of the motility on the synchronization processes in vessels

and periodic confinements. We conclude to what extent the techniques of static network analyzes are applicable. First insights into the underlying dynamics are deduced from a globally coupled network approach and we present analytical results for static networks with a multimodal distribution of the intrinsic frequencies. For identical oscillators, we estimate critical values of coupling strength for the onset of synchronization. In case of a bimodal frequency distribution, a manipulation of the oscillators' motility in the dependence of the degree of synchronization leads to a spatial separation of the two populations with different frequencies.

DY 62.24 Thu 16:00 Poster A

Anisotropic Finite Size Scaling of Orientation Correlation Functions in Stripe Phases Free of Topological Defects — ●CHRISTIAN RIESCH, GÜNTER RADONS, and ROBERT MAGERLE — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz

Recently, we discovered aging in the orientation dynamics of an ordered stripe-forming system in two dimensions, referred to as model B with Coulomb interactions [1]. Here, we study the influence of the aspect ratio and the size of the system on this dynamics. We find that the underlying mechanism governing the non-equilibrium evolution is the anisotropic coarsening of correlated regions within the orientation field. The spatial correlation functions perpendicular and parallel to the stripes coarsen as power laws of time with different exponents. The observed type of aging is also found in stripe phases described by the conserved and nonconserved Swift-Hohenberg model.

[1] C. Riesch, G. Radons, and R. Magerle, *Aging of orientation fluctuations in stripe phases*, Phys. Rev. E **90**, 052101 (2014).

DY 63: Physics of Sustainability and Human-Nature Interactions II (joint session SOE/ DY/ jDPG/ BP)

Time: Thursday 17:00–18:30

Location: MA 001

Topical Talk

DY 63.1 Thu 17:00 MA 001

Critical Transitions in Socio-econo-ecological Systems—A Global Adaptive Model of the Regional Transitions to Agriculture 8000 BC to AD 500 — ●CARSTEN LEMMEN and KAI W. WIRTZ — Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

Critical transitions in societies emerge as boundaries between cultural “ages”, e.g. the transition from the Industrial to the Information Age, or from the Holocene to the Anthropocene. Societal transitions are believed to emerge from nonlinear feedbacks between environment, economy, and society, but hypotheses have been difficult to test so far.

We propose to employ “numerical experiments in history” and consider one of the major critical transitions in world history—the abandonment of a foraging lifestyle in favor of agriculture and pastoralism. We investigate this transition with a deterministic and dynamic model of society. The global model resolves regional-scale human-environment interactions in space and time, based on only few prognostic adaptive societal traits and their co-evolutionary dynamics with population size.

We successfully reproduced the agropastoral transition as seen in archaeological data; we tested demic and cultural hypotheses about its expansion, finding both equally consistent with the data; we explored the stability of the expansion pattern facing large-scale palaeoenvironmental excursions and found strong resilience of populations and their key traits. Our model enabled us to quantify global and regional emissions of CO₂ and the sustainable population size for the past 10000 years.

DY 63.2 Thu 17:30 MA 001

Evaluating a Socio-environmental Complex Adaptive System: The Case of Self-Organized Socio-environmental Development in State Chiapas. — ●FELIPE LARA-ROSANO¹ and ADRIANA QUIROGA-CARAPIA² — ¹Universidad Nacional Autónoma de México (UNAM), Mexico City, Mexico — ²Colegio de la Frontera Sur (ECOSUR), San Cristobal las Casas, Mexico

The project “Social and Environmental Innovation for Development in Areas of High Poverty and Biodiversity in the Southern Border of

Mexico” was proposed by a research institute: the Colegio de la Frontera Sur (ECOSUR), and financed by the Mexican Research Council. Its central objective: to create opportunities for social and environmental innovation on the southern border of Mexico, seeking to strengthen the local capacity for sustainable management of natural resources and the welfare of its inhabitants. Because of the complex system and environment dynamics the solution of the problem is not a fixed one but it is a process that must be continuously evaluated and adapted based on the standpoint of the complex systems paradigm. The assessment of the socio-environmental development project is performed conceptualizing and organizing the community as a complex adaptive system in interaction with its environment. The system has properties expressed as state variables associated with a value that is changing through the development process. The analysis of the system dynamics is based on the behavior of its state variables. The Colegio de la Frontera Sur (ECOSUR) successfully applied this method in rural development projects in state Chiapas in 2013.

DY 63.3 Thu 17:45 MA 001

Macroscopic description of complex adaptive networks co-evolving with dynamic node states — ●MARC WIEDERMANN^{1,2}, JONATHAN F. DONGES^{1,3}, JOBST HEITZIG¹, WOLFGANG LUCHT^{1,2}, and JÜRGEN KURTHS^{1,2} — ¹Potsdam Institute for Climate Impact Research, Germany — ²Humboldt University, Berlin, Germany — ³Stockholm Resilience Centre, Stockholm University, Sweden

When investigating the causes and consequences of global change, the collective behavior of human beings is believed to have a considerable impact on natural systems. Here, we study opinion formation and imitation of nodes on a complex network depending on the state of individual resource stocks that are harvested by each node. Numerical simulations reveal that high interaction rates between nodes cause a likely depletion of the resource whereas low interaction rates ensure their sustainable existence. However, adaptively rewiring the nodes' neighborhood structure with an appropriate frequency guides the system into an equilibrium state where all nodes behave sustainably and a full depletion of the resource stocks is avoided. In order to explain these observations, we derive a consistent macroscopic description of

the system, which provides a general framework to model and quantify the influence of single node dynamics on the macroscopic state of a network and is applicable to many fields of study, such as epidemic spreading or social modeling. Our results suggest that with the current trend to faster imitation and ever increasing global network connectivity, societies are becoming more vulnerable to environmental collapse if they remain myopic at the same time.

DY 63.4 Thu 18:00 MA 001

Exploring the safe and just operating space in an inhomogeneous world — ●WOLFRAM BARFUSS^{1,2}, BOYAN BERONOV^{1,3}, MARC WIEDERMANN^{1,4}, and JONATHAN DONGES^{1,5} — ¹Potsdam Institute for Climate Impact Research, Germany — ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — ³Ludwig-Maximilians-Universität München, Germany — ⁴Humboldt-Universität zu Berlin, Germany — ⁵Stockholm Resilience Centre, Stockholm University, Sweden

The Anthropocene has become reality during the 20th century, meaning that our species is pressuring the Earth's ecosystems on a global scale. In the meantime the challenge of eradicating poverty has not yet come to an end. Effectively dealing with these issues requires us to better understand the driving forces, feedback loops and tipping elements in the whole earth system, constituted from natural and social components. To take a step forward in this direction, we refine an existing conceptual coevolutionary model between social and ecological domains by adding inhomogeneities modelled after real-world data. We then propose an analysis framework, 'the safe and just space'-plot, which aligns with the current debate of simultaneously staying within the Planetary Boundaries and ensuring the social foundations

and transforms it into a practical tool for studying socio-ecological models as well as real-world observations. First results from comparing the model outcome with real-world data indicate that the current state of the world is neither particularly safe nor particularly just.

DY 63.5 Thu 18:15 MA 001

Topology of Sustainable Management of Dynamical Systems with Desirable States — ●JOBST HEITZIG¹ and TIM KITTEL^{1,2} — ¹Potsdam Institute for Climate Impact Research — ²Humboldt University Berlin

The sustainable management of systems mainly governed by an internal dynamics for which one desires to stay in a certain region of their state space requires an understanding of the topology of the system's state space in terms of what regions are "safe" to stay in, and to what qualitative degree, and which of these regions can be reached from which others by the internal dynamics or by management.

The paradigm of optimal control on the one hand does not provide sufficient concepts for such a qualitative analysis and on the other hand typically requires quite a lot of structural knowledge about the problem, in particular, some or other form of quantitative evaluation of states.

