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

Walter Zimmermann (Sprecher)
Universität Bayreuth
Theoretische Physik I
Universitätsstrasse 30
D-95440 Bayreuth, Germany
Walter.Zimmermann@uni.Bayreuth.de

Joachim Peinke (Stellvertreter)
Carl-von-Ossietzky Universität Oldenburg
Institut für Physik, AG TWiSt
Carl-von-Ossietzky-Str. 9-11
D- 26111 Oldenburg, Germany
peinke@uni-oldenburg.de

Overview of Invited Talks and Sessions

(Lecture rooms H44, H46, H47, H48, and H36; Poster C)

Invited Talks

DY 3.1	Mon	9:30–10:00	H46	**History and Structure of Granular Sediments** — •Thorsten Pöschel
DY 11.1	Mon	15:00–15:30	H44	**Large deviation functionals in stochastic thermodynamics** — •Andreas Engel, Johannes Hoppenau, Daniel Nickelsen
DY 11.2	Mon	15:30–16:00	H44	**Thermodynamics with Continuous Information Flow** — •Massimiliano Esposito
DY 11.3	Mon	16:00–16:30	H44	**Measuring energy and information one molecule at a time** — •Felix Ritort
DY 11.4	Mon	16:45–17:15	H44	**Information reservoirs, bipartite systems, and the minimal energetic cost of uncertainty in biomolecular reactions** — •Andre C Barato
DY 11.5	Mon	17:15–17:45	H44	**Feedback control of transport in nanostructures.** — •Tobias Brandes
DY 16.1	Tue	9:30–10:00	H47	**Amoeboid swimming** — •Chaouqi Misbah
DY 35.1	Wed	9:30–10:00	H46	**Nonreciprocal forces in soft matter systems: passive particles become active** — •Hartmut Löwen
DY 41.1	Wed	15:00–15:30	H48	**Visualizing quantum chaos in four dimensions** — •Arnd Bäcker
DY 49.1	Thu	9:30–10:00	H46	**Patterns formation through elastic instabilities, from thin sheets to twisted ribbons** — •Pascal Damman
DY 50.1	Thu	9:30–10:00	H48	**A new look at atomic tunneling systems in glasses containing isotopes with nuclear quadrupol moments** — •Andreas Reiser
DY 54.1	Thu	15:00–15:30	H20	**Between Localization and Ergodicity in Quantum Systems** — •Boris Altshuler
DY 54.2	Thu	15:30–16:00	H20	**Canonical description of short-range interacting few-body quantum systems** — •Quirin Hummel, Benjamin Geiger, Juan Diego Urbina, Klaus Richter
DY 54.3	Thu	16:00–16:30	H20	**One, Two, Three, Many: Manipulating Quantum Systems One Atom at a Time** — •Selim Jochim
DY 54.4	Thu	16:45–17:15	H20	**Statistical Signatures of Many-Particle Interference** — •Mattia Walschaers
DY 54.5	Thu	17:15–17:45	H20	**Boson sampling with integrated quantum photonics** — •Fabio Sciarrino
DY 57.1	Thu	15:00–15:30	H46	**The Transition to the Ultimate State in Turbulent Thermal Convection** — •Eberhard Bodenschatz

Invited talks of the joint symposium SYCS

See SYCS for the full program of the symposium.

SYCS 1.1	Tue	9:30–10:00	H1	**Theory far from infinity: chimera states without the thermodynamic limit** — •Daniel Abrams
SYCS 1.2	Tue	10:00–10:30	H1	**Chimera patterns: Influence of topology, noise, and delay** — •Eckehard Schöll
SYCS 1.3	Tue	10:30–11:00	H1	**Chimera states in quantum mechanics** — •Victor Manuel Bastidas Valencia
SYCS 1.4	Tue	11:15–11:45	H1	**Synchronization in Populations of Chemical Oscillators: Phase Clusters and Chimeras** — •Kenneth Showalter
SYCS 1.5	Tue	11:45–12:15	H1	**Epileptic seizures: chimeras in brain dynamics** — •Klaus Lehnertz

Invited talks of the joint symposium SYSM

See SYSM for the full program of the symposium.

SYSM 1.1	Thu	9:30–10:00	H1	**Science Forecasts: Measuring, Predicting, and Communicating Scientific Developments** — •Katy Börner
SYSM 1.2	Thu	10:00–10:30	H1	**Mapping science with variable-order Markov dynamics reveal overlapping fields and multidisciplinary journals** — •Martin Rosvall
SYSM 1.3	Thu	10:30–11:00	H1	**Network algorithms for reputation and quality in scholarly data** — •Matúš Medo, Manuel Mariani, Yi-Cheng Zhang
SYSM 1.4	Thu	11:15–11:45	H1	**Modeling scientific networks in social media** — •Cassidy Sugimoto
SYSM 1.5	Thu	11:45–12:15	H1	**Modeling scientific collaboration across multiple scales: from individuals to Europe** — •Alexander Petersen

Invited talks of the joint symposium SYAD

See SYAD for the full program of the symposium.

SYAD 1.1	Thu	15:00–15:30	H15	**Phenomenology of Collective Chemotaxis in Artificial and Living Active Matter** — •Ramin Golestanian
SYAD 1.2	Thu	15:30–16:00	H15	**First-passage times of Markovian and non Markovian random walks in confinement** — •raphael Voituriez
SYAD 1.3	Thu	16:00–16:30	H15	**Cytoskeleton organization as an optimized, spatially inhomogeneous intermittent search strategy** — •Heiko Rieger, Yannick Schröder, Karsten Schwarz
SYAD 1.4	Thu	16:45–17:15	H15	**Ergodicity violation and ageing in living biological cells** — •Ralf Metzler
SYAD 1.5	Thu	17:15–17:45	H15	**Anomalous diffusion within cells** — Sarah Klein, •Cecile Appert-Rolland, Ludger Santen

Sessions

DY 1.1–1.3	Sun	16:00–18:30	H16	**Tutorial: Evolutionary Dynamics and Applications to Biology, Social and Economic Systems (SOE / DY / BP / jDPG)**
DY 2.1–2.6	Mon	9:30–11:00	H45	**Colloids and Complex Fluids I (joint Session BP/CPP/DY, organized by BP)**
DY 3.1–3.11	Mon	9:30–12:45	H46	**Granular Matter**
DY 4.1–4.12	Mon	9:30–12:45	H47	**Dynamics in many-body systems: Equilibriation and localization (joint session DY/TT)**
DY 5.1–5.11	Mon	9:30–13:00	H51	**Colloids and Complex Fluids II (joint session CPP/BP/DY)**
DY 6.1–6.6	Mon	10:00–11:30	H36	**Networks: From Topology to Dynamics I (joint session SOE / DY / BP)**
DY 7.1–7.5	Mon	10:30–12:35	H2	**SKM Dissertation-Prize 2016**
DY 8.1–8.4	Mon	12:15–13:15	H36	**Evolutionary Game Theory (joint session SOE / BP / DY)**
DY 9.1–9.1	Mon	14:00–14:45	H15	**Plenary Talk: Ehud Meron**
DY 10.1–10.11	Mon	15:00–18:00	H42	**Colloids and Complex Fluids III (joint session CPP/BP/DY)**
DY 11.1–11.5	Mon	15:00–17:45	H44	**Focus Session: Stochastic thermodynamics and information processing (joint session DY/BP)**
DY 12.1–12.4	Mon	15:00–16:00	H47	**Energy systems**
DY 13.1–13.9	Mon	15:00–17:15	H48	**Statistical Physics (general)**
DY 14.1–14.6	Mon	16:15–17:45	H47	**Complex Systems**
DY 15.1–15.5	Tue	9:30–12:15	H1	**Chimera State: Coherence-Incoherence Patterns in Complex Networks (joint symposium DY/SOE/BP)**
DY 16.1–16.12	Tue	9:30–13:00	H47	**Microswimmers I (joint session DY/BP)**
DY 17.1–17.12	Tue	10:00–13:15	H48	**Statistical Physics far from Thermal Equilibrium**
DY 18.1–18.4	Tue	12:00–13:00	H43	**Statistical Physics of Biological Systems I (Joint Session with DY)**
DY 19.1–19.6	Tue	14:00–15:45	H23	**Transport: Fluctuation and Noise (Joint session of DY and TT organized by TT)**
DY 20.1–20.4	Tue	14:00–15:00	H36	**Chimera State: Symmetry breaking in dynamical networks (joint session DY/SOE accompanying symposium SYCS)**
DY 21.1–21.5	Tue	14:00–15:15	H46	**Complex Fluids and Colloids IV (joint session DY/BP/CPP)**

DY 22.1–22.6	Tue	14:00–15:30	H47	**Anomalous Diffusion (joint session DY/BP)**
DY 23.1–23.5	Tue	14:00–15:15	H48	**Quantum Dynamics, Decoherence and Quanten Information**
DY 24.1–24.3	Tue	15:00–15:45	H36	**Networks: From Topology to Dynamics II (joint session SOE / DY / BP)**
DY 25.1–25.8	Tue	18:15–21:00	Poster B2	**Poster: Soft Matter Dynamics / Glasses**
DY 26.1–26.13	Tue	18:15–21:00	Poster C	**Poster - Quanten Systems**
DY 27.1–27.13	Tue	18:15–21:00	Poster C	**Poster - Statistical Physics, Critical Phenomena, Brownian motion**
DY 28.1–28.17	Tue	18:15–21:00	Poster C	**Poster - Complex Fluids, Granular Matter, Glasses**
DY 29.1–29.13	Tue	18:15–21:00	Poster C	**Poster - Active Matter, Microswimmers and -fluidics, Statistical Physics Biosystems**
DY 30.1–30.16	Tue	18:15–21:00	Poster C	**Poster - Complex nonlinear systems**
DY 31.1–31.13	Tue	18:15–21:00	Poster C	**Poster - Pattern Formation**
DY 32.1–32.3	Tue	18:15–21:00	Poster C	**Poster - Turbulence**
DY 33.1–33.13	Wed	9:30–13:15	H22	**Transport: Graphene (Joint session of DS, DY, HL, MA, O and TT organized by TT)**
DY 34.1–34.9	Wed	9:30–12:15	H42	**Crystallization, Nucleation, Self Assembly I (joint session CPP/DY, organized by CPP)**
DY 35.1–35.11	Wed	9:30–12:45	H46	**Active Matter (joint session DY/BP)**
DY 36.1–36.11	Wed	10:00–13:00	H47	**Complex Fluids and Colloids V (joint session DY/BP/CPP)**
DY 37.1–37.8	Wed	10:00–12:00	H48	**Nonlinear Dynamics, Synchronization and Chaos**
DY 38.1–38.4	Wed	11:30–12:30	H43	**Statistical Physics of Biological Systems II (Joint Session with DY)**
DY 39.1–39.6	Wed	11:30–13:00	H45	**Microswimmers II (joint Session BP/DY)**
DY 40.1–40.8	Wed	16:00–18:30	H42	**Crystallization, Nucleation, Self Assembly II (joint session CPP/DY, organized by CPP)**
DY 41.1–41.9	Wed	15:00–17:45	H48	**Quantum Chaos**
DY 42.1–42.9	Wed	15:00–18:15	H51	**Focus: Multiscale Simulations for Soft Matter: The Challenge of Dynamics (joint session CPP/DY, organized by CPP)**
DY 43.1–43.3	Wed	15:30–16:15	H46	**Statistical Physics in Biological Systems III (joint DY/BP)**
DY 44.1–44.7	Wed	15:30–17:15	H47	**Critical Phenomena and Phase Transitions**
DY 45.1–45.5	Wed	16:30–17:45	H46	**Brownian Motion and Transport**
DY 46.1–46.14	Wed	18:15–21:00	Poster B2	**Poster: Wetting, Nano- and Microfluidics**
DY 47.1–47.5	Thu	9:30–12:15	H1	**Scientometric Maps and Dynamic Models of Science and Scientific Collaboration Networks (SYSM)**
DY 48.1–48.11	Thu	9:30–12:45	H42	**Wetting, Nano- and Microfluidics I (joint session CPP/DY)**
DY 49.1–49.12	Thu	9:30–13:00	H46	**Pattern Formation (joint session DY/BP)**
DY 50.1–50.12	Thu	9:30–13:00	H48	**Glasses**
DY 51.1–51.5	Thu	10:00–11:15	H47	**Delay and feedback Dynamics**
DY 52.1–52.5	Thu	11:30–12:45	H47	**Extreme events**
DY 53.1–53.5	Thu	15:00–17:45	H15	**Anomalous Diffusion in Complex Environments (joint session BP/CPP/DY)**
DY 54.1–54.5	Thu	15:00–17:45	H20	**Focus Session: Many-Body Interference and Quantum Statistical Physics (joint session DY/TT)**
DY 55.1–55.13	Thu	15:00–18:30	H40	**Polymer Dynamics and Rheology (joint session CPP/DY, organized by CPP)**
DY 56.1–56.7	Thu	15:00–16:45	H42	**Wetting, Nano- and Microfluidics II (joint session CPP/DY)**
DY 57.1–57.13	Thu	15:00–18:45	H46	**Focus Session: Turbulence - From Pattern Formation to Stochastic Disorder**
DY 58.1–58.6	Thu	15:30–17:00	H47	**Networks: From Topology to Dynamics III (joint session DY/BP/SOE)**
DY 59.1–59.4	Thu	16:45–17:45	H43	**Networks - From Topology to Dynamics IV (Joint Session BP/SOE/DY)**
DY 60.1–60.9	Fri	9:30–12:00	H51	**Interfaces and Thin Films II (joint session CPP/DY, organized by CPP)**

Annual General Meeting of the Dynamics and Statistical Physics Division

10. März 2016 19:00–20:00 H47

- Bericht
- Frühjahrstagung 2017
- Verschiedenes

DY 1: Tutorial: Evolutionary Dynamics and Applications to Biology, Social and Economic Systems (SOE / DY / BP / jDPG)

Current model approaches for collective phenomena in biological, social and economic systems widely employ methods from statistical physics. This sequence of tutorial talks demonstrates how physical concepts allow the formulation of appropriate microscopic models, the numerical and analytical treatment to obtain phase diagrams and macroscopic equations of motion. Host-virus coevolution, social opinion formation and systemic risk of the interbank network are research frontiers illustrating fruitful applications (Session compiled by J.C.Claussen)

Time: Sunday 16:00–18:30 Location: H16

Tutorial DY 1.1 Sun 16:00 H16

Predicting evolution: statistical mechanics and biophysics far from equilibrium — •Michael Lässig — Institut für theoretische Physik, Zülpicher Strasse 77, D-50937 Köln

The human flu virus undergoes rapid evolution, which is driven by interactions with its host immune system. We describe the evolutionary dynamics by a fitness model based on two biophysical phenotypes of the virus: protein folding stability and susceptibility to human immune response. This model successfully predicts the evolution of influenza one year into the future, which has important consequences for public health: evolutionary predictions can inform the selection of influenza vaccine strains. Based on this example, we discuss the role of statistical mechanics and biophysics in making evolutionary biology a predictive science.

Tutorial DY 1.2 Sun 16:50 H16

Voter models of social opinion formation. — •Katarzyna Sznajd-Weron — Department of Theoretical Physics, Wroclaw University of Technology, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw

Among many different subjects, opinion dynamics is one of the most studied in the field of sociophysics. In my opinion there are at least two important reasons why physicists study this topic. The first motivation comes from social sciences and can be described as a temptation to build a bridge between the micro and macro levels in describing social systems. Traditionally, there are two main disciplines that study social behavior - sociology and social psychology. Although the subject of the study is the same for both disciplines, the usually taken approach is very different. Sociologists study social systems from the level of the social group, whereas social psychologists concentrate on the level of the individual. From the physicist's point of view this is similar to the relationship between thermodynamics and statistical physics. This analogy raises the challenge to describe and understand the collective behavior of social systems (sociology) from the level of interpersonal interactions (social psychology). The second motivation to deal with opinion dynamics is related to the development of non-equilibrium statistical physics, because models of opinion dynamics are often very interesting from the theoretical point of view. A good example of such an interesting model is a broad class of voter models, including linear voter model and nonlinear q-voter model introduced in along with its modifications.

Tutorial DY 1.3 Sun 17:40 H16

Maximum-entropy methods for network reconstruction, systemic risk estimation, and early-warning signals — •Diego Garlaschelli — Lorentz Institute for Theoretical Physics, University of Leiden, The Netherlands

The global financial crisis shifted the interest from traditional measures of "risk" of individual banks to new measures of "systemic risk", defined as the risk of collapse of an entire interbank system. In principle, estimating systemic risk requires the knowledge of the whole network of exposures among banks. However, due to confidentiality issues, banks only disclose their total exposure towards the aggregate of all other banks, rather than their individual exposures towards each bank. Is it possible to statistically reconstruct the hidden structure of a network in such a way that privacy is protected, but at the same time higher-order properties are correctly predicted? In this talk, I will present a general maximum-entropy approach to the problem of network reconstruction and systemic risk estimation. I will illustrate the power of the method when applied to various economic, social, and biological systems. Then, as a counter-example, I will show how the Dutch interbank network started to depart from its reconstructed counterpart in the three years preceding the 2008 crisis. Over this period, many topological properties of the network showed a gradual transition to the crisis, suggesting their usefulness as early-warning signals of the upcoming crisis. By definition, these early warnings are undetectable if the network is reconstructed from partial bank-specific information.

DY 2: Colloids and Complex Fluids I (joint Session BP/CPP/DY, organized by BP)

Joint session with CPP and DY organized by BP.

Time: Monday 9:30–11:00 Location: H45

DY 2.1 Mon 9:30 H45

Intracellular microfluidics to probe the role of hydrodynamic flows in embryonic cell polarization — Matthäus Mittasch[1], •Peter Gross[2], Stephan Grill[2], and Moritz Kreysing[1] — [1]MPI-CBG, Dresden, Germany — [2]Biotechnolgy Center, TU Dresden, Dresden, Germany

A hallmark of embryogenesis is the development of spatial structure. This process is orchestrated by gene regulatory networks coupled to physical transport mechanisms. Particularly, it was suggested that the polarization of the egg cell of the nematode worm Caenorhabditis elegans, prior to asymmetric cell division, relies on interaction of two protein networks (PAR proteins) coupled to active cortical flows. However, it remains a challenge to perturb intracellular fluid mechanics to demonstrate the causal role of hydrodynamic flows in embryogenesis. Towards this end, we exploited thermo-viscous pumping (Weinert & Braun, J. appl. Phys. 2008) in order to dynamically control hydrodynamic flows inside of living embryos. Specifically, well-defined flow patterns were generated on sub- and cellular length-scales with velocities exceeding wild-type flows significantly, without affecting the biological integrity of the embryo. By application of externally-induced flows we depleted membrane-bound PAR proteins locally, suggesting that hydrodynamic flows are essential to load PAR proteins at the posterior pole. Furthermore, we perform rescue experiments in a non-polarizing embryo, by which the omitted wild-type flow will be applied externally to test if the PAR polarity can be restored artificially.

DY 2.2 Mon 9:45 H45

Phase behavior of dense lysozyme solutions — •Julian Schulze[1], Johannes Möller[2], Michael Paulus[1], Julia Nase[1], Metin Tolan[1], and Roland Winter[3] — [1]Fakultät Physik/Delta, Technische Universität Dortmund,44221 Dortmund ,Germany — [2]ESRF - The European Synchrotron, 38043 Grenoble, France — [3]Fakultät für Chemie und Chemische Biologie, Technische Universität Dortmund, 44221 Dortmund, Germany

In previous studies, small-angle X-ray scattering (SAXS) in combination with liquid-state theoretical approaches and DLVO theory was used to study the intermolecular interaction potential V(r) of lysozyme solutions under the influence of varying environmental conditions such as protein concentration c, temperature T, and pressure p. While the repulsive Coulomb term of the DLVO potential remains almost con-

stant as a function of p, the depth of the attractive part, J(p), exhibits a non-monotonic p-dependence with a minimum at about 2 kbar at constant T. Adding 0.5 M NaCl leads to more prominent short range interactions, especially at high c and low T, and the homogeneous protein solution becomes turbid due to formation of a metastable liquid-liquid phase separation (LLPS) region, where lysozyme forms small droplets of high concentration within the more dilute liquid phase. At elevated pressures, this l-l phase separation is suppressed, but due to the non-monotonic behavior of J(p), a further pressure increase leads to a re-entrant LLPS regime. In this contribution, we will discuss the phase behavior of lysozyme as a function of c, p, and T.