In this talk, we will derive in a purely topological way a thorough qualitative classification of the possible states and management options of a system with respect to the possibility of avoiding or leaving some given undesired region by means of some given management options. Our results indicate that the sustainable management of a system may require discrete decisions such as choosing between ultimate safety and permanent desirability, or between permanent safety and increasing future options, etc.

DY 64: Annual General Meeting of the Dynamics and Statistical Physics Division

Jahresversammlung des Fachverbands Dynamik und Statistische Physik
Berichte
Wahlen - Sprecher und Stellvertreter
Verschiedenes

Time: Thursday 18:00–19:00

Location: BH-N 334

meeting

DY 65: Special Session in Honor of the 75th Birthday of Siegfried Hess: Non-equilibrium dynamics of anisotropic fluids

Time: Friday 9:30–11:30

Location: BH-N 243

Invited Talk DY 65.1 Fri 9:30 BH-N 243
The "shear-gradient concentration coupling instability": non-uniform flow of sheared hard-sphere glasses. — ●JAN K.G. DHONT — Forschungszentrum Juelich, Germany

There are several types of shear-induced instabilities in soft-matter systems, like vorticity- and gradient-banding. The microscopic origin of these two instabilities is by now well understood. There is, however, an instability that can be referred to as "the Shear-gradient Concentration Coupling instability" (the SCC-instability) that has been largely ignored since its phenomenological description a few decades ago. This instability is due to a postulated shear-gradient induced mass flux together with a strong coupling of the stress to concentration. The origin of the shear-induced mass flux resulting from direct interactions is so far not understood, and explicit expressions for the corresponding transport coefficient have therefore not been derived. In this presentation, the origin of this mass flux is discussed, an explicit expression for the transport coefficient is presented, and numerical results are discussed for the stationary non-uniform flow profiles and concentration profiles of an initially SCC-unstable system, which will be compared to experiments on hard-sphere glasses.

Invited Talk DY 65.2 Fri 10:00 BH-N 243
Active anisotropic fluids — ●SRIRAM RAMASWAMY — TIFR Centre for Interdisciplinary Sciences, Tata Institute of Fundamental Research, Hyderabad 500 075 India

The study of nonequilibrium phenomena in anisotropic fluids has taken interesting new directions recently thanks to the growing interest in the collective self-propulsion. My talk will summarise new developments from our group's work on fluids of self-driven orientable particles, in vibrated granular monolayers and active colloids.

Invited Talk DY 65.3 Fri 10:30 BH-N 243
Flow properties of anisotropic fluids — ●SEBASTIAN HEIDENREICH¹, SABINE H. L. KLAPP², and MARKUS BÄR¹ — ¹Physikalisch Technische Bundesanstalt, Berlin, Germany — ²Technische Universität Berlin, Berlin, Germany

From liquid crystal polymers to suspensions of bacteria anisotropic fluids are ubiquitous in nature and technology. The flow exhibits intriguing phenomena like flow alignment, shear banding, tumbling, shear thickening/thinning, large-scale correlation and mesoscale turbulence. The emergence of such fascinating aspects is often related to the anisotropy and to the out-of-equilibrium character of the considered system. In the first part of our presentation we review selected flow phenomena of passive fluids with anisotropy. We discuss the role of the order parameter like the alignment tensor for the description of the flow properties. In particular, we introduce the relaxation equation for the alignment tensor coupled to the hydrodynamic flow and discuss the orientational dynamics in the shear flow. In the second part of the talk we focus on active fluids like dense bacterial suspensions and we introduce the governing hydrodynamic equations for self-sustained

individuals that are swimming in a Newtonian fluid. We discuss the relationship to the passive counterpart and finally present recent work on mesoscale bacterial turbulence.

Invited Talk DY 65.4 Fri 11:00 BH-N 243

Concluding Remarks — ●SIEGFRIED HESS — Institut für Theoretische Physik, Technische Universität Berlin, Germany

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DY 66: Focus Session: Aging in Physical and Biological Systems (joint session DY/ BP)

Physical aging is known from a number of complex systems such as spin glasses or materials like polymer glasses, colloids and gels. On the other hand, biological aging refers to the increase in mortality and the associated loss of functions with age that occurs (almost) universally across the kingdoms of life. This focus session aims to confront these different manifestations of aging in order to identify possible conceptual and methodological interrelations between two largely disjunct fields of research. (Organizers J. Krug and H. Meyer-Ortmanns)

Time: Friday 9:30–12:00

Location: BH-N 334

Invited Talk DY 66.1 Fri 9:30 BH-N 334
Demographic perspectives on the evolution of senescence — ●ANNETTE BAUDISCH — University of Southern Denmark, Campusvej 55, 5230 Odense M

Senescence, the physiological decline that results in decreasing survival and/or reproduction with age, remains one of the most perplexing topics in biology. Most theories attempting to explain the evolution of senescence (i.e. antagonistic pleiotropy, mutation accumulation, disposable soma) were developed several decades ago. Confronted with empirical patterns of survival and reproduction, predictions of the theories do not hold. New theory is needed to shed light on the determinants of patterns of birth and death. At this point it might be feasible and instructive to broaden perspectives by cutting across disciplinary boundaries and seek for a general theory of determinants of birth and death patterns, i.e. life course trajectories, pertaining to animate or inanimate objects on any scale of observation.

Invited Talk DY 66.2 Fri 10:00 BH-N 334
Biological mechanisms of aging — ●BJÖRN SCHUMACHER — CECAD Research Center, University of Cologne

The Biology of aging has long been a descriptive research discipline. Only in the past 20 years mechanisms of aging have been uncovered through research in genetic model systems. A number of distinct an interconnected pathways that regulate longevity have been identified. However, the complexity of the aging process remains a challenge to modern aging research. Integration of quantitative data linking the age-dependent accumulation of harmful damage to macromolecules - particularly the genetic material- to the regulation of longevity assurance pathways have begun to unravel a more integrated and complete understanding the biological mechanisms of aging.

Invited Talk DY 66.3 Fri 10:30 BH-N 334
Aging in out-of-equilibrium systems: an overview — ●JEAN-PHILIPPE BOUCHAUD — Capital Fund Management, 75007 Paris, France

Aging is a particular type of out-of-equilibrium dynamics that is observed in a variety of systems, from glassy systems to atomic cooling and blinking dots, etc. I will review several distinct mechanisms that can lead to aging, discuss their theoretical underpinning and their experimental relevance.

Invited Talk DY 66.4 Fri 11:00 BH-N 334
Aging in coarsening systems with non-algebraic growth laws — ●MICHEL PLEIMLING — Virginia Tech, Blacksburg, VA, USA

Physical aging is generically encountered in systems far from equilibrium that evolve with slow dynamics. Well known examples can be found in structural glasses, spin glasses, magnetic systems, and colloids. Recent years have seen major breakthroughs in our understanding of aging processes in non-disordered systems characterized by an algebraic growth of the domains. Progress in understanding aging in systems with more complicated growth laws has been much slower though. After a brief introduction into the phenomenology of aging in simple coarsening systems, I discuss in this talk non-equilibrium relaxation and aging processes in systems characterized by a non-algebraic growth of the ordered domains. Disordered ferromagnets provide interesting examples where the relaxation process is dominated by a slow

crossover from an algebraic-like regime at early times to the slower asymptotic growth that prevails for large times. In order to study aging processes deep inside an anomalously slow growth regime we turn to different versions of the ABC model where the biased exchanges of particles of different types yield domains that only grow logarithmically with time.

This work is supported by the US Department of Energy through grant DE-FG02-09ER46613.

DY 66.5 Fri 11:30 BH-N 334
Aging of Classical Oscillators during a Noise-Driven Migration of Oscillator Phases — ●HILDEGARD MEYER-ORTMANN and FLORIN IONITA — Jacobs University Bremen, 28759 Bremen

We consider classical nonlinear oscillators like rotators and Kuramoto oscillators on hexagonal lattices of small or intermediate size. When the coupling between the elements is repulsive and the bonds are frustrated, we observe coexisting states, each one with its own basin of attraction. For special lattices sizes the multiplicity of stationary states gets extremely rich. When disorder is introduced into the system by additive or multiplicative Gaussian noise, we observe a noise-driven migration of oscillator phases in a rather rough potential landscape. Upon this migration, a multitude of different escape times from one metastable state to the next is generated. Based on these observations, it does not come as a surprise that the set of oscillators shows physical aging. Physical aging is characterized by nonexponential relaxation after a perturbation, breaking of time-translation invariance, and dynamical scaling. When our system of oscillators is quenched from the regime of a unique fixed point toward the regime of multistable limit-cycle solutions, the autocorrelation functions depend on the waiting time after the quench, so that time translation invariance is broken, and dynamical scaling is observed for a certain range of time scales. It is an open question as to whether physical aging as we have studied here, is also responsible for biological aging in these excitable or oscillatory systems in biological realizations.

F. Ionita, H. Meyer-Ortmanns, Phys. Rev. Lett. 112, 094101 (2014).

DY 66.6 Fri 11:45 BH-N 334
Parametrization and interaction analysis of survival curves — IVAN G. SZENDRO¹, RAHUL MARATHE², YIDONG SHEN³, ADAM ANTEBI³, and ●JOACHIM KRUG¹ — ¹Institute for Theoretical Physics, University of Cologne, Germany — ²Department of Physics, IIT Delhi, India — ³Max Planck Institute for Biology of Ageing, Cologne, Germany

A key signature of biological aging is the increase of mortality with age. Age-dependent mortality can be extracted from the survival curve, which monitors the surviving fraction of a population of individuals as a function of time. Experiments on longevity-related mutations and interventions in model organisms typically focus on mean life span only, thus neglecting much information contained in the shapes of survival curves. Here we present an exploratory study aimed at parametrizing experimental survival curves obtained for the nematode *Caenorhabditis elegans*. To this end, we fit survivorship data to models of varying complexity, including the classical Gompertz law as well as models based on reliability theory. We also analyze the multidimensional interactions between different interventions and mutations, using a published data set that contains all combinations of two interventions (di-

etary restriction and temperature) and two genetic mutations (daf-2 and clk-1).

DY 67: Networks: From Topology to Dynamics (joint session DY/ BP/SOE)

Time: Friday 9:30–12:45

Location: BH-N 128

DY 67.1 Fri 9:30 BH-N 128

Networks: From Dynamics to Topology — ●JOSE CASADIEGO^{1,3} and MARC TIMME^{1,2,3} — ¹Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — ²Institute for Nonlinear Dynamics, Faculty of Physics, University of Göttingen, 37077 Göttingen, Germany — ³IMPRS Physics of Biological and Complex Systems, Göttingen Graduate School for Neurosciences, Biophysics and Molecular Biosciences, 37077 Göttingen, Germany

How single units interact in a complex network fundamentally underlies its collective dynamics. Yet, identifying the physical structure of interactions from recorded time series still poses a great challenge. Up-to-date methods either require (i) a detailed pre-knowledge of the units' dynamical features, (ii) to externally drive the network or (iii) the network dynamics to be at stable states, such as fixed points or limit cycles. Here we develop a theory to reveal physical interactions of networks that relies on recorded time series only. By decomposing the dynamics of single units in terms of network interactions of different orders (pairs, triplets, quadruplets,...), we pose network reconstruction as an error minimization problem. We propose a greedy algorithm to solve such minimization problems. Our approach is principally model independent, ensuring its generality and applicability in different fields and making it particularly suitable when structural connections are desired, dynamical features are unknown and perturbing the network is unfeasible. Thus, our approach may serve as a key stepping stone for the expanding field of model-independent network reconstruction.

DY 67.2 Fri 9:45 BH-N 128

Revealing the Topology of Circulatory Networks in Nature — ●MIRKO LUKOVIC¹ and ERIK MARTENS^{2,3} — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Department of Biomedical Sciences, University of Copenhagen, Denmark — ³Department of Mathematical Sciences, University of Copenhagen, Denmark

Complex networks such as those used for communication, resource delivery and transportation are ubiquitous in nature and society. From the internet and urban traffic, to the intimate networks of the circulatory systems in our bodies, understanding how their topology and structure relate to their function and efficiency is an essential first step in their management. Given the wide variety of existing transport networks with structures that range from being tree-like to cases where there is an intricate arrangement of nested loops, our goal is to use circulation times of the flow in order to infer global properties of the underlying network structure. To this end we investigate circulatory transport networks by modeling the flow as a stochastic process whose first passage time properties we determine for a variety of different network topologies. We also set up a framework in which different branching rules of the flow can be tested and its effects on the first passage times analyzed. Our results will help develop an effective and non-invasive method for probing circulatory networks such as the human vascular system.

DY 67.3 Fri 10:00 BH-N 128

Symbolic Regression and Network Analysis for the prediction of El Nino — ●MARKUS ABEL¹, MARKUS QUADE¹, RUGGERO VASILE¹, AVI GOZ², SHLOMO HAVLIN³, and ARMIN BUNDE⁴ — ¹Ambrosys GmbH, Albert-Einstein Str. 1-5 Potsdam, Germany — ²Department of Solar Energy & Environmental Physics, Ben-Gurion University, Jerusalem, Israel — ³Department of Physics Bar-Ilan University Ramat-Gan 52900 Israel — ⁴Institute For Theoretical Physics, University of Giessen, Germany

In the context of the modeling of dynamical systems, statistical analysis and data-based modeling is a highly promising method. We use symbolic regression, in particular genetic programming and non-parametric regression to find effective models for the prediction of el Nino events. The data used consist of a novel method to form a network from the correlations of grid points in the El Nino basin. We compare our results with existing methods. Depending on the method

used a predictive power of up to 100% is achieved, i.e. all events are correctly predicted.

DY 67.4 Fri 10:15 BH-N 128

Model selection and hypothesis testing for large-scale network models with overlapping groups — ●TIAGO P. PEIXOTO — Institut für Theoretische Physik, Universität Bremen

The effort to understand network systems in increasing detail has resulted in a diversity of methods designed to extract their large-scale structure. Unfortunately, many of these methods yield diverging descriptions of the same network, making both the comparison and understanding of their results a difficult challenge. A possible solution to this outstanding issue is to shift the focus away from arbitrary methods, and move towards principled approaches based on statistical inference of generative models. In this talk we consider the comparison between a variety of generative models including features such as degree correction, where nodes with arbitrary degrees can belong to the same group, and community overlap, where nodes are allowed to belong to more than one group. Because such model variants possess an increased number of parameters, they become prone to overfitting. We present a method of model selection based on the minimum description length criterion and posterior odds ratios that is capable of fully accounting for the increased degrees of freedom of the larger models, and selects the best one according to the statistical evidence available in the data. In applying this method to many empirical datasets from different fields, we observe that community overlap is very often not supported by statistical evidence, and is selected as a better model only for a minority of them. On the other hand, we find that degree-correction tends to be almost universally favored by the available data.

DY 67.5 Fri 10:30 BH-N 128

Breakdown of quantum transport in scale-free networks — ●NIKOLAJ KULVELIS and OLIVER MÜLKEN — Uni-Freiburg, Deutschland

We apply the model of continuous time quantum walks (CTQW) to a subset of scale-free networks (SFN) containing solely trees. A quantity characterising the global transport for large time scales is introduced and, by means of estimating the dominant spectral degeneracy, calculated for given system size and branching strength. Taking the limit of infinite system size a phase transition resembling breakdown of transport is observed beyond a critical branching strength. All our analytic calculations are supported by Monte Carlo simulations and discussed.