DY 2.3 Mon 10:00 H45

Demixing and Ripening in Gradient Systems — •Christoph Weber[1], Chiu Fan Lee[2] und Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Department of Bioengineering, Imperial College, London

Ostwald ripening in homogeneous mixtures is described by the Lifshitz-Slyozov theory. It captures the phenomenon of smaller droplets that shrink, while larger ones grow. This process is driven by a difference in the Laplace pressures between the drops. Recently, liquid-like drops have been reported in living cells, which ripen in a gradient of a regulating protein component. This protein is known to affect the phase separation properties along the gradient such that drops dissolve at one and grow at the opposite side of the cell. An open question is how an inhomogeneous background affects the ripening law in contrast to the homogeneous Lifshitz-Slyozov theory.

To this end we analytically derived the corresponding growth law using a mean field theory. We find that there is a gradient of supersaturation that leads to a drift and an inhomogeneous growth of drops. The latter gives rise to a dissolution boundary that moves through the system leaving droplets only at one side of the system.

Using our mean field approach to describe the interactions between multiple drops we discover that a larger gradient of supersaturation not necessarily implies a faster ripening. Instead, droplets can be spatially sorted in size leading an arrest of the ripening dynamics for large times until homogeneous Ostwald-ripening sets in again.

DY 2.4 Mon 10:15 H45

New analysis method for passive microrheology — •kengo nishi[1], maria l. kilfoil[2], christoph f. schmidt[1], and fred c. macKintosh[3] — [1]Georg-August-Universität Göttingen, Göttingen, Germany — [2]University of Massachusetts, Amherst, USA — [3]Vrije Universiteit, Amsterdam, Netherland

Passive microrheology is an experimental technique used to measure the mechanical response of materials from the fluctuations of micron-sized beads embedded in the medium. Microrheology is well suited to study rheological properties of materials that are difficult to obtain in larger amounts and also of materials inside of single cells. In one common approach, one uses the fluctuation-dissipation theorem to obtain the imaginary part of the material response function from the power spectral density of bead displacement fluctuations, while the real part of the response function is calculated using a Kramers-Kronig integral. The high-frequency cut-off of this integral strongly affects the real part of the response function in the high frequency region. Here, we discuss how to obtain more accurate values of the real part of the response function by an alternative method using autocorrelation functions.

DY 2.5 Mon 10:30 H45

How to regulate droplet position in a heterogeneous chemical environment? — •Samuel Krüger[1,2], Christoph A. Weber[1], Jens-Uwe Sommer[2,3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Leibniz Institute of Polymer Research Dresden e.V., Dresden — [3]Technische Universität Dresden, Institute of Theoretical Physics, Dresden, Germany

Cells contain chemical components that are not separated from the cytoplasm by a membrane. An example are P-granules in the C. elegans embryo. They are liquid-like structures, that form droplets. They consist of RNA and proteins that are segregated spontanuously from the cytoplasm and are known to play a role in the specification of germ cells. During asymmetric cell division, P granules are segregated to one side of the cell. This segregation is guided by a spatial concentration gradient of the protein Mex-5. We simplify the multicomponent nature of the cytoplasm with a ternary model: The P granule material, the solvent (cytoplasm), and a regulator corresponding to Mex-5. Using this model we aim to understand the physical principles controlling the droplet position in a simplified scenario, where an external potential establishes the regulator gradient. We use the Flory-Huggins mean field theory and calculate the equilibrium solutions by minimizing the free energy functional. There are two equilibrium states. Droplets either localize at high external potential or low external potential. Changing the interaction between the regulator and the solvent we find that the free energy exhibits a kink indicating that the transition between both states being a discontinuous phase transition.

DY 2.6 Mon 10:45 H45

Finding descriptive features for the characterization of the coarsening dynamics of three dimensional foams — •Jonas Dittmann[1], Anja Eggert[2], Martina Lambertus[1], Jannika Dombrowski[3], Alexander Rack[4], and Simon Zabler[1,2] — [1]Lehrstuhl für Rötngenmikroskopie, Fakultät für Physik und Astronomie, Universität Würzburg, Germany — [2]Fraunhofer EZRT, Fürth, Germany — [3]Wissenschaftszentrum Weihenstephan, Technische Universität München, Germany — [4]European Synchrotron Radiation Facility (ESRF), Grenoble, France

Understanding the coarsening behavior of foams is essential for their deliberate design. The coarsening theories by Lifshitz, Slyozov and Wagner (LSW) as well as Glazier provide concise coarsening models with descriptive parameters that may enable systematic studies on the effects of different foam constituents.

Wet polydisperse beta-Lactoglobulin foam was imaged by fast synchrotron micro computed tomography over a period of 15 minutes in intervals of 2 to 5 minutes. The growth behavior of about 2×10^5 pores is individually observed and statistically analyzed as a function of pore radius as well as number of neighboring pores.

The three-dimensional analog of von Neumann's law by Glazier is confirmed as a fitting empirical description of the mean coarsening behavior, whereby the critical number of neighbors discriminating between shrinkage and growth is found to be 13.2 ± 5.5. Qualitative features of LSW theory are observed as well: the pore's growth rate increases with their size and a critical radius can be identified.

DY 3: Granular Matter

Time: Monday 9:30–12:45 Location: H46

Invited Talk DY 3.1 Mon 9:30 H46

History and Structure of Granular Sediments — •Thorsten Pöschel — Institute for Multiscale Simulation, Friedrich-Alexander Universität, Erlangen-Nürnberg, Germany

We consider the sedimentation of monodisperse granular particles under the influence of gravity. The history of the process is described by the surface of the sediment as a function of time. We show that the resulting structure of the sediment, characterized by the field of contact number is intimately related to the process of sedimentation such that the history of the process, can be completely deduced from the time-independent field of contact number of the sediment.

DY 3.2 Mon 10:00 H46

Mechanical properties of cohesive granular materials — •Arnaud Hemmerle, Matthias Schröter, and Lucas Goehring — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Understanding the mechanical properties of cohesive granular materials is important for various problems such as fracturing of rocks, fluid invasion, or seismology. By mixing glass beads with a curable elastic polymer, we create well-defined cohesive granular media, held together by solid capillary bridges. The mechanical response and the toughness of this model material can be tuned over a broad range by adjusting the strength and stiffness of the bridges, as well as the size and cohesion of its constituents. We thoroughly characterized the mechanical properties of this model cohesive granulate for various bead

sizes, volume fractions of polymer, and polymer stiffnesses to show the range of behaviors allowed, and their scaling. Using in situ stress-strain tests combined with X-ray micro-tomography, we investigated the links between these macroscopic properties and the microscopic modes of deformation, for example the elongation and the bending of connected neighboring beads.

Along with these fundamental studies of the mechanical response of this model system, we will briefly discuss potential applications of its customizable properties to geoengineering and biophysics, with, for example, investigations on biofouling and bio-deterioration.

DY 3.3 Mon 10:15 H46

Self-organization of wet granular hexagons under vertical agitations — •Manuel Baur and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

As each sand grain in nature has a peculiar shape, it is of practical importance to understand how shape matters in the collective beahvior of granular materials. As a starting point, we focus on the assembly of hexagonally shaped disks confined in a monolayer and agitated vertically against gravity. The particles are partially wet so as to introduce short ranged attractive interactions at each contact. We explore how the agitation strength and frequency, area fraction as well as cohesion influence the melting of wet granular hexagons by means of particle tracking. Using bond orientational order parameters, we identify the local structures of the particle, determine the nonequilibrium stationary states of the system and present them in a stability diagram. Moreover, we analyze the translational as well as orientational diffusivity of the particles in the vicinity of the melting transition.

DY 3.4 Mon 10:30 H46

$1/f$ noise on the brink of wet granular melting — •Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

The collective behavior of a two-dimensional wet granular cluster under horizontal swirling motions is investigated experimentally. Depending on the balance between the energy injection and dissipation, the cluster evolves into various nonequilibrium stationary states with strong internal structure fluctuations with time. Quantitative characterizations of the fluctuations with the bond orientational order parameter q_6 reveal power spectra of the form f^α with the exponent α closely related to the stationary states of the system. In particular, $1/f$ type of noise with $\alpha \approx -1$ emerges as melting starts from the free surface of the cluster, suggesting the possibility of using $1/f$ noise as an indicator for phase transitions in systems driven far from thermodynamic equilibrium.

DY 3.5 Mon 10:45 H46

Dynamical mesoscopic model for granular shear — •Sára Lévay and János Török — Department of Theoretical Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary

Flow law of dense granular material is of fundamental importance and is still an unsolved problem. Different methods are competing in the literature with similar properties yet they fail to predict correctly all empirical results [1]. We introduce a improved version of a simple mesoscopic model [2] based on the principle of minimal dissipation and random local dynamic effects to reproduce both quasi-static and dynamic flow laws. We test our model against other theories and numerical simulations and show that in spite of its simplicity it can provide more precise results than other methods.

[1] Alexander Ries, Lothar Brendel, and Dietrich E. Wolf. "Shearrate diffusion and constitutive relations during transients in simple shear." Computational Particle Mechanics (2015): 1-8.

[2] Tamás Börzsönyi, Balázs Szabó, Gábor Törös, Sandra Wegner, János Török, Ellák Somfai, Tomasz Bien, and Ralf Stannarius "Orientational Order and Alignment of Elongated Particles Induced by Shear" Phys. Rev. Lett. 108, 228302 (2012).

15 min. break.

DY 3.6 Mon 11:15 H46

Declustering in a granular gas as a finite size effect — •Mathias Hummel and Marco Giacomo Mazza — Max Planck Institute for Dynamics and Self-Organization

For realistic models of granular collisions, where the coefficient of restitution depends on the impact velocity, the existence of dense clusters has been shown to be a transient phenomenon. We report direct numerical simulations that elucidate the conditions for the disappearance of structures. We find that upon cluster formation the granular temperature and the convective kinetic energy couple and both follow Haff's law. Furthermore, we show that clusters will eventually dissolve in all finite size systems. We find the strong power law $t' \propto L^{12}$ for the declustering time. Our results imply that only in systems close to the initial critical system size both the clustering and declustering transitions are observable.

DY 3.7 Mon 11:30 H46

Structure and Mechanics of Ellipsoid Packings — •Simon Weis[1], Fabian Schaller[1], Gerd Schröder-Turk[2], and Matthias Schröter[3] — [1]Theoretische Physik 1, FAU Erlangen, Germany — [2]School of Engineering and IT, Murdoch University, Australia — [3]Institute for Multiscale Simulation, FAU Erlangen, Germany

Friction and adhesive forces are important parameters for the stability of granular packings. We examine the structural and mechanical properties of packings in respect to those parameters. Although friction has an impact on the mechanical characteristics, the analyzed local structural features remain unchanged.

The particles of interest are ellipsoids with two types of aspect ratios as well as spheres as a reference system. Interparticle friction is changed by grinding the particles with different abrasives as well as by applying liquid and dry lubricants, which also changes adhesive forces. The friction coefficient is measured using an inclined plane. Various packings with a range of friction coefficients are prepared using different preparation methods to obtain a range of packing fractions.

To obtain structural properties, the packings are recorded by X-ray tomography and the particles are detected. Structural characterization includes mean and local packing fractions, contact numbers as well as voronoi cell anisotropy by Minkowski tensors. The mechanical features are examined within a shear cell setup.

DY 3.8 Mon 11:45 H46

Hopper flow of shape-anisotropic grains — •Ahmed Ashour and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik

Granular materials have unusual and sometimes counterintuitive physical properties. For this reason, despite the fact that they have been involved in pharmaceutical, industrial, and agricultural applications since decades, centuries, and even millennia, they were and still are the subject of intense scientific research. One of the important problems in processing such materials is silo outlet, which has been studied with spherical grains in numerous publications before. We study experimentally the clogging of elongated granular materials during discharge from a flat bottom silo when the orifice size is not much bigger than the grain size. We check if there exists a critical radius of the orifice at which there is no clogging but continuous flow. The change in the flow velocity of the particles from the silo with changing radius of the orifice is studied, and we check the validity of Beverloo's equation for different geometric parameters

DY 3.9 Mon 12:00 H46

Hopper flow of nonspherical granular particles — •János Török[1], Gábor Szabó[2], Ellák Somfai[2], and Tamás Börzsönyi[2] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary — [2]Institute for Solid State Physics and Optics, Wigner Research Center for Physics,

We present experimental results of hopper flow with spherical and nonspherical granular particles. We show that the flow widens with the increasing hopper flow angle, but shrinks with the increasing particle aspect ratio, where the flow also gets more intermittent with a well defined frequency. The results are compared to a mesoscopic model based on the principle of minimal dissipation. We show that due the the elongated particles the shape of the flow changes and becomes more straight.

DY 3.10 Mon 12:15 H46

Spontaneous heaping and secondary flows in sheared granular materials — •David Fischer[1], Ralf Stannarius[1], and Tamás Börzsönyi[2] — [1]Otto von Guericke University, Magdeburg, Germany — [2]Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary

Cylindrical containers with a rotating bottom disk (so-called split-bottom geometry) are well established devices to shear granular mate-

rials in a continuous way, and to generate well-defined localized shear bands in the granular bed. When granular material composed of anisotropic grains is sheared in such a container, a secondary flow is generated that leads to the formation of a considerable heap of material near the rotation axis. Superficially, it reminds of the Weissenberg effect in polymer solutions. This process is analyzed for different materials, and its quantitative dependence upon geometric and dynamic parameters is investigated. We find secondary flow and heaping in all investigated anisometric granular materials, both for prolate and oblate shapes. For spherical or nearly-spherical grains, this phenomenon is completely absent.

DY 3.11 Mon 12:30 H46

Why Mikado is one of the easier granular problems — Cyprian Lewandowski[1], Pascal Wieland[2], Max Neudecker[3], Claus Heussinger[2], and •Matthias Schröter[3,4] — [1]Imperial College, London, UK — [2]Georg-August University of Göttingen, Germany — [3]MPI for Dynamics and Self-Organization, Göttingen, Germany — [4]Friedrich Alexander Universität, Erlangen, Germany

The mechanical stability of a granular packing depends on the number of contacts Z between its particles. For most particle shapes, predicting Z as a function of the average volume fraction ϕ is complicated by the spatial correlations between simultaneously contacting particles. However, in the dilute packings formed by cylinders with large aspect ratios α (length of the cylinder divided by its diameter) the individual contacts can be expected to become uncorrelated. Philipse (Langmuir **12**, 1127 (1996)) derived from this idea the Random Contact Model (RCM) which predicts $Z_{RCM} = 2\alpha\phi$. Using X-ray tomography of packings of frictional spaghetti and simulations of frictionless spherocylinders we measure how Z depends on α and ϕ. We find that a non-zero friction coefficient μ increases the range of ϕ where mechanically stable packings exist, but the average Z value seems to be not influenced by μ. For α in the range 15 to 80 the measured Z is smaller or equal to $0.85Z_{RCM}$. We show that this difference can be explained by the way the RCM defines contacts.

DY 4: Dynamics in many-body systems: Equilibriation and localization (joint session DY/TT)

Time: Monday 9:30–12:45 Location: H47

DY 4.1 Mon 9:30 H47

Dynamical thermalization in Bose-Hubbard systems — •Peter Schlagheck[1] and Dima L. Shepelyansky[2] — [1]Département de Physique, Université de Liège, Belgium — [2]Laboratoire de Physique Théorique du CNRS, IRSAMC, Université de Toulouse UPS, France

A bosonic many-body system can exhibit the Bose-Einstein distribution in its single-particle eigenstates not only if it is coupled to a heat and particle reservoir, but also if it is subject to a two-body interaction of moderately low strength which couples the single-particle eigenstates with each other. We numerically verify this dynamical thermalization conjecture within disordered Bose-Hubbard rings of finite size whose parameters are chosen such that the dynamics of the system can be expected to be ergodic [1]. This allows one to associate with each many-body eigenstate of the Bose-Hubbard system well-defined (positive or negative) values for the effective temperature and the effective chemical potential which depend on the energy per particle of the eigenstate under consideration [1]. With this information one can then predict the populations of single-particle eigenmodes within each many-body eigenstate of the system according to the Bose-Einstein distribution, without knowing more details about the quantum dynamics of the many-body system.

[1] P. Schlagheck and D. L. Shepelyansky, arXiv:1510.01864.

DY 4.2 Mon 9:45 H47

Stationary state after a quench to the Lieb-Liniger from rotating BECs — •Leda Bucciantini — Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

We study long-time dynamics of a bosonic system after suddenly switching on repulsive delta-like interactions. As initial states, we consider two experimentally relevant configurations: a rotating BEC and two counter-propagating BECs with opposite momentum, both on a ring. In the first case, the rapidity distribution function for the stationary state is derived analytically and it is given by the distribution obtained for the same quench starting from a BEC, shifted by the momentum of each boson. In the second case, the rapidity distribution function is obtained numerically for generic values of repulsive interaction and initial momentum. The significant differences for the case of large versus small quenches are discussed.

DY 4.3 Mon 10:00 H47

Short time propagation in interacting bosonic systems — •Benjamin Geiger, Quirin Hummel, Juan-Diego Urbina, and Klaus Richter — Institut für Theoretische Physik Universität Regensburg, 93040 Regensburg, Germany

We present a formalism to calculate thermodynamic properties of interacting bosonic gases as well as the smooth (Weyl) contribution to density of states by means of short-time propagation, and compare its analytical predictions against quantum integrable models. As an essential input of our approach, we were able to construct the many-body propagator for a one-dimensional unconfined bosonic gas with delta interactions of variable strength. Using this propagator we can give short-time approximations for the Lieb-Liniger model and non-integrable systems including external harmonic potentials. Furthermore we can think of using the spatial information and the time dependence of the propagator to calculate e.g. two-point correlations or to investigate quantum quenches.

DY 4.4 Mon 10:15 H47

Equilibration in many-body localised systems — Mathis Friesdorf, Albert Werner, •Marcel Goihl, Winton Brown, and Jens Eisert — Freie Universität Berlin

The effect of many-body localisation (MBL) is connected to an intriguing class of systems that fail to thermalise. Due to the randomness present in these models, both particles and energies remain largely confined to local regions. This prevents the relaxation of excitations and thus leads to a local memory of the precise initial conditions even after long evolution times. Based on a phenomenological model of MBL, we examine the time evolution of these systems and explore the role of local constants of motion, which are intrinsically present if energy is localised. We show that despite the fact that particles and energy are localised, information is able to propagate over arbitrary distances. Following this information theoretical viewpoint, we capture equilibration in MBL systems and derive time scales thereof. We connect our findings to signatures measurable in optical lattice architectures, thus allowing for the distinction of Anderson localisation and true MBL based solely on existing measurement techniques.

DY 4.5 Mon 10:30 H47

The eigenstate thermalization hypothesis as driving force behind initial state independent equilibration in closed quantum systems — •Christian Bartsch and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, D-49069 Osnabrück

We analyze the long time behavior of non-equilibrium expectation value dynamics for finite closed quantum systems considering very general Hamiltonians and observables. For a certain class of generic, i.e., experimentally realistic, initial states we analytically find that the long time expectation value depends on the concrete initial state and in general deviates from the expected average equilibrium value unless the eigenstate thermalization hypothesis (ETH) is fulfilled. We call this behavior stick effect. The initial states may be prepared by exposition of the system to a super bath in combination with an additional potential which depends on the regarded observable, thus the system is explicitly out of equilibrium and the initial state is correlated with both the Hamiltonian and the observable, i.e., the situation is not covered by established investigations involving typicality in terms of the Haar measure. The results suggest that the ETH may serve not only as a sufficient but also as a necessary condition for initial state independent equilibration. Numerics for a specific class of integrable quantum magnets, which does not fulfill the ETH, illustrate the findings.

DY 4.6 Mon 10:45 H47

Fluctuations, meta-stability and symmetry-breaking in open many-body systems — •Henrik Wilming[1], Albert H. Werner[1], Jens Eisert[1], and Michael J. Kastoryano[2] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [2]NBIA, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, DK

It is known that finite fluctuations of densities in thermal states correspond to the existence of several phases. In the case of fluctuations in order-parameters, they lead to the existence of spontaneous symmetry-breaking. Such results are purely kinematic in that they do not show how these states are prepared by nature.

Here, we consider the corresponding dynamical question: We assume that a state with finite fluctuations in a density is prepared by a dissipative Markovian short-range dynamics that is in detailed balance and show that such dynamics necessarily also has different meta-stable states, which converge to steady-states on (quasi-)local observables in the thermodynamic limit. In the case of fluctuating order-parameters we show the existence of explicitly symmetry-breaking meta-stable states and construct dissipative Goldstone-modes on top of them.

The existence of such meta-stable states shows that it is inherently difficult to prepare a many-body state with strong long-range correlations by short-range dissipative processes fulfilling detailed balance. Our results hold on regular lattices in arbitrary spatial dimensions and are constructive in the sense that we explicitly write down the meta-stable states.

15 min. break

DY 4.7 Mon 11:15 H47

Approaching equilibrium: Fermionic Gaussification — •Marek Gluza[1], Christian Krumnow[1], Mathis Friesdorf[1], Christian Gogolin[2,3], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Berlin, Germany — [2]ICFO-The Institute of Photonic Sciences, Mediterranean Technology Park, Barcelona, Spain — [3]Max-Planck-Institut für Quantenoptik, Garching, Germany

When and by which mechanism do closed quantum many-body systems equilibrate? This fundamental question lies at the very basis of the connection between thermodynamics, many-body quantum mechanics and condensed matter theory. In the setting of free fermionic evolutions, we rigorously capture the time evolution in abstract terms and uncover the underlying mechanism how local memory of the initial conditions is forgotten. Specifically, starting from an initially short range correlated fermionic states which can be very far from Gaussian, we show that if the Hamiltonian provides sufficient transport, the system approaches a state that locally cannot be distinguished from a corresponding Gaussian state. In this way, strongly correlated states, as encountered in the Fermi-Hubbard model, will become locally Gaussian during the evolution under a hopping Hamiltonian, leading to density-density correlations that factor according to Wick's theorem. For experimentally relevant instances of ultra-cold fermions in optical lattices, our result implies equilibration on realistic physical time scales. Moreover, we characterise the equilibrium state, finding an instance of a rigorous convergence to a Generalized Gibbs ensemble.

DY 4.8 Mon 11:30 H47

Controlling Fluctuations in Parametrically Driven Oscillators and Lattices — •Beilei Zhu and Ludwig Mathey — ZOQ/ILP, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

We consider an oscillator parametrically and periodically driven at a high frequency . In the quantum limit we obtain an effective Hamiltonian in the interaction picture analytically via Magnus Expansion. We compare this analytical result with a numerical one, which is developed in the classic limit in the Langevin formalism. The simulation results show that the fluctuations of the oscillator coordinates are reduced at high driving frequencies and moderate driving amplitudes. We also obtain qualitatively similar results in a lattice of parametric oscillators.

DY 4.9 Mon 11:45 H47

Equilibration of isolated quantum systems due to restrictions in the experimental set-up — •Ben Niklas Balz — Bielefeld University, Germany

We will explore in what sense and under which conditions isolated quantum many-body systems equilibrate. To estimate the deviations from the equilibrium state a more realistic distinguishability measure than the ones used in [1,2] will be developed, taking into account how often observables with a certain set of outcomes are measured. As a consequence new insights which physical parameters influence equilibration dynamics in what way can be gained. This might be of theoretical importance contributing to the understanding of thermalization [3] or can be used to give more accurate bounds on equilibration times [4,5].

[1]Peter Reimann. Physica Scripta, 86(5), 2012.
[2]Anthony J Short. New Journal of Physics, 13(5):053009, 2011.
[3]Peter Reimann. New Journal of Physics, 17(5):055025, 2015.
[4]D. Hetterich, M. Fuchs, and B. Trauzettel. ArXiv, June 2015.
[5]L. P. Garcia-Pintos, N. Linden, A. S. L. Malabarba, A. J. Short, and A. Winter. ArXiv e-prints, September 2015.

DY 4.10 Mon 12:00 H47

Reduced fluctuations in dissipative parametric oscillators — •Tobias Rexin, Beilei Zhu, and Ludwig Mathey — Zentrum für Optische Quantentechnologien und Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany

In this work we describe the non-equilibrium effects of a dissipative parametric oscillator system for which we derive an effective time-independent Hamiltonian via Magnus Expansion. The analytical result shows reduced variance in the high driving frequency and moderate driving amplitude regime, which also coincides with numerical results from the Langevin Equations. A chain of parametric oscillators exhibits similiar behavior.

DY 4.11 Mon 12:15 H47

Time evolution of the electron distribution function of thin copper films probed with broadband femtosecond optical pulses — •Manuel Obergfell and Jure Demsar — Universität Mainz

The time-resolved dynamics of the optical constants of thin copper films has been measured in the visible range. The photoinduced changes in reflectivity and transmission are based on the changes to the electron distribution function at the Fermi level. The dielectric function of copper is modelled at the d-band to Fermi level transition at photon energies up to 3 eV. With a low amount of sample dependent parameters the matching to the temperature dependence of the dielectric function of copper is achieved. Therefore we can reproduce standard thermomodulation. To extract the electron distribution function time dependently, the deconvolution is performed by matrix inversion. Our results demonstrate a highly non-thermal electronic distribution up to time delays of more than 1 ps depending on excitation density, at odds with the Two-Temperature model assumption. We extract the electron-phonon coupling constant from these data and compare the results to several recent theoretical models.

DY 4.12 Mon 12:30 H47

Adsorption-desorption kinetics of soft particles onto surfaces — •Brendan Osberg and Ulrich Gerland — Complex Biosystems, Physik-Department, Technische Universitaet Muenchen, Garching, Germany

A broad range of physical, chemical, and biological systems feature processes in which particles randomly adsorb on an extended substrate. Theoretical models usually assume hard (mutually impenetrable) particles, but in soft matter physics the adsorbing particles can be effectively compressible, implying soft interaction potentials. We recently studied the kinetics of such soft particles adsorbing onto one-dimensional substrates, identifying three novel phenomena: (i)gradual density increases, or 'cramming', replaces the usual jamming behavior seen in hard particles, (ii) a density overshoot can occur (only for soft particles) on a time scale set by the desorption rate, and (iii) relaxation rates of soft particles increase with particle size (on a lattice), while hard particles show the opposite trend. The latter occurs since unjamming requires desorption and many-bodied reorganization to equilibrate -a process that is generally very slow. Here we extend this analysis to a two-dimensional substrate, focusing on the question of whether the adsorption-desorption dynamics of particles in two dimensions are similarly enriched by the introduction of soft interactions. Application to experiments, for example the adsorption of fibrinogen on two-dimensional surfaces, will be discussed.

DY 5: Colloids and Complex Fluids II (joint session CPP/BP/DY)

Time: Monday 9:30–13:00 Location: H51

Invited Talk DY 5.1 Mon 9:30 H51

Dynamics of thermosensitive core-shell dumbbells as analyzed by rheo-SANS — •Matthias Ballauff — Helmholtz-Zentrum Berlin

We present a study of the dynamics of dumbbell-shaped colloids. The thermosensitive dumbbell-shaped microgels consist of a solid polystyrene core and a thermosensitive shell of cross-linked poly(N-isopropylacrylamide). These colloidal particles are nearly monodisperse as shown by cryogenic transmission electron microscopy. The aspect ratio L* defined by the ratio of the center distance L to the diameter D can be varied between 0.24 and 0.3. The effective volume fraction can be varied by temperature and high volume fractions can be achieved easily because of the thermosensitive shell [1]. We observe the formation of a plastic crystal in these suspensions about of volume fraction of 0.5 as predicted by theory. This is shown from rheological evidence and by the Bragg-reflections of the crystals. For higher volume fraction a glassy state is formed. Moreover, oscillatory experiments in the linear viscoelastic regime and flow curves up to volume fractions of nearly 0.7 have been obtained. Recent studies based on a combination of rheoSANS experiments and BD-simulations revealed the formation of a novel, partially oriented phase formed by dumbbells under shear. All data demonstrate that these particles present a novel model system for the study of the rheology of slightly anisotropic particles.

[1] F. Chu, et al., Macromol. Rapid Comm. 33 (2012) 1042.

DY 5.2 Mon 10:00 H51

Phase diagram of polydisperse colloidal dispersions — •Preecha Kiatkirakajorn[1], Joaquim Li[1], Bernard Cabane[2], Franck Artzner[3], Robert Botet[4], and Lucas Goehring[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Götingen, Germany — [2]LCMD, CNRS UMR 8231, ESPCI, 10 rue Vauquelin, 75231 Paris Cedex 05, France — [3]Institut de Physique, CNRS UMR 6626, Univ Rennes, 35042 Rennes, France — [4]Physique des Solides, CNRS UMR 8502, Univ Paris-Sud, F-91405 Orsay, France

Polydisperse colloidal dispersions have been predicted, for over twenty years, to have a rich and complex phase space of colloidal crystals. However, experiments have consistently suggested that such crystals are kinetically inaccessible, as small amounts of polydispersity poison crystal formation. Here, we show a result of small-angle X-ray scattering experiment of highly polydisperse (yet monomodal) colloidal dispersions in a range of sizes (average size from 8 to 50 nm), with soft, charge-mediated interactions. These dispersions were dialysed and compressed by aqueous solutions of poly(ethylene glycol) to reach 15% to 30% of volume fraction, and crystallize. Their phase diagrams, structure factors and crystal peaks were analysed by the x-ray scattering patterns. We found coexistences of complex crystal structures (two BCC structures and Laves AB2) for the small particle size, and BCC and FCC crystals for the larger particle size. These results show a fractionation among the particles. We further show how this is possible through numerical simulations, which explain how the fractionation occurs and how the particles distribute among the different coexisting phases.

DY 5.3 Mon 10:15 H51

Free energies, liquid and crystal phases of the Asakura–Oosawa model: a density functional theory study — •Mostafa Mortazavifar and Martin Oettel — Institut für Angewandte Physik, Uni Tübingen, Tübingen, Germany

The Asakura–Oosawa(AO) model is a well known model for studying colloid–polymer mixtures in which the depletion interaction between colloidal particles results in a phase diagram similar to molecular liquids. More importantly, it is a generic model system for short range attractive colloidal particles. We have studied the model by means of density functional theory (DFT) by applying a linearization of a two–component fundamental measure hard sphere tensor functional with respect to the second (polymer) component. The linearized functional gives a unified description of gas, liquid, and crystal phases. We have calculated the free energies and phase diagrams for a variety of colloid–polymer size ratios. The results are in good agreement with available simulations. For small size ratios, the model can be mapped exactly to a one–component system with a short–range attractive potential between the colloids. Standard mean field approximations fail in describing the liquid and crystal phases; here our functional offers novel insights how to construct generically density functional descriptions of interparticle attractions.

DY 5.4 Mon 10:30 H51

Crystallization of sheared nearly hard-spheres — •david richard and thomas speck — Staudingerweg 9, 55128 Mainz

Understanding crystallization pathways and kinetics is a long standing challenge in condensed matter science. Additionally, the effect of impurities and external fields is also a matter of debate. In this study, we look at the effect of a simple linear shear flow on the crystallization of nearly hard-spheres [1]. By varying the density from low to high supersaturation, we find a crossover from shear-suppressed crystallization to an enhanced crystallization kinetics. We attribute this crossover under shear to the vanishing nucleation barrier in the quiescent system, at which nucleation is changing from an activated to a diffusive limited process.

[1] Richard, David, and Thomas Speck. 'The Role of Shear in Crystallization Kinetics: From Suppression to Enhancement.' Scientific Reports 5 (2015).

DY 5.5 Mon 10:45 H51

On the influence of the softness of the potential on the phase diagrams of core-shell micelles - a simulation study — •Heiko G. Schoberth, Heike Emmerich, and Thomas Gruhn — Lehrstuhl Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth

Quasicrystals are of continuous interest due to their fascinating fundamental properties and their promising applications as advanced photonic materials in a range of optical devices. In the last years colloidal quasicrystals have been found in solutions with spherical polymer core-shell micelles. With these colloids and their intriguing possibility to self-assemble in a broad range of nanoscale and microscale quasicrystalline structures, the demand arises of understanding the complex formation mechanism and the thermodynamic stability of these structures. Especially, it is important to find a direct relation between the stability of the structures and the main parameters of the micelle-micelle interaction. We perform coarse-grained molecular dynamics simulation to investigate the dependence of the phase diagram on the softness of the interaction potential. The core-core interaction is modelled by infinite repulsion, whereas the shell-shell interaction is varied from a stiff to a very soft potential. Varying the core to shell radius and packing fraction we study systematically the change in the phase diagram finding domains with 10-,12-,18-,24-fold quasicrystalline symmetries. With increasing smoothness of the potential the phase diagram changes qualitatively and the geometry of the phase boundaries gets more regular.

DY 5.6 Mon 11:00 H51

Estimation of crystal nucleation barriers for colloidal crystals from computer simulations — •Peter Koss[1,2], Antonia Statt[1], Peter Virnau[1], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany

A fluid in equilibrium in a finite volume, with a density exceeding the onset of freezing, may exhibit phase coexistence of a crystal nucleus surrounded by liquid. In classical nucleation theory, the barrier of homogeneous nucleation is given by two contributions, the energy gain of creating a droplet and the energy loss due to surface tension of the newly created interface. Using a computational 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. Our novel analysis method is appropriate for crystal nuclei of all shapes without suffering from ambiguities occurring when one needs a microscopic identification of the crystalline droplet. We report that the nucleation barrier for a soft version of the effective Asakura-Oosawa model[1] is compatible with a spherical shape, and consistent with classical nucleation theory [2].

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

5771 (1999).

[2] A. Statt, P. Virnau, and K. Binder, Phys. Rev. Lett. 114, 026101 (2015).

DY 5.7 Mon 11:15 H51

Crystal nucleation in metastable hard sphere fluids by confocal microscopy — Achim Lederer[1] and •Hans Joachim Schöpe[2] — [1]Retsch Technology GmbH, Retsch-Allee 1-5, 42781 Haan, Germany — [2]Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

Crystal nucleation in colloidal hard spheres is a longstanding research topic. Light scattering and confocal microscopy as well as simulations had been carried out to characterize the nucleation process and to get a microscopic picture. In these studies results both differ and agree with each other. It is still unclear whether the large disagreement in the nucleation rate densities between the light scattering experiments and simulations are of physical nature or result from differing data analyses. Furthermore, the temporal evolution of the microscopic structure has not yet been characterized sufficiently. Using laser-scanning confocal microscopy we study crystal nucleation in colloidal hard spheres. The used system has been characterized with extreme care to allow for meaningful comparison with other experiments and simulations. Observing a large sample volume we can analyze the nucleation process with high accuracy. This allows us to obtain meaningful data of the nucleation rate density, critical nucleus size and nucleation barrier. Furthermore, we determine the time-dependent interfacial tension through how the cluster size distribution evolves. Analyzing the nucleation process on a microscopic scale, we confirm the scenario of precursor-mediated crystal nucleation. In addition we show in great detail the structure evolution from precursor to crystal.

15 min. break

Invited Talk DY 5.8 Mon 11:45 H51

Percolation in colloidal model systems — •Tanja Schilling[1], Hugues Meyer[1], Mohit Dixit[1], Mark Miller[2], and Paul van der Schoot[3] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Department of Chemistry, Durham University, United Kingdom — [3]Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, 5600 MB Eindhoven, The Netherlands

Connectivity percolation is the transition in which isolated clusters of solid particles in a fluid become connected in some sense to form a system-spanning network. This network has a significant effect on the transport properties of the material on a macroscopic scale. If, for example, an electrically insulating polymer is mixed with conductive fibres such as carbon nanotubes, the conductivity of the composite increases by ten or more orders of magnitude near the percolation transition of the filler material.

We discuss percolation in suspensions of fibres and of platelets. Our study covers the entire range of aspect ratios from spheres to extremely slender rods and infinitely thin disks. The percolation threshold for rod-like particles of aspect ratios below 1000 deviates significantly from the inverse aspect ratio scaling prediction, thought to be valid in the limit of infinitely slender rods and often used as a rule of thumb for fibres in composite materials. We also show the effects of polydispersity on the percolation transition. The main result is that the percolation threshold shows universal behaviour, i.e. it depends only on certain cumulants of the size distribution.

DY 5.9 Mon 12:15 H51

Towards flexible and dynamic self-assembly from colloids with magnetic anisotropy — •Gabi Steinbach[1,5], Dennis Nissen[2], Manfred Albrecht[2], Ekaterina V. Novak[3], Pedro Sánchez[4], Sofia Kantorovich[3,4], Sibylle Gemming[1,5], and Artur Erbe[5] — [1]Technische Universität Chemnitz, 09107 Chemnitz, Germany. — [2]University of Augsburg, 86159 Augsburg, Germany. — [3]Ural Federal University, 620000, Ekaterinburg, Russia. — [4]University of Vienna, 1090 Vienna, Austria. — [5]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany.

Magnetic colloidal particles are a suitable model system for the study of self-assembly and dynamic processes on the microscale. Here, we illustrate the potential of directed, but flexible bonds for tailored structure formation. As an example, we present a system of colloidal microspheres that have an off-centered net magnetic moment pointing perpendicular to the particle surface. They are an experimental realization of the theoretical model of spheres with radially shifted point dipole (sd-particles). Experimentally we observed the formation of branched structures as result of two coexisting self-assembly patterns, which is untypical for homogeneous systems. We show that the bistability can be explained by an extended model of sd-particles. This framework takes the broad magnetization distribution in the experimental particles into account. We will further show that the interacting particles exhibit interesting non-equilibrium dynamics when exposed to time-dependent fields, leading to reversible structural reconfigurations.

DY 5.10 Mon 12:30 H51

Enhanced magneto-optical response in dispersions of anisometric pigment particles — •Kathrin May, Alexey Eremin, and Ralf Stannarius — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

Colloidal suspensions of anisometric particles show a variety of unique properties depending on particle concentration and external electric fields, such as the formation of ordered phases, phase separation, electro-optical effects, and non-linear rheology. Electro- and magneto-optical properties of colloids are of particular interest because of the possible applications in electrophoretic ink displays and other technologies. We demonstrate a binary colloidal system with an unusually strong magneto-optical response which is comparable with that of thermotropic liquid crystals. This system is based on a binary mixture of elongated non-magnetic pigment particles and a small volume fraction < 0.1 v/% of spherical magnetic nanoparticles. The birefringence is caused by a partial alignment of the pigment particles, controlled by anisometric agglomerates of the magnetic particles that form in a magnetic field. This effect is discussed in the frame of the Onsager-Lekkerkerker theory of sterical alignment transfer in binary mixtures of colloidal particles.

The authors acknowledge the support by DFG (SPP 1681).

DY 5.11 Mon 12:45 H51

The initial magnetic susceptibility of cube-like magnetic colloids in dilute suspensions — •Joe Donaldson[1] and Sofia Kantorovich[1,2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Ural Federal University, Lenin av. 51, 620083, Ekaterinburg, Russia

Magnetic nano/micro-particles are currently applied in many diverse research and industrial disciplines. These particles exhibit a number of interesting properties that can be utilised, leading to a number of established and developing applications. Most notably: magnetic drug targeting; magnetic hyperthermia cancer treatment; and ferrofluids. In each of these applications, a crucial piece of information is required; namely, some sort of insight into the magnetic behaviour of these particles. Ideally, one would like some indication of this a priori. As such, we present here theoretical and simulation studies on permanently magnetised particles that are actually cube-like in shape [1]. We have investigated the differences in magnetic behaviour arising from this additional directional interaction, focussing on the initial magnetic susceptibility of low-density suspensions.