DY 67.6 Fri 10:45 BH-N 128

Two-dimensional unimodular Lattice Triangulations as small-world and scale-free networks — ●BENEDIKT KRÜGER, ELLA SCHMIDT, and KLAUS MECKE — Institut für Theoretische Physik, Staudtstr. 7, 91058 Erlangen

Triangulations are an important tool in physics for describing curved geometries. Unimodular triangulations on 2d lattices can also be considered as connected, simple, and maximal planar graphs, which allows the appliance of methods from graph theory on triangulations. We calculate the scaling behaviour of the degree distribution, clustering coefficient and the average shortest path length for random triangulations. Introducing a simple measure for the order of a triangulation and interpreting it as the energy of the triangulation we measure canonical averages of these observables using Monte-Carlo-Simulations. We find a crossover behaviour of all considered observables at small negative temperatures and hints for small-world and scale-free behaviour in certain temperature ranges.

15 min. break

DY 67.7 Fri 11:15 BH-N 128

Nonlinear elasticity of athermal networks: a critical phenomenon — ●ABHINAV SHARMA¹, ALBERT LICUP¹, MICHAEL SHEINMAN¹, KARIN JANSEN², GIJSE KOENDERINK², and FREDERICK MACKINTOSH¹ — ¹VU, Amsterdam, Netherlands — ²AMOLF, Ams-

terdam, Netherlands

Biopolymer networks exhibit highly interesting mechanical behavior. An instructive model system is that of a network composed of rope-like filaments—zero resistance to compression but finite resistance to stretching. For networks with connectivity below Maxwell point, there is no elastic modulus for small deformations. However, when networks are subjected to an external strain, stiffness emerges spontaneously beyond a critical strain. We demonstrate that the spontaneous emergence of elasticity is analogous to a continuous phase transition. The critical point is not fixed but depends on the geometry of the underlying network. The elastic behavior near the critical point can be described analogous to that of Magnetization in ferromagnetic material near the Curie temperature. Surprisingly, the critical exponents are independent of the dimensionality and depend only on the average connectivity in the network. By including bending interactions in the rope network, we can capture the mechanical behavior of biologically relevant networks. Bending rigidity acts as a coupling constant analogous to the external magnetic field in a ferromagnetic system. We show that nonlinear mechanics of collagen are successfully captured by our framework of regarding nonlinear mechanics as a critical phenomenon.

DY 67.8 Fri 11:30 BH-N 128

Coarsening dynamics of transient networks in an experiment with dipolar hard spheres — ●ARMIN KOEGEL and REINHARD RICHTER — Experimentalphysik 5, Universität Bayreuth, D-95440 Bayreuth, Germany

Permanent magnetic dipoles may self-assemble to linear chains and rings, even without an externally applied magnetic field. This has been investigated for nano-sized particles in ferrofluids; see e.g. [1,2] However, in this system the emerging structures and their dynamics are difficult to observe. Similar aggregates have also been observed in a mixture of glass beads and magnetized steel spheres, which are shaken in a vessel [3]. In the present contribution we focus on the formation of transient networks in this system, when quenching the amplitude of the vibrations [4]. We analyze the evolving networks by the number of spheres in a network cluster, its gyration radius, and its average shortest path length.

[1] P.G. De Gennes and A. Pincus, *Phys. Kondens. Mater.* **1**, 189 (1970).

[2] T. A. Prokopenko, V. A. Danilov, S. S. Kantorovich, Ch. Holm, *Phys. Rev. E* **80**, 031404 (2009).

[3] D. L. Blair, A. Kudrolli, *Phys. Rev. E* **67**, 021302 (2003).

[4] <http://www.ep5.uni-bayreuth.de/de/research/Magnetic-Soft-Matter/video/ferronetwerk.html>

DY 67.9 Fri 11:45 BH-N 128

Exclusion processes on networks — ●IZAAK NERI^{1,2}, NORBERT KERN³, and ANDREA PARMEGGIANI³ — ¹Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38 01187 Dresden Germany — ²Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108 01307 Dresden — ³Laboratoire Charles Coulomb UMR 5221 & CNRS, Université Montpellier 2, F-34095, Montpellier, France

We present a study of exclusion processes on complex networks, as a paradigmatic model for transport subject to excluded volume interactions. Building on the phenomenology of a single segment and

borrowing ideas from random networks we investigate the effect of connectivity on transport. In particular, we argue that the presence of disorder in the network crucially modifies the large scale transport features: disorder induces strong density heterogeneities in the network such that certain regions of the network are almost fully congested while other regions allow for free flow of matter.

DY 67.10 Fri 12:00 BH-N 128

Synchronization-Desynchronization Transitions in Complex Networks: An Interplay of Distributed Time Delay and Inhibitory Nodes — ●CAROLIN WILLE^{1,2}, JUDITH LEHNERT¹, and ECKEHARD SCHÖLL¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We investigate the combined effects of distributed delay and the balance between excitatory and inhibitory nodes on the stability of synchronous oscillations in a network of coupled Stuart–Landau oscillators. To this end a network model is proposed for which the stability can be investigated analytically. It is found that beyond a critical inhibition ratio synchronization tends to be unstable. However, increasing distributional widths can counteract this trend leading to multiple resynchronization transitions at relatively high inhibition ratios. All studies are performed on two distribution types, a uniform distribution and a Gamma distribution.[1]

[1] C. Wille, J. Lehnert, and E. Schöll, *Phys. Rev. E* **90**, 032908 (2014)

DY 67.11 Fri 12:15 BH-N 128

Efficient sampling of networks with high clustering — ●RICO FISCHER¹, JORGE LEITAO¹, TIAGO PEIXOTO², and EDUARDO ALTMANN¹ — ¹Max-Planck-Institut für Physik komplexer Systeme — ²University of Bremen

The problem in network generation is to obtain networks which satisfy specified properties but that are otherwise random. Traditional Markov Chain Monte Carlo methods (like Metropolis-Hastings) can be used in this problem but often fail in important cases, e.g., they do not correctly sample random networks with high clustering coefficients due to a rough \gg landscape, which typically leads to abrupt phase transitions, metastable states and hysteresis. In this talk we show how an efficient sampling of high-clustering networks is obtained using multicanonical Monte-Carlo methods. We characterize the efficiency of this method, we use it to investigate the phase transition methods, and we explore different applications.

DY 67.12 Fri 12:30 BH-N 128

Shape and scaling of spatially embedded transport networks — ●ROBIN DE REGT and CHRISTIAN VON FERBER — Coventry University, UK

Real world transport networks are usually embedded in two- or three-dimensional space. Here, we explore the shape and scaling properties of these spatially embedded complex networks. The work presented we focus on the interplay of spatial embedding and scaling statistics. In particular, complex transport networks of public transport appear to show that spatial and scaling properties within these networks are closely correlated. To support our claim we have analysed a number of public transport networks in a number of large scale conglomerations.

DY 68: Glasses and Glass Transition (joint session CPP/ DF/ DY)

Time: Friday 9:30–11:15

Location: C 243

DY 68.1 Fri 9:30 C 243

Stable glasses from strong liquids — ●YEONG ZEN CHUA¹, MATHIAS AHRENBURG¹, MICHAEL TYLINSKI², MARK D. EDIGER², and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706 USA

To date, only several materials have been observed to form ultra-stable glasses by vapor deposition. Some authors have suggested that fragility might be a controlling factor in the ability to form stable glasses by vapor deposition, with highly stable glasses only being possible for highly fragile liquids. Glasses of ethylcyclohexane, fragility index 56.5, and 1-pentene, a very small molecule, produced by physical vapor deposition have been characterized by in situ AC chip nanocalorimetry. Since the fragility index of 1-pentene was not available, it was determined as 52 from the calorimetric glass transition temperatures measured in the frequency range from 0.2 Hz to 4 kHz. Ethylcyclohexane and 1-pentene are both strong glass formers, for which possibility of stable glass formation has been questioned. On the contrary, we observed formation of highly stable glasses of ethylcyclohexane and 1-pentene. The results on ethylcyclohexane and 1-pentene will be presented and compared with literature data of other known glass formers.