[1] J. G. Donaldson and S. S. Kantorovich, Nanoscale, 2015, 7, 3217

DY 6: Networks: From Topology to Dynamics I (joint session SOE / DY / BP)

Time: Monday 10:00–11:30 Location: H36

DY 6.1 Mon 10:00 H36

Revealing physical interaction networks from nonlinear dynamics — Jose Casadiego[1], Dimitra Maoutsa[1], Hauke Hähne[1], Mor Nitzan[2], and •Marc Timme[1] — [1]Network Dynamics, MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Racah Institute of Physics, The Hebrew University of Jerusalem, Israel

Structural connectivity of networks reflects the direct physical interactions between pairs of dynamical units, as opposed to effective, functional or other statistical measures of connectivity. How to uncover physical interaction structure from measured time series of networked systems remains an open question. Here we present a dynamical systems' view on collective network dynamics, thereby proposing an approach to reveal physical interaction networks from the nonlinear dynamics they generate. Introducing the notion of *explicit dependency matrices*, we present two examples: one, where the time series consists of the full network states as a function of time, the other, where the time series exhibits only partial information about the full states. We apply the latter to neural circuit dynamics where the observables are spike timing data, i.e. only a discrete, state-dependent output of the neurons. These results may help revealing network structure for systems where direct access to dynamics is simpler than to connectivity.

For an introductory review of the state of the art, see
J. Phys. A: Math. Theor. 47 343001 (2014)
http://dx.doi.org/10.1088/1751-8113/47/34/343001

DY 6.2 Mon 10:15 H36

Theory and experiments on anomalous critical and supercritical connectivity transitions — •Jan Nagler — ETH Zurich

The emergence of large-scale connectivity on an underlying network or lattice, the so-called percolation transition, has a profound impact on the system's macroscopic behaviours. There is thus great interest in controlling the location of the percolation transition to either enhance or delay its onset and, more generally, in understanding the consequences of such control interventions. Here we report on the sudden emergence of large-scale connectivity that results from repeated, small interventions designed to delay the percolation transition. These transitions exhibit drastic, unanticipated and sometimes exciting consequences in complex networked systems but also pose experimental challenges. In particular, I will report on both theoretical and experimental progress (D'Souza & Nagler, Nature Physics 11:531, 2015; Nagler et al., unpublished).

DY 6.3 Mon 10:30 H36

What does Big Data tell? Sampling the social network by communication channels — •János Török[1,2], Yohsuke Murase[3], Hang-Hyun Jo[4,5], János Kertész[2,1,5], and Kimmo Kaski[5] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest H-1111, Hungary — [2]Center for Network Science, Central European University, Budapest H-1051, Hungary — [3]RIKEN Advanced Institute for Computational Science, Kobe, Hyogo 650-0047, Japan — [4]BK21plus Physics Division and Department of Physics, Pohang University of Science and Technology, Pohang 37673, Republic of Korea — [5]Department of Computer Science, Aalto University School of Science, P.O. Box 15500, Espoo, Finland

Big Data has become the primary source of understanding the structure and dynamics of the society at large scale. However, usually one has information only about one of the channels, which should be considered as a sample of the whole. We show by simulations and analytical methods that this sampling may lead to bias. For example, while it is expected that the degree distribution of the whole social network has a maximum at a value larger than one, we get with reasonable assumptions about the sampling process a monotonously decreasing distribution as observed in empirical studies of single channel data. Also we find, that assortativity may occur or get strengthened due to the sampling process. We analyze the far-reaching consequences of our findings.

DY 6.4 Mon 10:45 H36

Effective Distances in Complex Networks — Flavio Iannelli[1], •Andreas Koher[2], Philipp Hövel[2], and Igor M. Sokolov[1] — [1]Humboldt Universität zu Berlin, Germany — [2]Technische Universität Berlin, Germany

The analysis of global epidemics revealed that physical distances can hardly be used to forecast the outbreak dynamics. Instead, a network-based measure which has been introduced recently [1] allows to predict infection arrival times with a surprisingly high accuracy. The so-called effective distances are solely based on the (weighted) network topology.

We present an alternative approach, which is motivated by a fundamental property from the theory of random walks: The distribution of first passage times. This random walk based distance allows to forecast disease dynamics on various topologies. For the special case of highly heterogeneous networks it reduces to the previously introduced effective distance.

[1] Brockmann D, Helbing D "The hidden geometry of complex, network-driven contagion phenomena." Science. 2013;342(6164):1337–1342

DY 6.5 Mon 11:00 H36

A Geometrical Approach to Infection Dynamics on Temporal Networks — •Felix Herrmann[1], Philipp Hövel[1], Vitaly Belik[1], Andreas Koher[1], Hartmut H. K. Lentz[2], and Dirk Brockmann[3,4] — [1]Institut für Theoretische Physik, Technische Universität Berlin — [2]Friedrich-Loeffler-Institut, Greifswald — [3]Institut für Theoretische Biologie, Humboldt-Universität zu Berlin — [4]Robert Koch-Institut, Berlin

We investigate the extension of a recently introduced geometrical approach for the description of spreading processes on static undirected networks [1] to directed temporal networks. Its key quantity is a probabilistically motivated "effective distance" between nodes, which is based on the weights of the links and allows reliable predictions of disease arrival times and the identification of the origin of spreading processes. The approach has already been successfully applied to study infection dynamics on a static undirected air traffic network [1].

By demonstrating how this approach can be generalized, we contribute to a framework for the investigation of spreading dynamics on temporal networks. Specifically, we consider an empirical livestock trade network in Germany, consisting of 97,980 nodes (agricultural holdings) and 6,359,697 temporal edges (trade events) [2], and use a SIR model to simulate the local dynamics of the nodes. Strong fluctuations in the activity of the nodes render the application of the geometrical approach particularly challenging.

[1] D. Brockmann and D. Helbing, Science 342, 1337 (2013).
[2] H. H. K. Lentz et al., Phys. Rev. Lett. 110, 118701 (2013).

DY 6.6 Mon 11:15 H36

Controlling recurrent epidemics on temporal networks — •Vitaly Belik[1,2], Florian Fiebig[1], Hartmut H K Lentz[3], and Philipp Hövel[1,4] — [1]Institut für Theoretische Physik, Technische Universität Berlin — [2]Helmholtz Zentrum für Infektionsforschung, Braunschweig — [3]Institute of Epidemiology, Friedrich-Loeffler-Institute, Greifswald — [4]Bernstein Center for Computational Neuroscience Berlin, Humboldt Universität zu Berlin

We consider a rucurrent epidemic on a temporal network. The goal of the control is to reduce the prevalence or make the epidemic extinct, respectively. To this end we propose a protocol based on rewiring the edges away from infected nodes, after they are detected as those: instead of an infected node, we randomly choose a healthy one (or perceived as such). In contrast to coevolutionary adaptive networks, the intrinsic dynamics of the network is taken into account by our approach alongside with the adaptive rewiring. The proposed control scheme significantly expands the range of a disease-free parameter region. For example, on the network of German pig trade, diseases with detection times up to 10 days and infectious periods up to 3 months could be efficiently controlled by our method [1]. Thus changing the behaviour of trading partners could have significant impact on the epidemic outcome.

[1]V Belik, F Fiebig, HHK Lentz, P Hövel arXiv preprint arXiv:1509.04054

DY 7: SKM Dissertation-Prize 2016

Time: Monday 10:30–12:35 Location: H2

Invited Talk DY 7.1 Mon 10:30 H2

Parallel pumping: Novel means of spin-wave manipulation on the micro-scale — •Thomas Brächer — Univ. Grenoble Alpes, CNRS, CEA, INAC-SPINTEC, 17, rue des Martyrs 38054, Grenoble, France — Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany

Spin waves and magnons, their quanta, are highly promising candidates for the realization of a wave-based logic beyond CMOS, which transmits information in the form of amplitude and phase of spin waves. In this context, the amplification of spin waves is a central issue. Parallel pumping, i.e., the conversion of microwave photons into pairs of magnons at half the microwave frequency, is a versatile technique to realize frequency-selective generation and amplification of spin waves. I studied these effects in microstructured spin-wave waveguides of various geometries, proving its applicability on the micro-scale. Moreover, I demonstrated that beyond a mere amplification, parallel pumping can also be used to perform logic operations in the spin-wave system.

Invited Talk DY 7.2 Mon 10:55 H2

Self-referenced quantized current source — •Lukas Fricke — Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — CQC2T, UNSW, Sydney, Australia

Scheduled for 2018, the International System of Units is about to undergo a fundamental change by introducing seven defining constants, leading to a universal system of units based on constants of nature as proposed already by Maxwell and Planck. In the case of the Ampere, the defining constant will be the elementary charge e: Employing a single-electron pump, the current I is realized by transferring a precisely known number of electrons in a clocked manner, leading to the relation $I = \langle n \rangle\, ef$ with $\langle n \rangle$ the average number of charge carriers transferred per cycle and f the driving clock frequency.

Here, we demonstrate a complex circuit involving serially connected electron pumps and single-electron transistors attached to the interconnecting nodes. This allows to investigate electron pumps on the level of individual transfer cycles using full counting statistics. This method enables us to derive the single-electron transfer accuracy $1 - \langle n \rangle$ of the pump and to determine the underlying mechanisms of charge transfer.

Finally, the self-referenced single-electron source is discussed which enables the *in-situ* verification of the output current. By counting and attributing rare transfer errors, the uncertainty of the average number of transferred electrons $\langle n \rangle$ can be reduced by orders of magnitude, thereby making a practical realization of a quantum current standard based on a clocked single-electron source feasible.

Invited Talk DY 7.3 Mon 11:20 H2

Signatures of Majorana states in magnetic adatom chains — •Falko Pientka — Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

Recently, topological phases in superconductors hosting exotic Majorana states have become the subject of intense experimental and theoretical investigation. Majoranas exhibit nonabelian exchange statistics potentially useful for topologically protected quantum computing.

Possible signatures of Majorana states have been found in a recent STM experiment probing magnetic adatoms chains on the surface of a superconductor. In this talk, I will discuss the intriguing physics of the proximity effect in this system, which gives rise to a series of unexpected phenomena such as strongly localized Majorana states and an unconventional topological phase with long-range couplings.

I will also address experimental challenges of STM experiments on superconductors and show how an improved understanding of the relevant tunneling processes can be used to determine quasiparticle dynamics of superconducting bound states.

Invited Talk DY 7.4 Mon 11:45 H2

Imaging Spin Textures on Curved Magnetic Surfaces — •Robert Streubel[1,2], Peter Fischer[1,3], Florian Kronast[4], Oliver G. Schmidt[1], and Denys Makarov[1,5] — [1]Institute for Integrative Nanosciences, IFW Dresden, Dresden, Germany — [2]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA — [3]Physics Department, UC Santa Cruz, Santa Cruz, USA — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [5]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden, Germany

Extending 2D structures into the third dimension allows for modifying conventional or for launching novel functionalities. A proper characterization of 3D magnetic objects demands tomographic imaging reconstructing the magnetization vector field. State-of-the-art techniques, i.e. magnetic neutron tomography and vector field electron tomography, provide means to investigate macroscopic and nanoscopic samples; An characterization of mesoscopic specimens is not possible, yet highly demanded.

The main objective of the thesis was to develop a visualization technique that provides nanometer spatial resolution to image magnetic domain patterns on extended 3D curved surfaces. The proposed and realized concept of magnetic soft X- ray tomography (MXT), based on the X-ray magnetic circular dichroism (XMCD) effect with soft X-ray microscopies, is demonstrated by reconstructing the magnetic domain patterns on 3D curved surfaces resembling hollow cylindrical objects.

Invited Talk DY 7.5 Mon 12:10 H2

Observing Electron Dynamics in Two Dimensions — •Søren Ulstrup — Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, 94720 CA, USA - Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

Since the discovery of the all-carbon two-dimensional (2D) material graphene more than a decade ago the library of available 2D materials has been rapidly expanding. These materials not only host interesting physics, but may also lead to technological advances due to highly promising electronic and optical properties.

Here, I will discuss how we can directly study the energy and momentum distributions of the 2D electrons that give rise to many of these important properties in a variety of systems, including graphene and single layers of the semiconducting transition metal dichalcogenides (TMDCs). By using angle-resolved photoemission spectroscopy (ARPES), as well as recent advances of this method that have added either spatial resolution or femtosecond time-resolution, we are able to gain information that allows us to tailor new interesting 2D material systems, to investigate and tune the light-matter interaction in these materials and to discover new important physical phenomena.

DY 8: Evolutionary Game Theory (joint session SOE / BP / DY)

Time: Monday 12:15–13:15 Location: H36

DY 8.1 Mon 12:15 H36

Evolutionary ecological-economic modelling: Ecological instability and economic growth — •Sylvie Geisendorf[1], Frank Beckenbach[2], and Christian Klippert[1] — [1]ESCP Europe Campus Berlin, Heubnerweg 8-10, 14059 Berlin, Germany — [2]University of Kassel

The paper proposes an evolutionary ecological-economic model taking into account the complexity of the ecological as well as the economic system. We argue that Economics should consider ecological complexity and the co-dynamics of the economic and ecological system to better understand drivers and restrictions of economic evolution. At the same time, the development of a regenerative resource is affected by the internal growth dynamics of the economy. Given that no economic activity is conceivable without using natural resources and relying on natural systemic services, there is a surprising simplification of the natural system in economic models. The model we propose has three particularities distinguishing it from traditional resource economic models. (1) it implements a multi-dimensional link between the

economic and ecological system, considering side effects of the production process like waste or emissions. (2) it uses a difference equation approach for the biological resource instead of the typical differential one, to allow for the whole range of stability regimes and (3) it links this resource system to an evolving, agent-based economy instead of the standard optimization calculus.

DY 8.2 Mon 12:30 H36

Changing the rules of the game as an emergent feature of the dynamics — •Darka Labavić and Hildegard Meyer-Ortmanns — Jacobs University Bremen, Bremen, Germany

We consider (N, r) games of competition with N species and $r < N$ prey and predators. Basic reactions include predation, reproduction, decay, and diffusion, without a hard constraint on the occupation number per site. For special combinations of N and r we observe the option to see games within games for an appropriate choice of parameters. As one of the simplest examples we analyze a $(6, 3)$ game. Once the players segregate from a random initial distribution, domains on a coarse scale emerge, which play a $(2, 1)$-game at their boundaries, while agents inside the domains play rock-paper-scissors (that is, $(3, 1)$), leading to the formation of spirals with species chasing each other. The $(2, 1)$-game has a winner in the end, so that the coexistence of domains is transient, while agents inside the remaining domain coexist, until demographic fluctuations lead to the survival of only a single species. This means that we observe a dynamical generation of multiple scales in space and time with an emerging change of rules on the coarse scale starting from a simple set of rules on the unit scale of the grid. In view of predicting these features, we derive the deterministic limit within a van Kampen expansion. A linear stability analysis reproduces the number of forming domains and their composition in terms of species. A comparison of analytical predictions with Gillespie simulations also reveals the impact that the various sources of stochastic fluctuations have on the dynamics, even on its qualitative features.

DY 8.3 Mon 12:45 H36

A synthetic codon replicator with tRNA — •Simon Alexander Lanzmich and Dieter Braun — Systems Biophysics, Physics Department, Nanosystems Initiative Munich and Center for NanoScience, LMU Munich, Germany

Every evolving system requires the storage and replication of genetic information. Modern biology solves this using an RNA-dominated machinery (ribosome and a pool of tRNAs) to encode proteins. The proteins in turn replicate genetic information. In contrast, early life most probably replicated genes using a pool of short RNA sequences.

To approach above chicken and egg problem, we explore an autonomous, waste-free, and purely thermally driven replication mechanism. Instead of chemical base-by-base replication, it operates on successions of multi-base codons. The molecules used have a hairpin loop at each end and are derived from transfer RNA. They encode and replicate a binary code at the anticodon sites of tRNA.

Replication of a template succession of tRNAs is facilitated by temperature oscillations and proceeds in three logical steps. (1) Strands with matching anticodons bind to the template. (2) Fluctuations in the bound strands' hairpins allow for the hybridization to neighboring strands. (3) Subsequent heating splits the replicate from the template, freeing both for the next cycle. This physical ligation chain reaction proceeds cross-catalytically. Instead of chemical backbone ligation, matching strands are linked by physical base pairing.

DY 8.4 Mon 13:00 H36

Stepwise cooperation of molecular replicators — •Georg Urtel and Dieter Braun — Systems Biophysics, Ludwig-Maximilians-Universität München, Amalienstr. 54, D- 80799 München, Germany

Life emerged from the ability of informational polymers to pass on sequences to other polymers before they degrade. Before competition between living species, the first selection pressure was to replicate faster than degradation. What were the strategies the molecules could take?

Based on biological evidence, DNA or RNA replicators require a defined binding site to start replication. We study experimentally and theoretically three geometries of the binding site: linear single binding, hairpin binding and two opposing binding locations. The geometries have fundamentally different, increasing replication speeds.

Interestingly, two hairpin replicators cooperate readily and form the fastest replicating geometry. After incomplete replication, they bind by hybridization and cooperate by forming a crossbreed species. This cooperation of two replicators retains most of the sequence information of both hairpins. Under conditions where hairpins are doomed to degrade, their crossbreed is replicating fast enough to survive. As a result, two initially separated hairpins survive by diffusional mixing and the colocalized crossbreeding.

Our experiments show a stepwise evolution of replicator geometries. Already at a molecular level, cooperation was an advantageous strategy under Darwinian evolution.

DY 9: Plenary Talk: Ehud Meron

Time: Monday 14:00–14:45 Location: H15

Plenary Talk DY 9.1 Mon 14:00 H15

From patterns to function in living systems: dryland ecosystems as a case study — •Ehud Meron — Ben-Gurion University of the Negev, Beer-Sheva, Israel

Dryland landscapes show a variety of vegetation pattern-formation phenomena; banded vegetation on hill slopes and nearly hexagonal patterns of bare-soil gaps in grasslands ("fairy circles") are two striking examples. Vegetation pattern formation is a population-level mechanism to cope with water stress. It couples to other response mechanisms operating at lower and higher organization levels, such as phenotypic changes at the organism level and biodiversity changes at the community level, and plays a crucial role in understanding ecosystem response and ecosystem function in changing environments. In this talk I will present a platform of mathematical models for dryland ecosystems and describe some of the ecological questions we have studied using this platform. I will discuss the mechanisms that destabilize uniform vegetation and lead to periodic vegetation patterns, the variety of extended and localized patterns that can appear along a rainfall gradient, the impact of pattern formation on critical state transitions (regime shifts), pattern-induced species coexistence, and restoration of degraded landscapes as a spatial resonance problem. I will conclude with a discussion of two open problems, the coupling between pattern formation and biodiversity, and the reconciliation of human intervention and ecological integrity in disturbed ecosystems.
Reference: Ehud Meron, Nonlinear Physics of Ecosystems, CRC Press 2015.

DY 10: Colloids and Complex Fluids III (joint session CPP/BP/DY)

Time: Monday 15:00–18:00 Location: H42

DY 10.1 Mon 15:00 H42

Directed assembly of soft colloids through rapid solvent exchange — •Arash Nikoubashman[1], Victoria E. Lee[2], Chris S. Sosa[2], Robert K. Prud'homme[2], Rodney D. Priestley[2], and Athanassios Z. Panagiotopoulos[2] — [1]Institute of Physics, Johannes Gutenberg University of Mainz, Germany — [2]Department of Chemical and Biological Engineering, Princeton University, USA

We studied the directed assembly of soft nanoparticles through rapid micromixing of polymers in solution with a non-solvent. Both experiments and computer simulations were performed to elucidate the underlying physics and to investigate the role of various process parameters. In particular, we discovered that no external stabilizing agents or charged end-groups are required to keep the colloids separated from each other, when water is used as the non-solvent. The size of the

nanoparticles can be reliably tuned through the mixing rate and the ratio between polymer solution and non-solvent. Furthermore, we were able to fabricate a wide variety of patchy colloids, such as Janus particles, when polymer blends were used in the feed stream. Our results demonstrate that this mechanism is highly promising for the mass fabrication of uniformly-sized colloidal particles, using a wide variety of polymeric feed materials.

DY 10.2 Mon 15:15 H42

Directed Assembly of Janus Particles through Flow — •Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University of Mainz, Germany

We investigate the self-assembly of colloidal Janus particles under shear and Poiseuille flow, by employing hybrid molecular dynamics simulations that explicitly take into account hydrodynamic interactions. Under quiescent conditions, the amphiphilic colloids form spherical aggregates with a large size polydispersity. The solvophobic hemispheres are directed towards the core, whereas the solvophilic caps are exposed to the solvent. When sufficiently strong shear is applied, the micelles disaggregate with a consequent decay of the average cluster size. However, we find an intermediate regime where the balance between rearrangement and dissociation favors the growth of the aggregates, where the majority of clusters consist of 13 particles in an icosahedral arrangement. This bias is due to the high geometric symmetry of the icosahedron, which maximizes the internal bonding energy of the aggregate. Our findings demonstrate how self-assembly can be directed towards specific structures via external fields, and open up new applications for Janus particles, ranging from biotechnology to sensor systems.

DY 10.3 Mon 15:30 H42

Self-organized velocity pulses of dense colloidal suspensions in microchannel flow — •Philipp Kanehl and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Colloids in dense suspension exhibit shear-induced migration and size segregation under pressure driven flow [1]. If the density is increased further, the steady flow becomes unstable and regular oscillations in flow velocity emerge [2]. To develop a theoretical understanding of these oscillations, we simulate colloidal particles with frictional contact under pressure-driven flow in two dimensions using the mesoscale simulation technique of multi-particle collision dynamics.

We present a detailed parameter study on how friction generates transient jamming in the colloidal flow. The jammed regions are unjammed by rarefaction pulses travelling upstream similar to the experimental observations. Moreover, we address the role of fluid permeation and channel confinement.

Finally, a linear stability analysis of a newly developed continuum model predicts scaling laws for stability condition, wavenumber, and pulse speed, which agree well with our numerical data.

[1] P. Kanehl and H. Stark, J. Chem. Phys. 142, 214901 (2015).

[2] L. Isa, R. Besseling, A. N. Morozov, and W. C. Poon, Phys. Rev. Lett. 102, 058302 (2009).

DY 10.4 Mon 15:45 H42

An empirical correction for multiple scattering in integral laser Doppler velocimetry experiments — •Denis Botin[1], Ludmila Marotta Mapa[1,2], Christopher Wittenberg[1], Holger Schweinfurt[1], and Thomas Palberg[1] — [1]Institute of Physics, JGU, D-55099, Mainz, Germany — [2]Federal Univesity of Itajuba, Brazil

Super-heterodyne laser Doppler velocimetry (SHLDV) provides an integral measurement of the velocity distribution in electro-kinetic experiments[1]. This allows simultaneous evaluation of the electro-phoretic and electro-osmotic mobilities of the particles and along the cell wall, respectively [2]. Here, we introduce an extension of the method to the regime of concentrated samples, where multiple scattering affects the signal [3]. Multiple scattering distorts the signal shape, creating an additional hump in the background and prohibiting any meaningful fit. We use an empirical correction scheme for the spectra, in which we fit the multiple scattering contribution and subtract it from the raw data. This leaves the velocity dependent singly scattered contribution unaffected. First applications to measurements of the concentration dependence of the electro-phoretic mobility of charged colloidal spheres are reported.

[1]T. Palberg et al. J. Phys. Chem. 96, 8180 - 8183 (1992)

[2]T.Palberg et al. J. Phys.: Condens. Matter 24, 464109 (2012).

[3]H.C. Van de Hulst., *Multiple Light Scattering: Tables, Formulas, and Applications*, Academic Press, New York., (1980).

DY 10.5 Mon 16:00 H42

Multiscale modelling of complex (macro-)molecular fluid mixtures — •Christoph Junghans[1], Tiago E. de Oliveira[2,3], Paulo A. Netz[2,3], Debashish Mukherji[2], and Kurt Kremer[2] — [1]CCS Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — [2]Max-Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz Germany — [3]Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil

Many biophysical processes in water are determined by the interactions of cosolvents within the hydration shells of dissolved molecules. Computational approaches are mostly limited to the "mid sized" all-atom simulation protocols. While all-atom simulations are suitable in some cases, problems arise when concentration fluctuations are large, thus requiring efficient simulation methods. Therefore, we develop two distinct, yet related, multiscale methods. In one case, we develop a semi-grand canonical MD that heals the particle depletion [1] that uses the AdResS scheme [2], coupled with a metropolis particle exchange criterion. In AdResS, an all-atom region is coupled to a coarse-grained (CG) reservoir, where the particle exchange is performed. In the second protocol, we develop a "parameter free" CG model, which uses cumulative coordination within an iterative procedure [3]. Both methods preserve pair-wise structure of complex fluids and their solvation thermodynamics. We apply these methods to study several cases of (macro)molecular solvation in aqueous mixtures [1,3].

[1] D. Mukherji and K. Kremer, Macromolecules (2013). [2] S. Fritsch, et al. PRL (2012). [3] T. E. de Oliveira, et al. (2016).

DY 10.6 Mon 16:15 H42

Kinetics of liquid-liquid phase transition in protein solutions exhibiting LCST phase behavior studied by USAXS — •Fajun Zhang[1], Stefano Da Vela[1], Michal Braun[1], Michael Sztucki[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

We present the results of the early stage kinetics of liquid-liquid phase separation (LLPS) in protein-salt solutions studied by ultra-small angle x-ray scattering (USAXS). The model system of bovine serum albumin (BSA) with YCl_3 [1,2] shows LLPS and a lower critical solution temperature (LCST) phase behavior and can be rationalized using an ion-activated patchy-colloid model [3]. We focus on the phase transition of the dense liquid phases after a T-jump aiming at the arrested or slowed down kinetics. The USAXS curves of sample solutions after a T-jump exhibit a peak that grows in intensity and shifts to lower q values with time. The characteristic length (ξ) obtained from this scattering peak increases with time approximately as $t^{0.3}$. The interface between the dilute and dense phase is quickly established as a Porod region (q^{-4}) is visible within a few seconds. Thus the kinetics of the intermediate stage of phase transition was followed by USAXS. It is interesting to see that ξ(t) is nearly independent on the jump temperatures (below 40 °C). At a higher temperature jump (45 °C), a slowed down kinetics was observed indicating that the gelation line was approached. [1] F. Zhang, et al. Phys. Rev. Lett. 101, 148101 (2008) Proteins 78, 3450 (2010). [2] F. Zhang, et al. Soft Matter 8, 1313 (2012). [3] F. Roosen-Runge, et al. Sci. Rep. 4, 7016 (2014).

15 min. break

DY 10.7 Mon 16:45 H42

Hydration and hysteresis of triblock copolymers — •Bernhard Schummer, Stefan Gerth, and Randolf Hanke — Universität Würzburg, Lehrstuhl für Röntgenmikroskopie

Ternary polyether are block ABA copolymers consisting of polyethyleneoxide (PEO) (A) and polypropylenoxide (PPO) (B). They change their hydrophilic or hydrophobic balance dramatically with their temperature and their concentration in water. This change causes a micelleisation. In this case P123 will be used as a copolymer and SAXS will be the method of examination. For micelles an appropriate model is the core-shell model where the shell mostly consists of PEO and the core mainly of PPO. In this model the SLD's for core and for shell heavily depend on each other. A new parameter $\kappa = \frac{\rho_c - \rho}{\rho_s - \rho}$ is presented to describe the change of the conformation and hydration of the micelle while including the radii of shell and core. Here ρ_c is the SLD of the core ρ_s the SLD of the shell and ρ the SLD of the solvent. The new parameter indicates that the SLD of the core decreases and

thus dehydrates with increasing temperature. For instancethe SLD's of the poloxamer L51 show a similar dependency as P123. The heating and cooling curves of the sample for different small concentrations will be presented and show a hysteresis in the form phase diagram. This can be observed in a diagram where κ is ploted against the temperature. At higher concentrations poloxamers form a liquid crystal. It has already been shown that there is a hysteresis in the cell parameter at high concentrations. This effect can now be attributed to a single component of the system, the form change of the micelle.

DY 10.8 Mon 17:00 H42

Phase behaviour and interactions in a three components γ-globulin based depletion interaction system — •Stefano Da Vela[1], Fajun Zhang[1], Sarah El-Asfar[1], Christian Exner[1], Michael Sztucki[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

Aqueous solutions of bovine γ-globulin with polyethylene glycol (PEG) added as non-interacting polymer, provide a tunable protein system for the study of depletion-driven phase behaviour: range and strength of the interaction are adjusted by appropriate choice of PEG molecular weight and concentration. An extensive study of the phase behaviour of the system for different effective attraction strengths reveals a set of conditions for which a Liquid-Liquid Phase Separation (LLPS) phase boundary emerges above the freezing temperature of the solvent. Addition of bovine serum albumin (BSA), results into an effective three components system. BSA, while not inducing depletion interaction on its own, appears to enhance it in presence of PEG, shifting the LLPS boundary to higher temperatures while being preferentially excluded from the resulting protein-dense liquid phase. In order to investigate the effect of BSA on the phase boundaries and on the interaction, phase diagrams as a function of temperature, protein and PEG concentration are presented together with small angle X-ray scattering data. Optical microscopy, turbidimetry and size exclusion chromatography are employed as supplementary techniques. The findings are relevant to the understanding of protein mixtures and their separation.

DY 10.9 Mon 17:15 H42

Clusters of proteins – are they transient or static? — •Michal Braun[1], Marco Grimaldo[1,2], Felix Roosen-Runge[2], Christian Beck[1], Fajun Zhang[1], Frank Schreiber[1], and Tilo Seydel[2] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institut Laue-Langevin, Grenoble, France

Signatures of protein clusters have been observed for globular proteins such as lysozyme [1], crystallins and bovine serum albumin [2,3]. The nature of these clusters, whether static or transient, however, is still a debated question and depends sensitively on environmental conditions. A better understanding would be key to use protein clusters as precursors for protein crystallization or in drug delivery.

We report cluster formation in solutions of β-lactoglobulin (BLG), as systematically investigated using static and dynamic scattering techniques. From small-angle scattering (SAXS/SANS), we obtain a cluster signature from the missing shift of the correlation peak with concentration and related data fitting. Neutron quasi-elastic backscattering (QENS) evidences the formation of oligomers via the short-time self-diffusion coefficient at nanosecond time scales. Finally, neutron spin-echo spectroscopy (NSE) allows to compare structural information from the structure factor with the dynamical features of collective diffusion on time scales of several tens of nanoseconds, which ultimately allows to determine the nature of the observed protein clusters.

[1] Stradner et al. Nature 432 (2004) 492
[2] Soraruf et al. Soft Matter 10 (2014) 894
[3] Grimaldo et al. J. Phys. Chem. Lett. 6 (2015) 2577

DY 10.10 Mon 17:30 H42

Self-assembled micelles as drug carriers: Influence of molar mass and chain architecture — •Bart-Jan Niebuur[1], Xiaohan Zhang[1], Natalya Vishnevetskaya[1], Petr Chytil[2], Sergey K. Filippov[2], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Garching, Germany — [2]Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic

A promising way to achieve site-specific delivery of anticancer agents is to use the enhanced permeation and retention (EPR) effect of self-assembled polymeric micelles. At this, a low critical micelle concentration (CMC) and particle sizes in the range of 1-100 nm are of importance.

In the present work, we focus on the importance of (i) the overall molar mass and (ii) the chain architecture. We investigate both N-(2-hydroxypropyl) methacrylamide (HPMA) [1] homopolymers with randomly distributed cholesterol side groups and diblock copolymers having a pure HPMA block and an HPMA block with cholesterol. Using fluorescence correlation spectroscopy and small-angle neutron scattering (SANS), the CMC as well as the size and structure of the micelles are determined in phosphate buffer. We find that the CMC decreases with increasing molar mass, but does not depend on chain architecture. The micellar radius is with 4-5 nm in the desired range.

[1] Filippov, S.K. et al., *Biomacromolecules* **13**, 2594 (2012) and **14**, 4061 (2013)

DY 10.11 Mon 17:45 H42

Modeling Viscoelastic Properties of Complex Fluids — •Julius Schulz, Alexander Schlaich, Roland Netz, and Julian Kappler — Fachbereich Physik, Freie Universiät Berlin, 14195 Berlin

The viscoelastic response of a complex liquid like water differs significantly from more simple models such as a Lennard-Jones fluid or methane. Using all-atom molecular dynamics simulations, we calculate the frequency-dependent viscosity for two liquids: TIP4P/2005 water and a glycerol/water solution. The corresponding elastic spectrum exhibits two peaks and cannot be described by simple viscoelastic models. We discuss the origins of these features and present a novel extension of the Maxwell model for viscoelastic fluids which is capable of reproducing the relevant features of the frequency-dependent viscosity. Extracted shear relaxation times for the glycerol-water mixtures compare well with experiments.

DY 11: Focus Session: Stochastic thermodynamics and information processing (joint session DY/BP)

Over the last 10 years, stochastic thermodynamics has been established as a conceptual framework for describing small driven systems that are embedded in a heat bath of well-defined temperature like biomolecular machines and transport through nano-structures. Describing measurement and subsequent feedback operations of such systems requires to merge concepts from information theory with thermodynamic ones taking into account the crucial role of fluctuations. This focus session highlights recent developments in this field in theory and experiment.

Time: Monday 15:00–17:45 Location: H44

Invited Talk DY 11.1 Mon 15:00 H44

Large deviation functionals in stochastic thermodynamics — •Andreas Engel, Johannes Hoppenau, and Daniel Nickelsen — Institut für Physik, Universität Oldenburg

The thermodynamic description of fluctuating systems is based on probability distributions for thermodynamic quantities like heat, work, and entropy. Unlike traditional statistical mechanics the tails of these distributions quantifying the frequency of rare, exceptional events are of particular interest. Large deviation theory is the proper mathematical framework to analyse these tails by introducing large deviation functions that characterize the probability of exponentially unlikely realizations.

A whole class of important large deviation functions deriving from a stationary stochastic process may be deduced from a single large de-

viation *functional* for its empirical density. For systems with detailed balance an explicit expression for this functional was derived in a series of mathematical papers by Donsker and Varadhan quite some time ago. We rederive their result using a path-integral approach and generalize it to non-equilibrium steady states. To this end the proper incorporation of the empirical probability current turns out to be crucial. We give explicit results for the large deviation functional, elucidate its connection with the entropy production and discuss the contraction to large deviation functions of more specific quantities.

Invited Talk DY 11.2 Mon 15:30 H44

Thermodynamics with Continuous Information Flow — •Massimiliano Esposito — University of Luxembourg, 162a avenue de la Faïencerie, L-1511 Luxembourg, Luxembourg.

A unified thermodynamic formalism describing information transfers in autonomous as well as nonautonomous systems described by stochastic thermodynamics will be presented. Information is continuously generated in an auxiliary system and then transferred to a relevant system that can utilize it to fuel otherwise impossible processes. Indeed, while the joint system satisfies the second law, the entropy balance for the relevant system is modified by an information term related to the mutual information rate between the two systems. This formalism will be applied to various model systems, including an electronic Maxwell demon.

Main reference: J. M. Horowitz and M. Esposito, "Thermodynamics with continuous information flow", Phys. Rev. X 4, 031015 (2014)

Invited Talk DY 11.3 Mon 16:00 H44

Measuring energy and information one molecule at a time — •Felix Ritort — Universitat de Barcelona, Barcelona (Spain)

I will present recent developments in the non-equilibrium physics of small systems by emphasizing single-molecule experiments and their contribution to expanding our current understanding of fundamental concepts, such as temperature, energy, entropy, and information.

15 min. break

Invited Talk DY 11.4 Mon 16:45 H44

Information reservoirs, bipartite systems, and the minimal energetic cost of uncertainty in biomolecular reactions — •Andre C Barato — Max Planck Institute for the Physics of Complex Systems

First, we show that the theory of stochastic thermodynamics can be generalized to include information reservoirs. These reservoirs can be seen as a sequence of bits that have their Shannon entropy changed due to the interaction with the system. Second, we discuss bipartite systems that can be used to study cellular information processing, allowing for the definition of an entropic rate that quantifies how much a cell learns about a fluctuating external environment. This entropic rate is bounded by the thermodynamic entropy production, which quantifies the rate of dissipated heat. Third, we show a thermodynamic uncertainty relation for biomolecular processes that connects the uncertainty in a random variable such as the output of a chemical reaction with the free energy that must be dissipated in order to sustain the chemical reaction. An uncertainty ϵ requires an energy dissipation of at least $2k_BT/\epsilon^2$.

Invited Talk DY 11.5 Mon 17:15 H44

Feedback control of transport in nanostructures. — •Tobias Brandes — TU Berlin, Institut für Theoretische Physik

I will discuss some models for transport through nanostructures from the point of view of thermodynamics and information. I start with a feedback-controlled stochastic process that works by mapping onto time-dependent (open-loop) control in an enlarged space of counting events [1], which has been experimentally realized very recently. Conceptually, with its infinite-bias limit this is somewhat outside the usual modified fluctuation-theorem paradigm, but a model of particle transport through a large number of channels can be partly used for the thermodynamic analysis [2]. In the Gaussian limit of this Kardar-Parisi-Zhang-like model, the dynamics can be interpreted as a simple diffusive spreading of a feedback signal across the channels that displays scaling. This can be quantified via the flow of information, and becomes visible, e.g., in the spectral function of the particle noise.

I will also present recent work on feedback control of a correlation function, i.e., the waiting time statistics of transport [3], including optimization (with C. Emary) and an equivalent substitute ('hardwired') model for an analysis in terms of entropies.

[1] T. Brandes, Phys. Rev. Lett. 105, 060602 (2010). [2] T. Brandes, Phys. Rev. E 91, 052149 (2015). [3] T. Brandes, Ann. Phys. (Berlin) 17, No 7, 477-496 (2008).

DY 12: Energy systems

Time: Monday 15:00–16:00 Location: H47

DY 12.1 Mon 15:00 H47

Bridging KM-like power systems and real decentralized grids — Katrin Schmietendorf[1], •Oliver Kamps[2], and Joachim Peinke[1] — [1]ForWind, Universität Oldenburg, Germany — [2]CeNoS, Universität Münster, Germany

Kuramoto-like models describing networks of synchronous machines allow for the investigation of basic mechanisms of power grid stability and the interplay between dynamics and topology from the viewpoint of self-organized synchronization. Several key issues of modern power systems are concerned with the integration of fluctuating renewables into decentralized grids. To address these questions, some model extensions have to be implemented before-hand.

In the course of ongoing decentralization, small and medium renewable generating units are progressively being connected to the low and medium voltage level where, in contrast to the previous studies on the extra-high voltage transmission grid, transfer losses can not be neglected. Furthermore, in particular solar power is fed into the grid via inverters, whose behaviour is different from generators with inertia. Hence, the network of synchronous machines has to be complemented by simple units mimicking inverter characteristics. In addition, we introduce a simple local voltage regulator, which may support the system in keeping tolerance bounds.

We discuss the impact of transmission losses and voltage regulation on the dynamics and stability of both a small two-machine component and a complex power grid and we present a how-to for the implementation of inverter units.

DY 12.2 Mon 15:15 H47

Cascading Failures in AC Electricity Grids — •Martin Rohden, Samyak Tamrakar, Daniel Jung, and Stefan Kettemann — Department of Physics and Earth Sciences, Jacobs University Bremen, 28759 Bremen

The severity of power grid failures is often measured by the number of affected consumers. Data from real-world power grids show that the probability to disconnect more than a certain number of consumers often decays like a power law [1]. Here we are using an oscillatory power grid model [2] to model cascading failures, induced by the failure of single transmission lines. We analyse the effect of different cascading failures by counting the number of affected consumers for both artificial regular topologies and the topology of the German power grid. We show that depending on parameter values different distributions of disconnected consumers can be found. Furthermore we analyse the effect of different cluster sizes of generators and consumers and determine the vulnerability of small and large clusters against cascading failures.

[1]: I. Dobson et al., Chaos **17**, 026173 (2007)
[2]: M. Rohden et al., Chaos **24**, 013123 (2014)

DY 12.3 Mon 15:30 H47

Long-range Response in AC Electricity Grids — •Daniel Jung and Stefan Kettemann — Department of Physics & Earth Sciences, Focus Area Health, Jacobs University Bremen, 28759 Bremen, Germany.

The transition towards renewable energy sources (RES) leads naturally to a decentralized and fluctuating production of electrical power. Furthermore, it is well known not only among grid operators that local changes to the grid topology – regardless if intentional or accidental – can have global effects on the flow of power within the entire network [1]. Thus it can be expected that ensuring stable grid operation

becomes more challenging with an increasing share of RES. In a model-based ansatz focussing on decentral power production, the impact of single-line additions on the long-range response of DC electricity grids has recently been studied numerically [2]. By solving the real part of the static AC load flow equations, we conduct a similar investigation for AC grids. For intermediate distances in a regular 2D grid, we find a power law behavior for the change of power flow as a function of distance to the disturbance. Furthermore, the power exponent saturates in the limit of large system sizes. We also compare the results of the regular 2D grid topology to a model topology of the German transmission grid.