DY 68.2 Fri 9:45 C 243

Broadband dielectric spectroscopy of ionic liquids — ●PIT SIPPEL¹, MICHAEL AUMÜLLER¹, STEPHAN KROHNS^{1,2}, PETER LUNKENHEIMER¹, and ALOIS LOIDL^{1,2} — ¹Experimental Physics V, University of Augsburg, Germany — ²Institute for Materials Resource Management, University of Augsburg, Germany

Due to their high potential for applications, e.g., in energy-storage devices such as supercapacitors or batteries, during recent years ionic liquids have come into the focus of research [1]. Ionic liquids are composed of organic cations and weakly coordinating anions. An essential method for the study of ionic transport is dielectric spectroscopy. Our results on a large variety of ionic liquids cover a broad frequency and temperature range. This allows obtaining valuable information on phenomena like dc charge transport, the glass transition, electrode polarization, and relaxation. We analyze the dielectric spectra using an equivalent-circuit approach [2]. Amongst others, this enables the deduction of the relaxation times of the involved dynamic processes. We conclude that the main reorientational relaxation process of these ionic liquids, the α relaxation, is closely linked to the dc-conductivity. This provides insight into the underlying conductivity mechanisms and, thus, the mobility of the ionic charge carriers. Moreover, a number of secondary relaxation processes is found, including hints at the presence of a Johari-Goldstein relaxation process [3].

[1] M. Armand *et al.*, Nat. Mat. **8**, 621 (2009). [2] S. Emmert *et al.*, Eur. Phys. J. B **83**, 157 (2011). [3] G.P. Johari and M. Goldstein, J. Chem. Phys. **53**, 2372 (1970).

DY 68.3 Fri 10:00 C 243

Dielectric spectroscopy on glycerol and water confined in metal-organic frameworks — ●JONAS FISCHER¹, PIT SIPPEL¹, PETER LUNKENHEIMER¹, DMYTRO DENYSENKO², DIRK VOLKMER², and ALOIS LOIDL¹ — ¹Experimental Physics V, University of Augsburg, Germany — ²Chair of Solid State and Material Chemistry, University of Augsburg, Germany

Approaching the glass transition, the slowing down of molecular dynamics generally proceeds much stronger than expected for thermally activated motions. This can be ascribed to a temperature-dependent activation energy arising from the cooperative motion of increasing numbers of molecules at low temperatures [1]. The number of correlated molecules can be controlled by confining the glass-forming liquid in small pores. Previously, glass formers have been confined in porous glasses, zeolites and other silicates [2]. Recently, metal-organic frameworks (MOFs) have become available. This class of porous coordination polymers consists of metal-containing units and organic linkers. MOFs are tunable in many regards [3], thus allowing confinement in pores of different inner surfaces and varying sizes. Here, we present broadband dielectric spectroscopy data of glycerol and water confined in different MOFs, of the MFU-type [4]. It is shown that MOFs are well-suited for the measurement of confined liquids.

- [1] T. Bauer *et al.*, Phys. Rev. Lett. **111**, 225702 (2013).
 [2] A. Huwe *et al.*, Phys. Rev. Lett. **82**, 2338-2341 (1999).
 [3] H. Furukawa *et al.*, Science **341**, 1230444 (2013).
 [4] D. Denysenko *et al.*, Chem Commun. **48**, 1236 (2012).

DY 68.4 Fri 10:15 C 243

Dynamics of the glass transition in confined glycerol under hard and soft confinement, investigated by ²H NMR — ●MICHAEL LANNERT, MATTHIAS SATTIG, THOMAS BLOCHOWICZ, and MICHAEL VOGEL — Hochschulstraße 6-8, 64289 Darmstadt, Germany
²H NMR allows us to access correlation times of molecular rotational dynamics, ranging from $\tau=10^{-12}$ s to $\tau=10^{-1}$ s, by using longitudinal relaxation, solid echo, and stimulated echo sequences. Findings for confined glycerol, which is subjected to spherical soft confinement (using AOT/toluene micro-emulsions) and cylindrical hard confinement (using microporous silica, namely MCM-41) are compared, and a shift in correlation times to shorter times is observed for the hard confinement, but not for the soft confinement. Various diameters (2nm to 9nm) were used in order to gain a comprehensive understanding of the finite size effect. Investigation of the dynamics of the glycerol in the supercooled regime proved to be a challenging enterprise in soft confinement, because of the onset of rotational diffusion of the whole microemulsion droplet, which exceeds the contribution of molecular rotational dynamics. Therefore droplet size-dependence and viscosity-dependence of the dynamics were investigated additionally, in order to evaluate the impact of these results.

DY 68.5 Fri 10:30 C 243

Structure and Dynamics of Asymmetric Poly(styrene-*b*-1,4-isoprene) Diblock Copolymer under 1D and 2D Nanoconfinement — ●WYCLIFFE K. KIPNUSU¹, MAHDY M. ELMAHDY¹, EMMANUEL U. MAPESA¹, JIANGI ZHANG², DETLEF-M. SMILGIES³, CHRISTINE M. PAPADAKIS⁴, and FRIEDRICH KREMER¹ — ¹Institute of Experimental physics I, Linnstr.5, 04103, Leipzig — ²National Center for Nanoscience and Technology (NCNST), No.11 ZhongGuanCun BeiYiTiao, 100190 Beijing, P.R. China. — ³Cornell High Energy Synchrotron Source (CHESS), Wilson Laboratory, Cornell University, Ithaca, NY 14853, USA — ⁴Technische Universität München, Physik-Department, Physik weicher Materie, James-Frank-Straße 1, 85748 Garching, Germany.

The impact of 1- and 2-dimensional (2D) confinement on the structure and dynamics of poly(styrene-*b*-1,4-isoprene) P(S-*b*-I) diblock copolymer is investigated by a combination of Grazing-Incidence Small-Angle X-ray Scattering (GISAXS), Atomic Force Microscopy (AFM) and Broadband Dielectric Spectroscopy (BDS). 1D confinement is achieved by spin coating the P(S-*b*-I) to form nanometric thin films on silicon substrates, while in the 2D confinement, the copolymer is infiltrated into cylindrical anodized aluminum oxide (AAO) nanopores. GISAXS and AFM reveal hexagonally packed cylinders of PS in a PI matrix. The dynamic glass transition of the styrene and isoprene blocks is independent of the dimensionality and the finite sizes (down to 18 nm) of confinement but the normal mode is influenced by both factors with 2D geometrical constraints exerting greater impact.

DY 68.6 Fri 10:45 C 243

High frequency laser heated AC-chip calorimeter for dynamic glass transition investigation in room temperature ionic liquids — ●EVGENI SHOIFET^{1,2,3,4}, HEIKO HUTH¹, SERGEY VEREVKIN^{2,4}, CHRISTOPH SCHICK^{1,4}, and EGON HASSEL³ — ¹Institute of Physics, University of Rostock, 18057 Rostock, Germany — ²Institute of Physical Chemistry, University of Rostock, 18059 Rostock, Germany — ³Department of Technical Thermodynamics, Faculty of Mechanical Engineering and Marine Technology, Rostock, 18051 Rostock, Germany — ⁴Faculty of Interdisciplinary Research, Department "Life, Light and Matter", University of Rostock, Germany

Many ionic liquids are good glass formers. Nevertheless, for the relaxation behavior only a few studies of the dynamic glass transition in ionic liquids are available so far. Particularly the frequency dependence of the dynamic glass transition (α -relaxation) is not known for most ionic liquids. The standard technique for such studies - dielectric spectroscopy - is not easily applicable to ionic liquids because of the high electrical conductivity. In addition, dielectric spectroscopy is equally

sensitive to the segmental relaxation (α -relaxation) and secondary relaxation but calorimetry is sensitive solely to segmental relaxation.

We try to use calorimetric techniques to obtain complex heat capacity and to investigate the dynamic glass transition of room temperature ionic liquids (RTILs) in a wide frequency range. This can give an insight in cooperative motions of ions and ion clusters in RTILs. Particularly the influence of alkyl chain length on the α -relaxation in the frequency range from 1 mHz to 0.1 MHz [Shoifet. E. et. al. (2013)].