[1] D. Witthaut and M. Timme, Eur. Phys. J. B **86**, 377 (2013).
[2] D. Labavić, R. Suciu, H. Meyer-Ortmanns, and S. Kettemann, Eur. Phys. J. Spec. Top. **223**, 2517 (2014), arXiv:arXiv:1406.4699v1.

DY 12.4 Mon 15:45 H47

Model order reduction for network based whole energy systems — •Frank Hellmann — Potsdam Institute for Climate Impact Research

I will discuss recent work on applying non-linear model order reduction techniques to power system models. The aim of this work is to obtain models that are simple enough that methods which were previously only available for conceptual models can be applied in practice. To do so we develop reduction methods that make use of and preserve the network structure of the system under consideration.

DY 13: Statistical Physics (general)

Time: Monday 15:00–17:15 Location: H48

DY 13.1 Mon 15:00 H48

Numerische Simulation zur Hochtemperatur-Supraleitung — •Ingo Morgenstern — Universtätsstraße 31, 93053 Regensburg

Gezeigt werden numerische Simulationen zum Hubbard-Modell in zwei Dimensionen für U=2 und U=3. Verwendet wird ein auf dem Weltrekordalgorithmus (2009 weltweit eine der besten 50 Erfindungen) basierendes Verfahren mit korrekter Mitnahme des Minussigns. Das Modell zeigt in diesem Falle Hochtemperatur-Supraleitung. Für größere U bricht die Simulation zusammen. Ein Bias im Minussign unterdrückt darüber hinaus die Supraleitung. Es wird gezeigt, dass die nichtlineare Ankopplung des Apex-Sauerstoffs zu einer Absenkung der effektiven Hubbard-Abstoßung zu Werten von U=3 vom realistischen Wert führt. Damit ist der Apex-Sauerstoff nicht ursächlich für die Hochtemperatur-Supraleitung verantwortlich, sondern nur für die Absenkung des effektiven Us. Andere Mechanismen, die ebenfalls in ein effektives U zwischen 2 und 3 verursachen, führen demnach auch zu Hochtemperatur-Supraleitung.

DY 13.2 Mon 15:15 H48

Determining the size at which neutral gold clusters turn three-dimensional at finite temperature — •Bryan Goldsmith[1], André Fielicke[2], Matthias Scheffler[1], and Luca Ghiringhelli[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstrasse 36, D-10623 Berlin

Discerning the ground state structure of free gold clusters, and in particular the critical size when Au clusters begin favoring three-dimensional (3D) structures over planar structures at 0 K, has been a topic of longstanding interest. At finite temperature, however, Au clusters exhibit coexistence of many structural isomers. To move beyond the monostructure description of clusters at 0 K, we performed *ab initio* replica-exchange molecular dynamics (REMD) on Au_n clusters (n=5-14) to identify metastable states, their relative stability, and to examine the influence of entropy and van der Waals (vdW) on the isomer energetics. REMD calculations used PBE with the scalar ZORA correction and either Tkatchenko-Scheffler or Many-Body-Dispersion vdW. Free energies of Au isomers are estimated using the Multistate Bennett Acceptance Ratio and the planar and 3D isomer populations are examined between 100-1000 K. The distribution of bond coordination numbers is used to discriminate isomers along the dynamical trajectories. Isomer energetic ordering is verified using renormalized second-order perturbation theory. Computed anharmonic IR spectra of Au_n are compared with experimental spectra.

DY 13.3 Mon 15:30 H48

Effects of Local Measurements on Quantum Statistical Ensembles — •Walter Hahn[1] and Boris Fine[1,2] — [1]Institute for Theoretical Physics, University Heidelberg, Germany — [2]Skolkovo Institute of Science and Technology, Moscow, Russia

We investigate the effect of local measurements on quantum statistical ensembles for macroscopic systems. The system chosen is a lattice of spins 1/2 subject to projective measurements of individual spins. We find that the effect of measurements depends on system's Hamiltonian and on the initial statistical ensemble. The above findings justify prescriptions for protecting unconventional statistical ensembles.

DY 13.4 Mon 15:45 H48

Q–tensor Density Functional Theory of Non–spherical Hard–Body Mixtures — •Rodrigo Lugo-Frias and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In nature there are numerous examples of polydisperse systems composed of molecules with different shapes and concentrations. The behavior of these complex fluids in and out of equilibrium is a long–standing problem with relevance in material science, engineering and soft matter theory.

On the basis of density functional theory and the phase–field–crystal model for liquid crystals [1] we derive in detail a free energy functional of an N component hard–body mixture in terms of a set of tensorial order parameters $\{\mathbf{Q}^i\}$. In contrast to previous works on binary non–spherical mixtures [2], our free energy functional includes gradients of the order parameters. Thus, our description can be used as a starting point to explore liquid–crystalline phases of mixed systems with spatial inhomogeneities, or as an input to mesoscopic dynamical equations for the orientational order parameters.

[1] R. Wittkowski, H. Löwen and H. R. Brand, Phys. Rev. E, **82**, 031708 (2010).
[2] R. Lugo-Frias and S. H. L. Klapp, J. Phys.: Condens. Matter, *submitted* (2015).

DY 13.5 Mon 16:00 H48

From Shapiro-Steps to frozen Kinks — •Thorsten Brazda and Clemens Bechinger — Pfaffenwaldring 57, 70550 Stuttgart, Germany

Although friction is ubiquitous in our everyday lives, a microscopic understanding is still lacking. This is partially due to the small length scales, which are not easily accessible in experiments. To overcome this problem and to observe individual particle motion during sliding, we studied a two-dimensional commensurate colloidal crystal which is driven across a (111) substrate, the latter created by a laser interference pattern [1]. In order to study the effect of substrate lattice vibrations on the sliding motion we have periodically modulated the substrate strength U. For small driving forces F, we observe a cooperative, phase-locked, particle motion which leads to characteristic Shapiro-steps in the mobility-force plane. At higher F, the colloids form an increasing number of local compression zones (kinks) which are still mobile during time-intervals where U is small. On the contrary, for large U, the particle motion is entirely stopped and the kinks are frozen. The formation of kinks leads to an incoherent particle motion which leads to the blurring of Shapiro-steps until they finally disappear at high F.

[1] T. Bohlein J. Mikhael and C. Bechinger, Observation of kinks and antikinks in colloidal monolayers driven across ordered surfaces, Nat. Mater. 11, 126 (2011).

DY 13.6 Mon 16:15 H48

Melting in 2D and a Fresh Perspective on Monte Carlo — •Sebastian Kapfer[1] and Werner Krauth[2] — [1]Theoretische Physik 1, FAU Erlangen — [2]LPS, Ecole Normale Superieure, Paris

The melting transition of two-dimensional solids has been the subject of continued research for more than fifty years, with the prevalent sce-

narios 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]. A key problem in these simulations are the large correlation lengths, which we tackle using a new rejection-free global-balance Monte Carlo algorithm [2].

We show that the hard disk 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.

The new algorithm is very versatile, and could also be applied to spin systems, polymers, path integral problems, etc. It can be augmented to treat long-range force laws such as Coulomb without any artificial truncation.

[1] E. P. Bernard, W. Krauth, Phys. Rev. Lett. 107, 155704 (2011). [2] M. Michel et al., J. Chem. Phys. 140, 054116 (2014). [3] S. C. Kapfer, W. Krauth, Phys. Rev. Lett. 114, 035702 (2015).

DY 13.7 Mon 16:30 H48

Apparent non-universality due to competing anisotropies in 3D Zq models — •Thomas Lottermoser[1], Andres Cano[2], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — [2]CNRS, Université de Bordeaux, ICMCB, UPR 9048, 33600 Pessac, France

3D Z_q models ($q > 4$) like the q-state clock model, antiferromagnetic Potts model or the XY model with discrete q-fold anisotropy, are known to belong all to the XY-universality class at criticality, whereas the Z_q anisotropy is dangerously irrelevant at T_C. This leads to a new length scale associated to the fluctuations of the phase of the order parameter with a critical exponent $\nu_q > \nu$. Here ν is the standard XY critical exponent for the correlation length ξ of the order parameter amplitude. While there is a general agreement on this behavior in the literature, due to contradicting simulation results the question of the universality of ν_q aroused. We propose that these contradictions can be explained by the existence of competing anisotropies. Therefore, in our extensive Monte-Carlo study we investigated the critical behavior of a 12-state clock model with competing 6-fold anisotropy. As a result we found that the apparent non-universality of ν_q can indeed be traced back to the strength of the competing anisotropy we introduced in our model system. This allows us to continuously tune the value of ν_q between the universal values for the 6-state and 12-state clock models, respectively.

DY 13.8 Mon 16:45 H48

Analytical one-dimensional approach of understanding water anomalies and phase transitions — •Katharina Ferling and Andreas Heuer — Institut für Physikalische Chemie, WWU Münster, Germany

The understanding of the water behaviour, including its anomalies, can play an important role in improving the description of water. Here the emphasis lies on the property of building H-bonds which is believed to be one major factor for many anomalies such as the density change or the liquid-liquid phase transition at low temperatures. For the present investigation a simple model has been chosen which focuses on the distinction between a close-packed and an open structure. The one dimensional model - which was first introduced by Ben-Naim [1] - has now been extended by terms, capturing the interaction of second-nearest neighbours as well as the transition to the gas phase at high temperatures. Here, two different analytical approaches are evaluated via explicit calculation of the partition function, and selected properties are discussed with the aim to show water-like behaviour such as a high-density liquid and low-density liquid (HDL-LDL) transition. One model shows a clear first order phase transition between a high-density and a low-density phase and both models have a (theoretical) transition line with negative slope in the p-T plane. Furthermore, anomalous behaviour of several properties, such as the density, heat capacity and isothermal compressibility, is visible, as can be seen in real water.

[1] Arieh Ben-Naim, J. Chem. Phys. 128, 024505 (2008)

DY 13.9 Mon 17:00 H48

Metadynamics for Nucleation studies in Potts-Models — •Ralf Schmid and Peter Nielaba — Universität Konstanz, Konstanz, Baden-Württemberg

Simulating nucleation processes in particle based systems can be time consuming due to large barriers in the free energy landscape. So new simulation techniques like Umbrella Sampling, Thermodynamic Integration and Metadynamics were invented for accelerating rare events. In molecular dynamics studies of nucleation the Metadynamics protocol was successfully used to accelerate the process and to calculate the free energy landscape in given reaction coordinates like cluster size.

We use the Metadynamics tool in Potts-Model systems to study nucleation and crystallization. The underlying dynamics of the system is a Metropolis Monte-Carlo simulation in the semi-grand canonical ensemble. The use of different reaction coordinates leads to insights into the basic processes that enable nucleation.

DY 14: Complex Systems

Time: Monday 16:15–17:45 Location: H47

DY 14.1 Mon 16:15 H47

An integrative quantifier of multistability in complex systems based on ecological resilience — •Chiranjit Mitra[1,2], Jürgen Kurths[1,2,3,4], and Reik V. Donner[1] — [1]Potsdam Institute for Climate Impact Research, Transdisciplinary Concepts & Methods - Research Domain 4, Potsdam, 14412, Germany — [2]Humboldt University of Berlin, Department of Physics, Berlin, 12489, Germany — [3]University of Aberdeen, Institute for Complex Systems and Mathematical Biology, Aberdeen, AB24 3UE, United Kingdom — [4]Nizhny Novgorod State University, Department of Control Theory, Nizhny Novgorod, 606950, Russia

The abundance of multistable dynamical systems calls for an appropriate quantification of the respective stability of the (stable) states of such systems. Motivated by the concept of ecological resilience, we propose a novel and pragmatic measure called 'integral stability' which integrates different aspects commonly addressed separately by existing local and global stability concepts. We demonstrate the potential of integral stability by using exemplary multistable dynamical systems such as the damped driven pendulum, a model of Amazonian rainforest as a known climate tipping element and the Daisyworld model. A crucial feature of integral stability lies in its potential of arresting a gradual loss of the stability of a system when approaching a tipping point, thus providing a potential early-warning signal sufficiently prior to a qualitative change of the system's dynamics.

Reference: Mitra, C. et al. An integrative quantifier of multistability in complex systems based on ecological resilience. Sci. Rep. 5 (2015).

DY 14.2 Mon 16:30 H47

Fractional interpolation methods for two phase flow in porous media — •Pradeep Kumar, Rouven Steinle, Bakkyraj Thangarashu, and Rudolf Hilfer — Institute for Computational Physics, University Stuttgart, Germany

Two phase flow in porous media is described macroscopically using the generalized Darcy theory with hysteresis. Recently, numerical solutions for various hysteresis models were found to exhibit non-monotone profiles [1] and [2]. In this talk, we will focus on analytical solutions of this model by using the theory of semigroups and fractional interpolation methods [3]. In this framework uniqueness, global existence and maximal regularity of the solutions are also discussed.

[1] Hilfer, R. and Steinle, R., Eur. Phys. J. ST, **223**, 2323 (2014)
[2] Steinle, R. and Hilfer, R., Transp. Porous Media, (in print) 2016
[3]. Yagi, A., *Abstract parabolic evolution equations and their applications*, Springer-Verlag, Berlin (2010)

DY 14.3 Mon 16:45 H47

Scale dependent complexity measure for time series — •Eckehard Olbrich[1] and Georg Martius[2] — [1]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany — [2]IST Austria, Klosterneuburg, Austria

The predictive information - also known as effective measure complexity or excess entropy - is a natural complexity measure for temporal se-

quences. It measures the amount of information that the past contains about the future which is equal to the non-extensive part of the entropy of the sequence. In order to apply it to dynamical systems with continuous states one has to partition the state space first. But, then the result will depend on the partition and will be different even for different generating partitions. Here we will study the excess entropy using scale dependent entropies. We show that the excess entropy becomes infinite in the limit of infinite resolution for deterministic systems. The attractor dimension controls, how the excess entropy diverges with increasing resolution while the resolution independent offset provides a complexity measure on its own — if appropriately rescaled — that is related to the correlations. Moreover, we show that the excess entropy remains finite for noisy systems, and discuss how it is determined by the noise levels and the entropy rate on the large scales. We demonstrate the usefulness of the scale dependent excess entropy using it for quantifying the effects of autonomously learned behavior of simulated robots using task independent objective functions.

G. Martius and E. Olbrich, Quantifying Emergent Behavior of Autonomous Robots, Entropy 17(10), 2015, 7266-7297.

DY 14.4 Mon 17:00 H47

Anisotropic Gaussian random fields characterized by Minkowski tensors — •Michael A. Klatt[1,2], Max Hörmann[2], and Klaus Mecke[2] — [1]KIT, Institut für Stochastik, Englerstraße 2, 76131 Karlsruhe — [2]FAU, Institut für Theoretische Physik, Staudtstraße 7, 91058 Erlangen

Anisotropic Gaussian random fields are important models of anisotropic disordered structures that appear in very different physical and biological systems. Often physical insight is best achieved by a rigorous structure characterization, for which comprehensive shape descriptors are needed. We here show how the Minkowski tensors as sensitive and robust measures of anisotropy, which extend the notion of volume and surface area to scalar and tensorial morphometric measures [1], comprehensively characterize the shape of level sets of Gaussian random fields.

We give explicit expressions for the mean values and compare them to simulation results. We also provide explicit integral expressions for the second moments of the Minkowski functionals. Which additional information is contained in higher rank Minkowski tensors? We find that tensors of higher rank indeed contain additional anisotropy information as compared to the tensor of rank two. Surprisingly, we can show that the latter is nevertheless sufficient to estimate the model parameters which are necessary to determine all Minkowski tensors of arbitrary rank. Using this relation a null hypothesis test for non-Gaussianities in anisotropic random fields can be defined.

[1] G. E. Schröder-Turk et al., Adv. Mater. 23:2535, 2011.

DY 14.5 Mon 17:15 H47

Propagation, growth and decay of saturation overshoot — •Rouven Steinle and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

A sequence of drainage and imbibition shocks within the traditional theory of two-phase immiscible displacement can give rise to shallow non-monotone saturation profiles [1]. This phenomenon depends sensitively on model parameters and initial conditions. The systematical investigation of saturation overshoot on initial conditions allows to determine regions in the parameter space for the observation of saturation overshoot and to explore limitations of the underlying idealized hysteresis model. Numerical solutions of the nonlinear partial differential equations of motion reveal a strong dependence of the overshoot phenomenon on the boundary and initial conditions [2]. Overshoot solutions with experimentally detectable height are shown to exist numerically. Extensive parameter studies reveal different classes of initial conditions for which the width of the overshoot region, can decrease, increase or remain constant.

[1] Hilfer, R. and Steinle, R., Eur.Phys.J.ST, **223**, 2323 (2014)
[2] Steinle, R. and Hilfer, R., Transp. Porous Media, (in print) (2016)

DY 14.6 Mon 17:30 H47

A novel experimental technique for analyzing spreading droplets — •Roghayeh Shiri[1], Ali Najafi[1], and Mehdi Habibi[2] — [1]University of Zanjan, Zanjan, Iran — [2]Institute for advanced studies in basic sciences, Zanjan, Iran

Recently, a simple and accurate phase measurement method, called the sampling moiré method was developed for thickness distribution measurement of transparent plates from a single image. A single image taken from a Ronchi grating that encoded the optical characteristics of transparent sample is the main experimental element of the sampling moiré method. This method can obtain small displacements up to 1/500 of the grating pitch by analyzing the phase distribution of the moiré fringe of each single grating image before and after deformation.

Therefore, Sampling moiré method can provide an accurate technique to investigate the dynamical properties of a spreading droplet of a transparent fluid over a rigid substrate where the air-liquid interface evolves in time. Studying the dynamics of such a multi-phase flow interface is interesting either from fundamental or technical point of view.

We have performed the spreading experiment with silicone oils with different viscosities and compared them with a universal scaling relation that quantifies the early time dynamics in non-gravitational regime as:$h(t) \sim t^{-0.2}$. In our experiments, all droplets with different viscosities show a linear dynamics with slope -0.2 in the logarithmic scale that are in good agreement with the theoretical results.

DY 15: Chimera State: Coherence-Incoherence Patterns in Complex Networks (joint symposium DY/SOE/BP)

Time: Tuesday 9:30–12:15 Location: H1

Invited Talk DY 15.1 Tue 9:30 H1

Theory far from infinity: chimera states without the thermodynamic limit — •Daniel Abrams — Northwestern University, Evanston, IL, USA

Chimera states are surprising symmetry-broken patterns in networks of coupled oscillators which often coexist with fully symmetric states. Much of the theory for chimera states focuses on networks with an infinite number of oscillators. In this talk, I will discuss some new results for the finite-N case, showing that stable chimera states are possible with as few as 4 oscillators. This suggests that they may be easily constructed in experimental or engineered systems, and may even occur naturally.

Invited Talk DY 15.2 Tue 10:00 H1

Chimera patterns: Influence of topology, noise, and delay — •Eckehard Schöll — Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Chimera patterns, which consist of coexisting spatial domains of coherent and incoherent dynamics, are studied in networks of oscillators involving amplitude as well as phase dynamics, complex hierarchical (fractal) topologies, noise, and delay. We show that a plethora of novel chimera patterns arise if one goes beyond the Kuramoto phase oscillator model. For the FitzHugh-Nagumo system, the Van der Pol oscillator, and the Stuart-Landau oscillator with symmetry-breaking coupling we find various multi-chimera patterns [1], including amplitude chimeras and chimera death [2]. To test the robustness of chimera patterns, we study small-world and hierarchical topologies. We also address the robustness of amplitude chimera states in the presence of noise [3], and the emergence of coherence-resonance chimeras [4]. If delay is added, the lifetime of transient chimeras can be drastically increased, and novel phenomena like stochastic resonance of delayed-feedback chimeras can arise.