DY 68.7 Fri 11:00 C 243

Dynamic glass transition measurements on nm-thin films of Indomethacin using AC chip-nanocalorimetry — ●MATHIAS AHRENBURG, CHRISTOPH SCHICK, and GUNNAR SCHULZ — Institut für Physik, Universität Rostock

We are using AC chip nano-calorimetry for the in-situ investigation of

the dynamic glass transition of vapor-deposited thin films of toluene and indomethacin of thicknesses between several hundred nm down to ten nm. With these experiments on low molecular mass substances we complement our data on similar thin polymer films. Firstly, the deposition-related thermodynamic state (stable glass) of each film is erased by transforming them into ordinary glasses. Secondly, upon reheating the thin ordinary glass films a direct comparison of the subsequently measured frequency-dependent dynamic glass transition temperatures becomes possible. The frequency of temperature modulation can be varied from 1 Hz up to about 1000 Hz. Film thicknesses for indomethacin are measured ex-situ with an atomic force microscope directly on the membrane of the chip-sensors. Similar to the thin polymer films no thickness dependence of the dynamic glass transition temperature (main relaxation) is seen. The results are in agreement with the explanation given by Cangialosi et al.

DY 69: Complex Fluids and Soft Matter (joint session BP/DY/PPP)

Time: Friday 9:30–12:15

Location: H 1058

DY 69.1 Fri 9:30 H 1058

Anisotropic Diffusion of Macromolecules in the Contiguous Nucleocytoplasmic Fluid during Eukaryotic Cell Division — NISHA PAWAR, CLAUDIA DONTH, and ●MATTHIAS WEISS — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Protein diffusion in intracellular fluids is a crucial determinant of many vital biochemical pathways. Frequently an anomalous diffusion of macromolecules in the cytoplasm and nucleoplasm of eukaryotic cells has been reported, and associated changes in biochemical reactions have been discussed in some detail. Here we show that the contiguous nucleocytoplasmic fluid in dividing cells features an anisotropically varying diffusion of macromolecules [1]. In metaphase, diffusion in the contiguous nucleocytoplasmic fluid appears less anomalous along the spindle axis as compared to perpendicular directions. As a consequence, the long-time diffusion of macromolecules preferentially points along the spindle axis, leading to a prolonged residence of macromolecules in the spindle region. An anisotropic diffusion may support the dynamic formation of a spindle matrix which guides later steps in mitosis.

[1] N. Pawar, C. Donth, and M. Weiss, *Curr. Biol.* 24, 1905 (2014).

DY 69.2 Fri 9:45 H 1058

Optical Shaking of Single Cells — ●CARLA ZENSEN^{1,3}, ISIS E. FERNANDEZ^{2,3}, OLIVER EICKELBERG^{2,3}, THEOBALD LOHMÜLLER^{1,3}, and JOCHEN FELDMANN^{1,3} — ¹Chair for Photonics and Optoelectronics, Physics Department and CeNS, Ludwig-Maximilians-Universität, Munich, Germany — ²Comprehensive Pneumology Center, Institute of Lung Biology and Disease, Ludwig-Maximilians-Universität and Helmholtz Zentrum, Munich, Germany — ³Nanosystems Initiative Munich (NIM), Schellingstr. 4, Munich, Germany

We report on a new strategy to dynamically manipulate single cells by exposing them to an applied optical force field which varies periodically in time and space. The mechanical transient response of the cell is monitored both by optical imaging and by a microfluidic detector bead [1] positioned in the cell vicinity. These optical 'shaking' experiments give insight into the mechanobiological properties of single cells.

A predefined array of NIR laser beams is spatially varied with a periodic dynamics in order to optically 'shake' single cells. A detector bead, which is optically trapped with an independent laser beam, is used to simultaneously map the resulting microfluidic flow. We demonstrate a first application of this novel technique by resolving mechanobiological differences in the hypotonic state of individual human erythrocytes. By analyzing the Fourier spectra of cell and detector bead movements, we show that tracking a single detector particle is sufficient to distinguish between soft and hard cells.

[1] A. Ohlinger, A. Deak, A.A. Lutich, and J. Feldmann, *Phys. Rev. Lett.* 108, 018101 (2012)

DY 69.3 Fri 10:00 H 1058

In vivo mechanics measurements using ferrofluid droplets — ●FRIEDHELM SERWANE, ALESSANDRO MONGERA, PAYAM ROWGHANIAN, DAVID KEALHOFER, and OTGER CAMPÀS — Department of Mechanical Engineering, University of California, Santa Barbara, USA

The development of living tissues and organs depends on cell behav-

ior strongly influenced by the mechanics of their microenvironment. A prime example is the ability of a tumor to spread which has been linked directly to the elasticity of the surrounding matrix.

This interplay between mechanical inputs and biological responses has remained poorly understood, mainly due to a lack of techniques to measure mechanical properties while characterizing the molecular signals *in vivo*.

Here we present a technique to measure the mechanics of cellular microenvironment within living tissues and organs. We use ferrofluid oil droplets as mechanical actuators. Once injected in developing zebrafish embryos, we obtain the mechanical properties by tracking the dynamical response of the droplet when actuated by an external magnetic field. In particular, this technique allows us to measure the changes in mechanical properties underlying zebrafish gastrulation.

This technique opens the door to experiments which uniquely relate biological signals to the underlying mechanical properties.

DY 69.4 Fri 10:15 H 1058

Biomolecule dynamics in microfluidic pH gradients and prebiotic FeS membranes — ●FRIEDERIKE M. MÖLLER¹, DOMINIC BERCHTOLD¹, FRANZISKA KRIEGEL¹, LAURA BARGE², MICHAEL RUSSELL², and DIETER BRAUN¹ — ¹Systems Biophysics, LMU München, Germany — ²Jet Propulsion Laboratory, Pasadena, USA

What are possible driving forces to reduce local entropy in early evolution? Early earth creates a marked redox potential of >600mV between the CO₂-dominated atmosphere, creating an ocean around pH 6 and the alkaline outflow of geological serpentinization reactions at pH 10. A rocky FeS membrane forms upon contact from the sulfuric S⁻ and the Fe⁺⁺ ions. Its equilibrium version was studied by Huber and Wächtershäuser to form the first organic molecules starting from CO. The FeS clusters created in the membrane are central parts in ancient electron-transfer proteins.

What are the physical characteristics of this membrane? In a microfluidic replica, the pH gradient leaks through the membrane. However, we find yet unexplained attractive forces: hydrophobic and charged molecules are strongly attracted towards the membrane center. As reference system, we create pH gradients in water by uncaging of OH⁻ or H⁺ ions. The phoretic motions and pH gradients are measured by fluorescence. The rich non-equilibrium dynamics are explained with finite element modeling. They offer a microscopic view back in time into the geological setting of early Earth.

DY 69.5 Fri 10:30 H 1058

Dynamics of biological membrane mimics - A combined QENS and MD simulation study — ●LISA LAUTNER¹, MARTIN SCHMIELE¹, SEBASTIAN BUSCH², MICHAELA ZAMPONI³, and TOBIAS UNRUH¹ — ¹Chair for Crystallography and Structural Physics, FAU Erlangen-Nuremberg, Germany — ²University of Oxford, United Kingdom — ³Heinz Maier-Leibnitz Zentrum, Garching

Phospholipids are of high interest in the fields of biology and biophysics. As a main component of biological cell membranes the lipids are involved in lipid-lipid and lipid-protein interactions and therefore essential in a variety of cell functions. Many of these processes, e.g. binding to or transport through the membrane, are coupled to their structure and dynamics. Quasielastic Neutron Scattering (QENS) ex-

periments and state-of-the-art Molecular Dynamics (MD) simulations yield a complementary view on these processes, with high spatial as well as temporal resolution.

A combination of QENS experiments and MD simulations was used to obtain a detailed understanding of the dynamics of biomimetic POPC (1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine) bilayers in the liquid crystalline (L_α) phase. Special emphasis was thereby the study of the temperature dependent behaviour of the phospholipid dynamics. The results of both the QENS experiments and the MD simulations coincide nicely and confirm the benefit of the combination of these complementary methods. These results provide a basis for extended studies on more complex systems e. g. lipid mixtures and lipid-protein interactions. First results of such experiments will be presented as well.

15 min break

DY 69.6 Fri 11:00 H 1058

Bridging the scales: How is the large-scale deformation of a cellular network related to cell-scale processes? — ●MATTHIAS MERKEL¹, RAPHAEL ETOURNAY², SUZANNE EATON², and FRANK JÜLICHER¹ — ¹MPI for the Physics of Complex Systems, Dresden — ²MPI of Molecular Cell Biology and Genetics, Dresden

We propose a method to study the deformation of two-dimensional cellular networks. To this end, we focus on biological tissues, which typically undergo large-scale deformations during the development of an organism. However, how these large-scale deformations correspond to the collective behaviour of individual cells is not fully understood yet. Today, experimentalists are able to image tissues with up to 10 000 cells at sub-cellular spatial resolution and at a time resolution of minutes. Nevertheless, there is still a lack of methods allowing us to exploit the full depth of this huge amount of information.

Here, we propose a geometrical framework that exactly decomposes large-scale deformations into contributions by different kinds of cellular processes, which comprise cell shape changes, cell rearrangements (T1 transitions), cell divisions, and cell extrusions (T2 transitions). As the key idea, we introduce a tiling of the cellular network into triangles. This allows us to define the precise contribution of each of kind of cellular process to large-scale deformation. Additionally, our rigorous approach reveals subtle effects of correlated cellular motion, which constitute a novel source of large-scale tissue deformation. Finally, we demonstrate our new method on the wing of the fruit fly, which undergoes large-scale deformations during development.

DY 69.7 Fri 11:15 H 1058

Bridging from ionic to non-ionic thermophoresis — ●MANUEL WOLFF, MICHAEL NASH, and DIETER BRAUN — Center for Nanoscience, LMU, Munich, Germany

Thermal gradients drive molecules in solutions, an effect termed thermophoresis. Interest in aqueous thermophoresis was recently triggered by its widespread application in biomolecule affinity analysis using infrared-illuminated capillaries.

Theoretical models are debated, not least due to the fact that molecules in water seem to behave significantly different in non-aqueous fluids. By designing fluorescently labeled polymers that are either completely uncharged or whose charge can be tuned by a change in pH, we find that the temperature dependence of ionic and non-ionic polymers is very distinct. Building upon previous models, we find that increasing thermophoresis for rising temperature, often fitted by a heuristic formula proposed by Piazza and attributed to hydrophobic effects, can be fully explained by the Seebeck effect: the temperature dependence of ionic thermophoresis is dominated by the temperature dependent thermophoresis of the small ions in solution. While this dependence is not yet fully known for H^+ and OH^- , the thermophoresis of peptide nucleic acid (PNA) with its pH dependent charge is described well across a wide range of pH with reasonable assumptions. These findings offer a new bridge from aqueous thermophoresis to non-aqueous solutions.

DY 69.8 Fri 11:30 H 1058

How to regulate droplet position in a heterogeneous chemical environment? — ●SAMUEL KRÜGER^{1,2}, CHRISTOPH WEBER¹, JENS-UWE SOMMER^{2,3}, and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden — ²Leibniz Institute of Polymer Research Dresden e.V., Dresden — ³Technische Universität Dresden, Institute of Theoretical Physics, Dresden, Germany

P granules are droplet-like structures consisting of RNA and proteins. They occur in *Caenorhabditis elegans* embryo and are known to determine its germ lineage. Interestingly, P granules are segregated to one side of the cell. There is evidence that the droplet position is regulated by a spatially inhomogeneous protein called Mex-5. Here we propose a model that simplifies the multicomponent nature of the cytoplasm as a ternary mixture: The P granule material, the background fluid, and a regulator mimicking Mex-5. Using our model we aim to understand the physical principles controlling the droplet position. To this end we consider lattice-based Monte Carlo simulations for a ternary mixture, where the microscopic interactions between the components are captured by three Flory-Huggins parameters. Considering a linear regulator gradient we observe two stationary states. Droplets localise in regions of lowest regulator concentration if the regulator exhibits a high affinity to the solvent, and vice versa. We present evidence that the transition between the localisation at highest and lowest regulator concentration can be regarded as a phase transition. Beyond biology, understanding how the droplet positions can be regulated offers the possibility to design switchable units for chemical computing.

DY 69.9 Fri 11:45 H 1058

Mechanical regulation of vein morphogenesis in plant leaves — ●JONATHAN E. DAWSON¹, FRANCK A. DINTENGOU², IRINA KNEUPER², WILLIAM TEALE², KLAUS PALME², and ELENI KATIFORI¹ — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Institute of Biology II, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany

Development of leaf veins is a highly dynamic and regulated process. However, mechanisms that regulate the formation of veins and vascular architecture are largely unknown. In a growing leaf, in addition to genetic regulation, cell mechanics must also play an important role in forming veins. To what extent cell mechanics and the interplay between mechanics and biochemistry plays a role in vascular patterning is not well understood. Using a cell based model in which cells are polygons, here we describe the vascular development in early stages of growing leaf primordia. We investigate the formation of leaf primary vein by simulating tissue growth driven by inter-cellular diffusion of the plant hormone auxin, from auxin synthesizing cells. We show that dynamic modulation of the cell mechanical properties based on cell auxin concentration can reproduce realistic primary vein as observed in growing leaf primordia. We further tested our model by comparing with experiments in which auxin transport is affected.

DY 69.10 Fri 12:00 H 1058

Osmolyte effects: Impact on the aqueous solution around charged and neutral spheres — ●JENS SMIAŁEK — Institut für Computerphysik, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

We have performed atomistic molecular dynamics simulations to study the solvation characteristics of model spheres for low concentrations of urea and hydroxyectoine in aqueous solution. The spheres are either positively or negatively charged with a valency of one or charge neutral. Our results illustrate that the presence of osmolytes influences the solvation properties of the spheres significantly. We have conducted a detailed investigation of water properties like the mean dipolar relaxation times, water orientation parameters around the spheres, dielectric constants, preferential binding behavior, water self-diffusion coefficients, and free energies of solvation by thermodynamic integration to study the influence of osmolytes in detail. Our findings indicate that several factors like the charge of the spheres as well as the characteristics of the osmolytes significantly influence the thermodynamic and dynamic properties of the local water shell and the solvation process with regard to varying enthalpic and entropic contributions.

DY 70: Microswimmers, Active Liquids - Part III (joint session CPP/ BP/ DY)

Time: Friday 9:30–11:30

Location: C 264

Invited Talk

DY 70.1 Fri 9:30 C 264

From chemical nanomotors to biological microswimmers — ●PEER FISCHER — Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart — Institut für Physikalische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart

Building, powering, and operating structures that can navigate complex fluidic environments at the sub-mm scale is challenging. Moving through fluid environments at the scale of micro-organisms for instance presents a different set of challenges compared to those encountered by macroscopic swimmers. Artificial means of realizing motion in microparticles often makes use of local gradients that are established across the colloid, resulting in slip velocities at the particle surface, which in turn drives the motion. In its simplest form this can be realized with Janus-like colloids. I describe what, to the best of my knowledge, are the smallest synthetic chemical nanomotors that have been made and show that their active motion can be tracked with light scattering. Moving from enhanced diffusion to propulsion, I present recent results where colloidal nanopropellers can be moved in water by external magnetic fields similar to a bacterial flagellum and show how the motion of these structures can benefit from the complex rheology in biological media. Although strong Brownian forces dominate in water we achieve controlled propulsion in biological gels, which paves the way for applications inside biological media and the extracellular matrix. Finally, I present an example of a microscallop that does not move in water, but that swims in non-Newtonian liquids.