[1] I. Omelchenko et al., Phys. Rev. Lett. 110, 224101 (2013). I. Omelchenko et al., Phys. Rev. E 91, 022917 (2015). I. Omelchenko et al., Chaos 25, 083104 (2015). [2] A. Zakharova, M. Kapeller, and E. Schöll, Phys. Rev. Lett. 112, 154101 (2014). [3] S. Loos, J. C. Claussen, E. Schöll, and A. Zakharova, Phys. Rev. E (2016), arXiv:1508.04010v2. [4] N. Semenova, A. Zakharova, V. Anishchenko, and E. Schöll (2016), arXiv:1512.07036.

Invited Talk DY 15.3 Tue 10:30 H1

Chimera states in quantum mechanics — •Victor Manuel Bastidas Valencia — Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, 117543 Singapore, Singapore

Chimera states are a hallmark of self-organization in non-linear dynamical systems [1]. These intriguing states are characterized by the spatial coexistence of synchronized and desynchronized motion in a complex network [2,3]. In this talk, I will discuss the emergence of Chimera states in a network of N coupled quantum van der Pol oscillators with a ring topology. Among the diverse quantum signatures of Chimera states, I will describe the formation of Chimera-like quantum correlations in the network. In addition, I will show how Chimera states can be characterized by using concepts of quantum information theory such as the quantum mutual information. By using this approach, one can show that Chimera states exhibit lower mutual information than a synchronized state, but higher mutual information than a desynchronized one, which extends in a natural way the definition of chimera states to quantum mechanics [4].

[1] M. J. Panaggio and D. M. Abrams, Nonlinearity **28**, R67 (2015).
[2] Y. Kuramoto and D. Battogtokh, Nonlin. Phenom. in Complex Syst. **5**, 380 (2002)
[3] D. M. Abrams and S. H. Strogatz, Phys. Rev. Lett. **93**, 174102 (2004).
[4] V. M. Bastidas, I. Omelchenko, A. Zakharova, E. Schöll, and T. Brandes, Phys. Rev. E **92**, 062924 (2015).

15 min. break

Invited Talk DY 15.4 Tue 11:15 H1

Synchronization in Populations of Chemical Oscillators: Phase Clusters and Chimeras — •Kenneth Showalter — West Virginia University, Morgantown, USA

We have studied heterogeneous populations of chemical oscillators to characterize different types of synchronization behavior. The formation of phase clusters in stirred suspensions of Belousov-Zhabotinsky oscillators is described, where the (global) coupling occurs through the medium. We then describe the formation of phase clusters and chimera states in populations of photosensitive oscillators. The nonlocal coupling occurs via illumination intensity that is dependent on the state of each oscillator. The behavior of oscillators in ring configurations as a function of the number of oscillators is described, including traveling cluster states.

References: A. F. Taylor et al., Angewandte Chemie Int. Ed. 50, 10161 (2011); M. R. Tinsley et al., Nature Physics 8, 662 (2012); S. Nkomo et al., Phys. Rev. Lett. 110, 244102 (2013); J. F. Totz et al., Phys. Rev. E 92, 022819 (2015).

Invited Talk DY 15.5 Tue 11:45 H1

Epileptic seizures: chimeras in brain dynamics — •Klaus Lehnertz — Universität Bonn

Epilepsy is a complex malfunction of the brain that affects approximately 50 million people worldwide. Epileptic seizures are the cardinal symptom of this multi-facetted disease and are usually characterized by an overly synchronized firing of neurons. Seizures can not be controlled by any available therapy in about 25% of individuals, and knowledge about mechanisms underlying generation, spread, and termination of the extreme event seizure in humans is still fragmentary.

There is now increasing evidence for the existence of large-scale epileptic networks in which all constituents can contribute to the generation, maintenance, spread, and termination of even focal seizures as well as to the many pathophysiologic phenomena seen during the seizure-free interval. Using concepts and analysis tools from nonlinear dynamics, statistical physics, synchronization and network theory, significant progress has been made over the last decade in characterizing the connection structure of large-scale epileptic networks and in understanding their long-term dynamics. Model simulations of complex oscillator networks with connection structures seen in human epilepsies indicate that seizure-like activities can be regarded as self-initiated and self-terminated chimera states. Altogether, findings open promising directions for the development of new therapeutic possibilities.

DY 16: Microswimmers I (joint session DY/BP)

Time: Tuesday 9:30–13:00 Location: H47

Invited Talk DY 16.1 Tue 9:30 H47

Amoeboid swimming — •Chaouqi Misbah — CNRS and Univ. Grenoble, France

Microorganisms, such as bacteria, algae, or spermatozoa, are able to propel themselves forward thanks to flagella or cilia activity. By contrast, other organisms employ pronounced changes of the membrane shape to achieve propulsion, a prototypical example being the Eutreptiella gymnastica. Cells of the immune system as well as dictyostelium amoebas, traditionally believed to crawl on a substratum, can also swim in a similar way. We develop a model for these organisms. It is shown that fast propulsion can be achieved with adequate shape adaptations. We investigate the effect of confinement. A complex picture emerges. In particular it is found that optimal swimming can be obtaiend for a special confinement, and that the nature (pusher or puller) of the swimmer depends on confinement. The swimmer is often found to excecute ample excursion (navigation) in the channel.

DY 16.2 Tue 10:00 H47

Meandering liquid crystal droplet swimmers — •Carsten Krüger, Corinna Maass, Christian Bahr, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Liquid crystal microswimmers immersed in an aqueous surfactant solution at concentrations above the critical micelle concentration show self-propelled motion. The droplets dissolve into surfactant micelles [1], producing an inhomogeneous surfactant distribution in the continuum, propelling the droplets via Marangoni flows at the interface [2,3].

Below the nematic-isotropic transition we observe regular meandering trajectories, which change to a persistent random walk when the droplets are made isotropic by heating. This offers a unique possibility to tune the swimming behavior. We observe a distortion of the nematic director field, with the central defect pulled towards the droplet apex, but angled away from the direction of motion. This is consistent with a constant torque caused by a distortion of the defect pattern by the external and internal flow fields, acting against the elastic field associated with the nematic order. It also gives rise to the twofold symmetry break required for helical motion, as proposed by theory, e.g. in [4].

We use polarized microscopy to observe defect structures, PIV to image flow fields and are able to track freely moving droplets in 3D with a light sheet setup. [1] K. Peddireddy et al., Langmuir 28, 12426 (2012). [2] S. Herminghaus et al., Soft Matter 10, 7008 (2014). [3] C. C. Maass et al., Annu. Rev. Cond. Mat. 7, in press (2016). [4] H. Crenshaw, Amer. Zool. 36, 608 (1996).

DY 16.3 Tue 10:15 H47

Dynamical density functional theory of microswimmers — •Andreas M. Menzel, Arnab Saha, Christian Hoell, and Hartmut Löwen — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Microswimmers are found in nature in the form of self-propelling microorganisms, or they can be realized artificially, e.g. as Janus particles propelling due to self-induced phoretic effects. To describe and predict the collective behavior of many such interacting microswimmers on the mesoscopic level, statistical approaches are necessary.

Along these lines, we here report on a newly established dynamical density functional theory (DDFT). This theory includes steric as well as hydrodynamic interactions between individual swimmers within dilute and moderately concentrated suspensions of microswimmers. Minimal model microswimmers are considered. They self-propel by setting the surrounding fluid into motion, which leads to additional hydrodynamic interactions. Both pusher and puller swimming mechanisms are taken into account.

Via numerical simulations, our DDFT is demonstrated to reproduce effects recently observed in agent-based simulations. In a spherical trapping potential, this includes the formation of density rings and the self-organization in a symmetry-breaking state that resembles a hydrodynamic fluid pump. An additional instability is predicted that

destabilizes the pumping state.

DY 16.4 Tue 10:30 H47

Dynamics of a single self-propelled particle — •Christina Kurzthaler, Sebastian Leitmann, and Thomas Franosch — Department for Theoretical Physics, University of Innsbruck, Innsbruck, Austria

The dynamics of a single self-propelled particle in two dimensions is analyzed in terms of the intermediate scattering function, i.e. the characteristic function of the random displacements. Its analytical solution is derived by solving the Fourier transform of the Fokker-Planck equation which has the form of a complex Mathieu equation. Exact expressions for the mean-square displacement and non-Gaussian parameter are obtained as derivatives of the intermediate scattering function. For large wave numbers, oscillations in the intermediate scattering function reflect the persistent swimming motion, whereas at small wave numbers diffusive behavior emerges with an effective diffusion coefficient depending on the velocity and rotational diffusion of the swimmer.

DY 16.5 Tue 10:45 H47

Droplet swimmers in complex geometries: Autochemotaxis and trapping at pillars. — •Chenyu Jin, Corinna Maass, Carsten Krüger, and Stephan Herminghaus — MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany

Many organisms communicate by trail mediated signalling or autochemotaxis: their motion is influenced by their own emission of a chemical attractant or repellent, diffusing slowly compared to typical agent velocities. This causes gradient forces acting both on themselves as well as on other individuals. Meanwhile, geometrical confinement also influences the behaviour of microswimmers, e.g., pusher-type swimmers attach to curved interfaces depending on the interplay of hydrodynamic interaction and trajectorial persistence. It is of high biological relevance to have a well-controlled, tunable artificial model system exhibiting these traits.

A promising candidate are self-propelling liquid crystal droplets in an aqueous surfactant solution. They gain propulsion energy by micellar solubilisation, with filled micelles acting as a chemical repellent. We can tune the key parameters swimmer size, velocity and persistence length. We use microfluidic pillar arrays of variable radii to provide a convex wall to attract the swimmer, bend its trajectory and to force it to revert to its own trail. Hence, we investigate the interplay of wall attraction, persistence of motion, and negative auto-chemotaxis. We observe repulsion for highly curved surfaces, stable trapping at large pillars, and a narrow transition region, where negative autochemotaxis makes the swimmers detach after a single orbit.

15 min break

DY 16.6 Tue 11:15 H47

Dimensionality matters in the collective behaviour of active emulsions — •Corinna Maass, Carsten Krüger, and Stephan Herminghaus — MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany

Microswimmer systems like plankton constitute an important part of our ecosystem. The description of such systems is complex, as it involves large numbers of agents, long range hydrodynamic interactions and nontrivial boundary conditions like turbulent flows and complex interfaces. They exhibit rich and sometimes puzzling behaviour like the high species diversity referred to in the Plankton Paradox, or self organised bioconvection of gravitactic bacteria. This complexity makes them hard to treat analytically and numerically. Large scale simulations usually have dimensional restrictions or exclude hydrodynamic interactions, which has to be considered in comparisons with natural systems. Simple, tunable artificial swimmer systems can help bridging this gap.

Our experimental system consists of an active emulsion of self propelling liquid crystal droplets under variable microfluidic confinement and with tunable buoyancy. While changing the system's geometry from a quasi 2D confinement to a full 3D bulk reservoir, we observe a pronounced transition from only transient local aggregation over line formation to a large scale clustering phase stabilised by self-generated convection patterns. We studied this clustering behaviour in more detail with respect to reservoir height and buoyancy.

DY 16.7 Tue 11:30 H47

Quantification of modular phoretic micro-swimmers — •Ran Niu, Christopher Wittenberg, Julian Weber, Denis Botin, and Thomas Palberg — Institut f. Physik, JGU Mainz, Staudingerweg 7, D-55128 Mainz, Germany

We have studied the swimming behavior of modular phoretic 2D micro-swimmers with particular focus on collective and cooperative effects[1,2]. These were exploited to proceed from isolated electrolyte releasing particles, driven by electro-osmotic flow field across a charged substrate, to multi-component complex, capable of self-generated, self-directed motion, transport and release of cargo and mutual long ranged interactions. Using optical techniques, such as microscopy and superheterodyne laser doppler velocimetry, we accurately measured and characterized the swimmer properties and dynamics. From PH gradient measurements and particle tracking, we quantified the electric field and flow field around electrolyte releasing particle. The dependence of field strength on time and the size of electrolyte releasing particle were also determined. This provides the base for the quantitative understanding and establishing of a reliable model.

[1] T. Palberg, H. Schweinfurth,T. Koller,H. Muller,H.J. Schope, and A Reinmuller, European Physics Journal Special Topics 2013, 222:2835-2853. [2] A. Reinmuller, H.J. Schope, and T. Palberg, Langmuir 2013, 29:1738*1742.

DY 16.8 Tue 11:45 H47

Confinement of Single Microswimmers in Circular Microfluidic Chambers — •Tanya Ostapenko, Thomas Böddeker, Christian Kreis, Fabian Schwarzendahl, Marco G. Mazza, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

The characteristics of active fluids, such as suspensions of biological microswimmers, may not only originate from the mutual interactions between the constituents, but also from interactions with interfaces and confining walls. In fact, the natural habitats of many living organisms are complex geometric environments, rather than bulk situations. The influence of interfaces on the dynamics was recognized as an important factor, and there are differences in the way that pusher-type swimmers (e.g. *E. coli*) and puller-type swimmers (e.g. *C. reinhardtii*) behave close to flat interfaces. Using experiments and simulations, we report on the dynamics of single puller-type swimmers in 2D circular microfluidic chambers. We find that the radial probability distribution of trajectories displays a characteristic wall hugging effect, where swimmers remain trapped at a concave interface for decreasing chamber size. For trajectories in the vicinity of the concave wall, an alignment of the local swimming direction with the local wall tangent is observed. In contrast, the swimmers tend to scatter off convex interfaces with short interaction times. Based on geometric arguments involving the swimmer's persistence length, we explain this entrapment effect at concave interfaces.

DY 16.9 Tue 12:00 H47

Tumbling of an E. coli: role of rotation-induced polymorphism and external shear — •Tapan Chandra Adhyapak and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D - 10623 Berlin, Germany

Many multiflagellated bacteria such as E. coli adopt a run-and-tumble strategy to detect and direct themselves in chemical gradients in their surroundings. Tumbles are events which mark nearly abrupt changes in the direction of straight runs of the bacterium. Reversal of rotation of one or more of the flagella, which under normal rotation act as the propelling part of the bacterium, initiates these tumbles. Simultaneously, flagella that are reverse rotated are observed to undergo a series of polymorphic transitions between different flagellar states [1].

To understand the need, if there is any, of these transitions for an effective tumbling event has remained a long-standing problem. We present here a detailed numerical investigation unraveling the correlation between flagellar conformational changes and an efficient tumbling strategy for E. coli. Importance of these transitions in comparison to the contribution from hydrodynamic and steric interactions [2] will be addressed. At the end the nature of a tumbling event in sheared environment will also be discussed.

[1] R. Vogel and H. Stark, Phys. Rev. Lett. **110**, 158104 (2013).
[2] T.C. Adhyapak and H. Stark, Phys. Rev. E **92**, 052701 (2015).

DY 16.10 Tue 12:15 H47

Sperm Cells in Structured Microchannels — •Sebastian Rode, Jens Elgeti, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems (ICS-2) , Forschungszentrum Jülich, 52425 Jülich, Germany

At low Reynolds numbers and in confinement, the directed motion of a self-propelled microswimmer is strongly influenced by steric and hydrodynamic surface interactions [1-2]. Our mesoscale hydrodynamics simulation allow the study of various flagellated and ciliated microorganisms in this environment, ranging from a single flagellated sperm cell to multiciliated microswimmers. In particular, we have studied the motion of sperm in geometrically structured (zig-zag) microchannels. This is an interesting geometry for the manipulation and sorting of sperm cells. In general, sperm swim along the channel walls, but can be deflected from the wall at sharp bends. We found that the effective adhesion of a sperm cell to a curved surface depends both on the envelope of its sinusoidal beating shape and on the orientation of its beating plane. We present a heuristic argument explaining this dependence by an interplay of steric and hydrodynamic surface interactions. Our results are in qualitative agreement with recent microfluidic experiments and might provide a better insight in the mechanisms of sperm navigation under strong confinement.

[1] J. Elgeti et al., Rep. Prog. Phys. 78, 056601 (2015)
[2] J. Elgeti et al., Biophys. J. 99, 1018 (2010)

DY 16.11 Tue 12:30 H47

Cross-stream transport of asymmetric particles driven by oscillating shear — •Matthias Laumann[1], Paul Bauknecht[2], Stephan Gekle[2], Diego Kienle[1], and Walter Zimmerman[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Biofluid Simulation and Modeling, Universität Bayreuth, 95440 Bayreuth, Germany

We study the dynamics of asymmetric, deformable particles in oscillatory, linear shear flow. By simulating the motion of a dumbbell, a ring polymer, and a capsule we show that cross-stream migration occurs for asymmetric elastic particles even in linear shear flow if the shear rate varies in time. The migration is generic as it does not depend on the particle dimension. Importantly, the migration velocity and migration direction are robust to variations of the initial particle orientation, making our proposed scheme suitable for sorting applications of various elastic Janus-like particles.

DY 16.12 Tue 12:45 H47

Calibration method for pH measurements with spatial and temporal resolution — •Julian Weber — Staudingerweg 7, 55128 Mainz

According to the framework of modular microswimmers, the field flow around involved particles is of great interest and can be measured by Doppler velocimetry. Here I present a special method for measuring the pH gradient around a cationic exchange resin. First gradient measurements are demonstrated.

DY 17: Statistical Physics far from Thermal Equilibrium

Time: Tuesday 10:00–13:15 Location: H48

DY 17.1 Tue 10:00 H48

First-passage fluctuation theorems — •Izaak Neri[1,2,5], Édgar Roldán[1,5], Meik Dörpinghaus[3,5], Heinrich Meyr[3,4,5], and Frank Jülicher[1,5] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for Cell and Molecular Biology, Dresden, Germany — [3]Vodafone Chair Mobile Communications Systems, Dresden — [4]Institute for Integrated Signal Processing Systems, Aachen — [5]Center for Advancing Electronics Dresden, Dresden

The Second Law of Thermodynamics states that entropy of an isolated system out of equilibrium increases until the equilibrium state is reached. Statistical physics allows to define entropy of a single trajectory in the microscopic phase space. A universal relation for the fluctuations of entropy production of stochastic systems far from thermal equilibrium follows. The entropy production fluctuation theorem states that a steady state process produces exponentially more likely a positive amount of entropy than an equal but negative amount. In this presentation we show an equivalent relation for the first-passage times of entropy production. The probability to produce for the first time a positive amount of entropy is exponentially more likely than the probability to produce for the first time an equivalent but negative amount of entropy. This novel fluctuation relation is illustrated on a couple of examples of stochastic systems.

DY 17.2 Tue 10:15 H48

Sensory capacity: an information theoretical measure of the performance of a sensor — •David Hartich[1], Andre C. Barato[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Stuttgart, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

For a general sensory system following an external stochastic signal, we introduce the sensory capacity [1]. This quantity characterizes the performance of a sensor: sensory capacity is maximal if the instantaneous state of the sensor has as much information about a signal as the whole time-series of the sensor. We show that adding a memory to the sensor increases the sensory capacity. This increase quantifies the improvement of the sensor with the addition of the memory. Our results are obtained with the framework of stochastic thermodynamics of bipartite systems, which allows for the definition of an efficiency that relates the rate with which the sensor learns about the signal with the energy dissipated by the sensor, which is given by the thermodynamic entropy production. We demonstrate a general tradeoff between sensory capacity and efficiency: if the sensory capacity is equal to its maximum 1, then the efficiency must be less than 1/2. As a physical realization of a sensor we consider a two component cellular network estimating a fluctuating external ligand concentration as signal. This model leads to coupled linear Langevin equations that allow us to obtain explicit analytical results.

[1] D. Hartich, A. C. Barato, and U. Seifert (2015) arXiv:1509.02111

DY 17.3 Tue 10:30 H48

Variational principles and information measures for nonequilibrium processes — •Matteo Polettini — 162 A, avenue de la Faïencerie L-1511 Luxembourg (Grand Duchy of Luxembourg)

We critically review several variational principles for nonequilibrium processes. In particular, we discuss the general form of observable constraints for the correct formulation of the minimum entropy production principle close to equilibrium (minEP), we contest the validity of the so-called maximum entropy production principle, discuss the information-theoretic structure of MAXENT far from equilibrium, and reject a conjectured convexity principle for the relative entropy of a system. Part of our analysis is based on the Fisher information metric, a statistical tool that allows to put bounds on the precision of an estimation of a random variable. We digress on possible roles of this quantity in the context of information processing in nonequilibrium systems.