DY 70.2 Fri 10:00 C 264

Optothermal Manipulation of Plasmonic Nanoparticles in Viscous Solvents — ●FELIX WINTERER^{1,2}, CHRISTOPH MAIER^{1,2}, THEOBALD LOHMÜLLER^{1,2}, and JOCHEN FELDMANN^{1,2} — ¹Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Munich, Germany — ²Nanosystems Initiative Munich (NIM), Munich, Germany

We present an all-optical approach to move and manipulate single plasmonic nanoparticles with high accuracy in viscous solvents.

Gold nanoparticles are subject to optical forces and heat generation upon irradiation with a focussed laser beam. Tuning the laser wavelength with respect to the plasmon resonance frequency allows for switching between repulsive and attractive optical forces, which renders it possible to trap or push individual nanoparticles in two and three dimensions. At the same time, laser light can induce heat in the surrounding medium.

We explore how both effects can be employed to control nanoparticle movement by a combination of thermal gradients and optical forces and discuss further applications of this approach for nanolithography and nanoscale physics.

DY 70.3 Fri 10:15 C 264

Dynamics of a carpet of self-propelled surfactant particles covering a liquid film — ANDREY POTOTSKY¹, ●UWE THIELE², and HOLGER STARK³ — ¹Department of Mathematics, Swinburne University of Technology, Hawthorn, Victoria, 3122, Australia — ²Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — ³Institut für Theoretische Physik, Technische Universität Berlin, 10623, Berlin, Germany

We consider a carpet of self-propelled surface-active particles that move along the liquid-gas interface of a liquid film on a solid substrate and whose swimming direction changes in time due to rotational diffusion. We study the intricate influence of these self-propelled insoluble surfactants on the stability of the film surface and show that depending on the strength of in-surface rotational diffusion and the absolute value of the in-surface velocity several instability modes can occur [1]. In particular, the rotational diffusion can have a stabilizing or destabilizing influence and may even suppress the instability entirely. In the limit of purely upwards swimming we recover the destabilisation described in the literature [2]. The results of the linear analysis are confirmed by fully nonlinear simulations of the complete continuum model and as well through a hybrid discrete self-propelled surfactant particles - continuous film model. [1] A. Pototsky, U. Thiele and H. Stark, *Phys. Rev. E* **90**, 030401(R) (2014). [2] S. Alonso and A.S. Mikhailov, *Phys. Rev. E* **79**, 061906 (2009).

DY 70.4 Fri 10:30 C 264

Tangled Flagella: Importance in Bacterial Propulsion — ●TAPAN CHANDRA ADHYAPAK and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D - 10623 Berlin

It has been well established that hydrodynamic interactions between flagella of peritrichous bacteria such as *E. coli*, leads to synchronization of rotation and bundling of those flagella [1,2]. Flagella are rotated at their bases by rotary motors embedded in the cell body. In response, the cell body has to rotate in the opposite sense such that total torque acting on the bacterium is zero. Often, such cell rotation causes flagella to tangle before they are synchronized completely. We show that tangling has a profound effect on the overall synchronization and bundling dynamics. In particular, we observe abrupt synchronization and bundling on time scales much shorter than those required when the cell movement is switched off to avoid entanglement. Although hydrodynamic interactions still play an important role, through a comparative investigation we conclude that flagellar entanglement generated by cell rotation predominantly affects the total time to synchronize and bundle. Cell movement modifies stationary bundling states too. Specifically, the length over which a bundle is closely packed varies over time, having an oscillatory behavior whose amplitude decreases with increasing number of flagella. At the end we discuss how strongly all these findings affect the overall propulsion of the bacterium.

[1] M. Reichert and H. Stark, *Eur. Phys. J. E* **17**, 493 (2005).[2] S.Y. Reigh, R.G. Winkler, and G. Gompfer, *Soft Matter* **8**, 4363 (2012).

DY 70.5 Fri 10:45 C 264

Reorientation of passive Janus type swimmer in an external temperature profile — ●ANDREAS BREGULLA and FRANK CICHOS — University of Leipzig, department for experimental physics, leipzig, germany

Swimming on the micrometer length scale is dominated by omnipresent Brownian fluctuations and overwhelming viscous forces. Self-phoretic swimmers are an example how to overcome those limitations. Most of those particles are driven by phoretic surface flows generated by surface gradients. In the last decade many different phoretic swimming mechanisms have been proposed. When such self-propelled objects are starting to interact at higher densities, coherent collective motions are observed in which the swimmers align and form flocks, swarms or other complicated patterns. About the origin and details of these complex interactions only little is known. The lack of understanding is mostly due to the lack of control of such particles. Here we want to present a method which extends the existing photon nudging algorithm to gather and collect a specific number of particles and study their interactions. The interactions themselves can be mediated through many different aspects like charges, flow fields or through external profiles created by each active swimmer. The last mentioned interaction will be discussed in detail. An immobile gold colloid acts as an external heat source and mimics the temperature profile that an active swimmer would create in its surrounding. The motion of a passive Janus particle in this temperature field is investigated and the relative motion and alignment with respect to the heat source is quantified.

DY 70.6 Fri 11:00 C 264

Thermophoretic Trapping of Single and Multiple Nano-Objects by Actively Controlled Temperature Fields — ●MARCO BRAUN and FRANK CICHOS — Molecular Nanophotonics, Fakultät für Physik und Geowissenschaften, Universität Leipzig, Deutschland

The understanding of nano-scale soft-matter science benefited enormously from the ability to study single molecules, such as DNA or proteins. In solution Brownian motion lets a molecule disappear quickly from the observation volume, which is why it is typically immobilized in a polymer matrix or by chemical interactions, generally accepted due to a lack of alternatives. However, this strongly changes the local physical and chemical properties. Here, we present an all-optical technique to trap single nano-objects in solution which exploits highly localized temperature fields. The so-called thermophoretic trap exploits thermophoretic interactions of a particle with a temperature gradient, which e.g. locally distorts the screening of the surface charges and by that induces a drift of the particle. In our approach the tempera-

ture field is generated by an optically heated gold nano-structure. Due to the small dimensions of the heat sources, even a small temperature increase introduces large temperature gradients causing a strong thermophoretic drift by which the motion of a Brownian particle can be manipulated. In our experiment an appropriate gold structure is heated locally by a focused laser beam with feedback to the Brownian particles position. The real-time control of the laser beam thereby allows for arbitrary effective trapping potentials for single and multiple particles.

DY 70.7 Fri 11:15 C 264

Low-tech, high-throughput tracking of bacteria in 3D —
•KATJA TAUTE, SANDER TANS, and TOM SHIMIZU — FOM Institute AMOLF, Science Park 102, Amsterdam 1098XG, The Netherlands

Many bacteria swim in liquids and execute complex motility patterns. The increasingly recognized diversity of motility strategies has sparked a growing interest in their characterization via 3D tracking. The only 3D tracking techniques thus far to have passed the benchmark of re-

solving the model bacterium *E. coli*'s run-tumble motility suffer from being limited to single individuals [1]; and/or are technically challenging and require specialized experimental setups [1,2,3].

Here we present a broadly applicable high-throughput 3D bacterial tracking technique which requires only a standard biological phase contrast microscope. We exploit the relationship between an object's distance to the focal plane (z) and the observed intensity pattern, and assign z positions by maximizing image cross-correlations to a reference stack. We achieve micron-scale resolution in z , $<0.5 \mu\text{m}$ resolution in x and y , a range of $\sim 350 \times 300 \times 200 \mu\text{m}$ (x,y,z), a throughput of tens of bacteria, and a temporal resolution that is only limited by the detector readout rate. We demonstrate the application of this technique to a range of bacterial species, verify that we recover previously observed motility patterns, and reveal that bacterial individuality, rather than stochasticity, underlies the broad population distribution observed for a key motility parameter of *V. alginolyticus*.

[1] Berg & Brown, *Nature* 239:500, 1972. [2] Vater et al., *PLoS ONE* 9:e87765, 2014. [3] Molaei et al., *PRL* 113:068103, 2014.