DY 17.4 Tue 10:45 H48

Universal bounds on current fluctuations — •Patrick Pietzonka[1], Andre C. Barato[2], and Udo Seifert[1] — [1]II. Institut für theoretische Physik, Universität Stuttgart — [2]Max Planck Institute for the Physics of Complex Systems, Dresden

For current fluctuations in non-equilibrium steady states of Markovian processes, we derive four different universal bounds valid beyond the Gaussian regime. Different variants of these bounds apply to either the entropy change or any individual current, e.g., the rate of substrate consumption in a chemical reaction or the electron current in an electronic device. The bounds vary with respect to their degree of universality and tightness. A universal parabolic bound on the generating function of an arbitrary current depends solely on the average entropy production. A second, stronger bound requires knowledge both of the thermodynamic forces that drive the system and of the topology of the network of states. These two bounds are conjectures based on extensive numerics. An exponential bound that depends only on the average entropy production and the average number of transitions per time is rigorously proved. This bound has no obvious relation to the parabolic bound but it is typically tighter further away from equilibrium. An asymptotic bound that depends on the specific transition rates and becomes tight for large fluctuations is also derived. Our bounds generalize a recently derived relation for the relative uncer-

tainty in current fluctuations [1] and provide a new general class of constraints for nonequilibrium systems.
[1] A. C. Barato and U. Seifert, Phys. Rev. Lett. **114**, 158101 (2015)

DY 17.5 Tue 11:00 H48

On the difference between information and heat reservoirs — •Johannes Hoppenau and Andreas Engel — Universität Oldenburg, Germany

In classical thermodynamics, there are two kinds of reservoirs: heat and work reservoirs. While the work reservoirs allow for an exchange of energy without a change of their entropy, for heat reservoirs at temperature T the exchange of the energy Q comes along with a change Q/T of the entropy. Hence, a work reservoir can be seen as a heat reservoir at infinite temperature.

With the advent of stochastic thermodynamics, during the past years the concept of Maxwell's demons has regained increased interest. An integral part of all Maxwell's demons is a memory or information reservoir. A key characteristic of an information reservoir is that its entropy can be increased without the cost of energy exchange. Hence, an obvious question to ask is, if an information reservoir can be seen as a heat bath at zero temperature. This however is not that easily possible since correlation play an essential role in memory, that are not present in heat reservoirs.

To illustrate this difference, we present a model of a tape that stores information and has an intrinsic temperature and derive general bounds of efficiency for engines in contact with this tape. Depending on the perspective, this tape is an imperfect information reservoir or an imperfect heat reservoir and engines acting on this tape are Maxwell's demons or heat engines.

DY 17.6 Tue 11:15 H48

Decision making in the arrow of time — •Édgar Roldán[1,5], Izaak Neri[1,2,5], Meik Dörpinghaus[3,5], Heinrich Meyr[3,4,5], and Frank Jülicher[1,5] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstraße 108, 01307 Dresden, Germany — [3]Vodafone Chair Mobile Communications Systems, Technische Universität Dresden, 01062 Dresden, Germany — [4]Institute for Integrated Signal Processing Systems, RWTH Aachen University, 52056 Aachen, Germany. — [5]Center for Advancing Electronics Dresden, cfaed, Germany.

We show that the steady state entropy production rate of a stochastic process is inversely proportional to the minimal time needed to decide on the direction of the arrow of time. Here we apply Wald's sequential probability ratio test to optimally decide on the direction of time's arrow in stationary Markov processes. Furthermore the steady state entropy production rate can be estimated using mean first-passage times of suitable physical variables. Our results are illustrated by numerical simulations of two simple examples of nonequilibrium processes.

15 min. break

DY 17.7 Tue 11:45 H48

Work and Entropy Production in Generalized Gibbs Ensembles — Martí Perarnau-Llobet[1], Arnau Riera[1], Rodrigo Gallego[2], •Henrik Wilming[2], and Jens Eisert[2] — [1]ICFO-Institut de Ciencies Fotoniques, 08860 Castelldefels, Barcelona, Spain — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

Thermodynamics can be put into contact with quantum mechanics by assuming that systems at thermal equilibrium can be effectively described by the Gibbs ensemble.

Here, we consider thermodynamic protocols in situations where the systems in question cannot be described accurately by a Gibbs ensemble – either because they are strongly coupled to a heat bath or because conserved quantities require the use of an effective description by a so-called Generalized Gibbs ensemble (GGE) to describe their equilibrium state after a quench, as, for example, in the case of localized systems.

In particular we study the validity of the "minimum work principle" and entropy production in optimal work-extraction protocols – both analytically and numerically. Our findings show that the minimum-work principle can break down in the presence of a large number of conserved quantities, while we can show that it remains intact if system and bath together can be well described by a Gibbs ensemble, even in the strongly interacting regime. Since we consider large but finite baths, our results can also be understood as corrections to the usual assumption of ideal infinite heat baths, which do not degrade when used in thermodynamic protocols.

DY 17.8 Tue 12:00 H48

Defining work from operational principles — •Rodrigo Gallego, Jens Eisert, and Henrik Wilming — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

In recent years we have witnessed a concentrated effort to make sense of thermodynamics for small-scale systems. One of the main difficulties is that, at the nano-scale, thermal fluctuations of energy in general render it conceptually difficult to distinguish work from heat. Despite of several attempts to resolve this issue, many of which inspired by quantum information theory, there is still remarkable little consensus on it. In this work, we attempt to define work in a strictly operational way. In our resource-theoretic approach, agents wish to agree upon how much work needs to be invested to effect a transition from one state of an arbitrary quantum work-storage device to another. We introduce basic operational principles, and deduce from them a strict set of mathematical properties that any reasonable function quantifying such work has to fulfill. We show that one work quantifier satisfying all the required properties is the difference of the non-equilibrium free energy of the initial and final state of the work-storage system. More generally, for any work quantifier fulfilling the stated properties, we can derive a quantitative second law in the sense of bounding the work that can be performed using some non-equilibrium resource by the work that is needed to create it. We furthermore discuss the role of path dependence for work quantifiers and the connection to the concept of probability-distributions of work.

DY 17.9 Tue 12:15 H48

Performance of a nanoscale refrigerator — •Obinna Abah and Eric Lutz — Department of Physics, University of Erlangen-Nuremberg, Germany

We consider a quantum Otto refrigerator cycle of a time-dependent frequency harmonic oscillator. We investigate the coefficient of performance at maximum figure of merit for adiabatic and nonadiabatic frequency modulations. We further derive the characteristic time bounding the refrigerator functionality for nonadiabatic transformations. The validity of both cases in both high- and low-temperature limits are discussed.

DY 17.10 Tue 12:30 H48

Nonequilibrium thermodynamics of open degenerate quantum systems — Gregory Bulnes Cuetara[1], Massimiliano Esposito[2], and •Gernot Schaller[3] — [1]Dept. of Chemistry & Biochemistry, UCSD, Urey Hall, 9500 Gilman Dr., La Jolla, CA 92093-0340, USA — [2]University of Luxembourg, Physics and Materials Science Research Unit, Campus Limpertsberg BRB 0.03, 162a avenue de la Faïencerie, L-1511 Luxembourg, G. D. Luxembourg — [3]Institut für Theoretische Physik, Technische Universität Berlin, Eugene-P.-Wigner-Gebäude PN 147, Hardenbergstr. 36, 10623 Berlin

We establish quantum stochastic thermodynamics for open systems with degenerate energy eigenstates. The Born-Markov-secular quantum master equation (QME) leads in this case to couplings between degenerate populations and their coherences. We show that our genuine quantum formulation nevertheless reduces to conventional stochastic thermodynamics with time-dependent rates satisfying local detailed balance, when the QME is represented in the time dependent basis diagonalizing the system density matrix. We illustrate our findings by considering transport through a parallel double quantum dot junction with degenerate levels, where the coupling to two different environments may drag the system towards a pure state.

DY 17.11 Tue 12:45 H48

Causal Entropic Forces: Dynamics and Pattern Formation — •Hannes Hornischer, Stephan Herminghaus, and Marco G. Mazza — MPI for Dynamics and Self-Organization, Göttingen

One basic principle of evolution is survival, that is, organisms distance themselves from situations threatening their physical health and thereby enlarge their accessible space of possible futures. We use a path-based entropy, causal entropy, which can be viewed as a measure for the diversity of future options, and examined the dynamics of a particle solely driven by a causal entropic force towards states of highest entropy production. Without any extra information about the system and solely due to entropic force those particles are able to

adapt to changes in their environment, overcome potential barriers, find the fastest escape paths in evacuation scenarios. Many particles in a confined space would develop stable spatial patterns. This basic and general approach has the potential to give deeper understanding in social interactions in the context of behavioral ecology, for example applied to insects, fish or humans.

DY 17.12 Tue 13:00 H48

Switching kinetics of a roadblock particle in an exclusion process — •Mamata Sahoo[1] and Stefan Klumpp[2,3] — [1]Computational Modelling & Simulation Section, National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram - 695019, India — [2]Department of Theory and Bio-Systems, Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany — [3]Institute for Nonlinear Dynamics, Georg August University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Motivated by complex transport processes occurring in nature, we study the switching dynamics of a "roadblock" particle in a totally asymmetric simple exclusion process (TASEP). The roadblock particle blocks the traffic of moving particles while bound to the lattice, but can stochastically unbind or switch off, thus enabling the traffic to pass. We use simulations to study the dependence of the particle flux on the on/off switching dynamics of the roadblock, which exhibits a surprisingly rich dynamic behaviour. In particular, unlike in other studied TASEP variants with defects, here we observe that the particle flux is affected by the roadblock even in the initiation-limited or low density phase if the roadblock dynamics is slow. Rapid switching off the roadblock results in the typical behaviour of a TASEP with a defect/pause with reduced maximal current, but no effect of the roadblock on the flux in the initiation-limited phase. Moreover, in an intermediate range of roadblock rates, the particle current is found to be system-size dependent.

DY 18: Statistical Physics of Biological Systems I (Joint Session with DY)

Joint session with DY organized by BP.

Time: Tuesday 12:00–13:00 Location: H43

DY 18.1 Tue 12:00 H43

Interplay of directed transport and diffusive motion inside cellular protrusions — •Isabella Krämer and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität, München, Deutschland

Linear cellular protrusions are characterized by their finger-like structure that is connected to the cell body at one end, the base, and extends into the surroundings at the other end, the tip. A membrane enclosing the protrusion separates the inside from the extracellular and prevents in- and outflux other than at the base. Inside the protrusion bundles of parallel actin filaments are embedded into cytoplasm so that different types of motion interact: directed transport of cargo towards the tip on the actin filaments and diffusive motion inside the cytoplasm.

Motivated by this biological process we study the steady-state behaviour of a totally asymmetric simple exclusion process (TASEP) that is weakly coupled to different diffusive environments and focus on systems that are closed at the tip of the TASEP. We derive an exact equation that relates the average total occupation on the TASEP to the average total occupation on the diffusive lattice coupled to it. This mass balance equation represents a global detailed balance for the exchange between the two lattices, where detailed balance does not hold locally for any pair of sites but for the two lattices in total. We show that the steady-state profile on the TASEP is given by a localized domain wall whose position can be determined using the mass balance equation. By further exploiting this equation we find an analytic expression for the nearest-neighbour correlations on the TASEP.

DY 18.2 Tue 12:15 H43

Physical driving of chemical reactions — •Vladimir Palyulin and Ulrich Gerland — Theory of Complex Biosystems, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Out-of-equilibrium physical processes can generate a chemical disequilibrium, if a suitable coupling mechanism exists. Such a physical driving of chemical reactions is relevant in contexts ranging from prebiotic evolution to atmospheric chemistry. Inspired by recent microfluidic experiments, we introduce a minimal model that couples biased diffusion as a generic form of physical non-equilibrium to reversible dimerization as the simplest nonlinear reaction. The model demonstrates explicitly that the effective coupling strength, i.e. the amplitude of the chemical response to a given amount of physical driving, depends on the boundary conditions as well as the relative speeds of the physical and chemical kinetics.

DY 18.3 Tue 12:30 H43

Growth and Division of Active Droplets: A Model for Protocells — David Zwicker[1,2], •Rabea Seyboldt[1], Christoph A. Weber[1], Anthony A. Hyman[3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA — [3]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany

It has been proposed that during the early steps in the origin of life, small droplets could have formed by phase separation from a surrounding complex mixture. These droplets could have provided chemical reaction centers to generate and evolve organic molecules. However, whether these droplets could divide and propagate is unclear. Here we study the dynamics of such droplets by combining the physics of phase separation with chemical reactions that are maintained away from thermodynamic equilibrium by an external supply of energy. Outside the droplets, these reactions turn precursors into droplet material, which then gets incorporated into droplets, where it is eventually converted into a waste product that leaves the droplet. Surprisingly, our theoretical study shows that the resulting chemically driven fluxes can lead to shape instabilities that trigger division of droplets into two smaller daughters, which can then grow again. Therefore, chemically active droplets can exhibit cycles of growth and division that resemble the proliferation of living cells. Dividing active droplets could serve as a model for prebiotic protocells, where chemical reactions in the droplet play the role of a prebiotic metabolism.

DY 18.4 Tue 12:45 H43

Robustness of nucleosome patterns in the presence of DNA sequence-specific free energy landscapes and active remodeling — •Johannes Nuebler[1], Benedikt Obermayer[2], Wolfram Moebius[3], Michael Wolff[1], and Ulrich Gerland[1] — [1]Physik-Department, TU München, James-Franck-Str. 1, 85748 Garching — [2]Max-Delbrück-Center for Molecular Medicine, Robert-Rössle-Str. 10, 13125 Berlin — [3]Department of Physics, Harvard University, Cambridge, MA 02138, USA

Proper positioning of nucleosomes in eukaryotic cells is important for transcription regulation. When averaged over many genes, nucleosome positions in coding regions follow a simple oscillatory pattern, which is described to a surprising degree of accuracy by a simple one-dimensional gas model for particles interacting via a soft-core repulsion. The quantitative agreement is surprising given that nucleosome positions are known to be determined by a complex interplay of mechanisms including DNA sequence-specific nucleosome affinity and active repositioning by remodeling enzymes. We rationalize the observed robustness of the simple oscillatory pattern by showing that the main effect of several known nucleosome positioning mechanisms is a renormalization of the particle interaction. For example, "disorder" from sequence-specific affinities leads to an apparent softening, while active remodeling can result in apparent softening for directional sliding or apparent stiffening for clamping mechanisms. We suggest that such parameter renormalization can explain the apparent difference of nucleosome properties in two yeast species, S. cerevisiae and S. pombe.

DY 19: Transport: Fluctuation and Noise (Joint session of DY and TT organized by TT)

Time: Tuesday 14:00–15:45 Location: H23

DY 19.1 Tue 14:00 H23

Super-Poissonian shot noise of squeezed-magnon mediated spin transport — •Akashdeep Kamra and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

The magnetization of a ferromagnet (F) driven out of equilibrium injects pure spin current into an adjacent conductor (N). Such F|N bilayers have become basic building blocks in a wide variety of spin based devices. We evaluate the shot noise of the spin current traversing the F|N interface when F is subjected to a coherent microwave drive. We find that the noise spectrum is frequency independent up to the drive frequency, and increases linearly with frequency thereafter. The low frequency noise indicates super-Poissonian spin transfer understood in terms of dipolar interaction mediated squeezing of F eigenmodes, which results in quasi-particles with effective spin $\hbar^* = \hbar(1+\delta)$. For experimentally relevant parameters, we estimate $\delta \approx 0.4$ for yttrium iron garnet and $\delta \approx 3.0$ for iron thin films. The spontaneous squeezing of F eigenmodes suggests novel possibilities for their applications in quantum optics and related fields.

DY 19.2 Tue 14:15 H23

Statistics of transmission eigenvalues in diffusive star-shaped multi-terminal structures — •Sven Essert, Viktor Krueckl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We study transport in diffusive star-shaped devices with more than two leads. We find that the eigenvalue distribution $p(t)$ of the transmission matrix between any pair of terminals is typically not showing the bimodal distribution that is found in two-lead devices. Instead, the distribution displays a cutoff t_c, i. e., $p(t) = 0$ for $1 \geq t \geq t_c$. We explain the origin of this cutoff by deriving analytical expressions in the limit of low transmission for fully symmetric stars and for some limiting cases of extreme asymmetry. Using numerical calculations we probe the validity of these results away from the low-transmission limit.

In addition, we note that the bimodal distribution can be recovered when combining the leads of the star into meta leads in such a way that the total number of such meta leads is two. Then the transport between these is again bimodal, thus showing "open channels" with transmissions close to 1. Related to this, we propose the study of a new observable, which we call eigenvector splitting, that quantifies the distribution of outgoing flux among the constituent leads of the meta lead. This quantity becomes particularly interesting, when studying devices in the low-transmission limit, where it directly relates to the eigenvalue distribution. We present analytical solutions for the eigenvector splitting in some limiting geometries and supplement them by numerical calculations.

DY 19.3 Tue 14:30 H23

Detection of interactions via generalized factorial cumulants in systems in and out of equilibrium — •Philipp Stegmann[1], Björn Sothmann[2], Alfred Hucht[1], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

We introduce time-dependent, generalized factorial cumulants $C_s^m(t)$ of the full counting statistics of electron transfer as a tool to detect interactions in nanostructures [1]. The violation of the sign criterion $(-1)^{m-1}C_s^m(t) \geq 0$ for *any* time t, order m, and parameter s proves the presence of interactions. For given system parameters, there is a minimal time span $t_{\min}$ and a minimal order m to observe the violation of the sign criterion. We demonstrate that generalized factorial cumulants are more sensitive to interactions than ordinary ones [2, 3] and can detect interactions even in regimes where ordinary factorial cumulants fail. We illustrate our findings with the example of a quantum dot tunnel coupled to electronic reservoirs either in or out of equilibrium.

[1] P. Stegmann, B. Sothmann, A. Hucht, and J. König, PRB **92**, 155413 (2015)
[2] D. Kambly, C. Flindt, and M. Büttiker, PRB **83**, 075432 (2011)
[3] D. Kambly and C. Flindt, J. Comput. Electron. **12**, 331 (2013)

DY 19.4 Tue 14:45 H23

Time-resolved statistics of entangled photon pairs in Josephson photonics — •Simon Dambach, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany

The interplay of the tunneling transfer of charges and the emission and absorption of light can be investigated in a setup where a voltage-biased Josephson junction is placed in series to a microwave resonator. Such circuits combine phenomena and observational tools originally known from the fields of charge transfer physics and quantum optics (Josephson photonics). Due to the inherent nonlinearity of the Josephson junction, tunneling Cooper pairs can create a variety of nonclassical states of light. This is reflected in form of characteristic signatures in the second-order correlation function $g^{(2)}(\tau)$ and the waiting-time distribution $w(\tau)$. We find that this device represents a versatile source of nonconventional light which can be tuned from photon-pair creation and strong bunching to single-photon creation and complete antibunching [1].

In this talk, we will investigate theoretically the simultaneous creation of two photons within different modes and, in particular, address the question of intermode entanglement by means of different entanglement witnesses.

[1] S. Dambach et al., PRB **92**, 054508 (2015).

Invited Talk DY 19.5 Tue 15:00 H23

Dynamical Coulomb Blockade theory of resonantly enhanced light emission from a tunnel junction — •Wolfgang Belzig[1], Fei Xu[1], and Cecilia Holmqvist[2] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

Inelastic tunneling of electrons generates emission of photons, whose energies intuitively should be limited by the applied bias voltage. However, experiments indicate that more complex processes involving the interaction of electrons with plasmon polaritons lead to photon emission characterized by over-bias energies. We have proposed a model of this observation [1] in analogy to the dynamical Coulomb blockade, originally developed for treating the electronic environment in mesoscopic circuits, and explained the experimental finding quantitatively by the correlated tunnelling of two electrons interacting with an LRC circuit modelling the local plasmon-polariton mode. Furthermore, we calculate the over-bias emission at finite temperature and discuss the possibility of non-classical light emission.

[1] F. Xu, C. Holmqvist, W. Belzig, PRL **113**, 066801 (2014).

DY 19.6 Tue 15:30 H23

Correlations of weak quantum measurements in a non-Markovian detection scheme — •Johannes Bülte[1], Adam Bednorz[2], Christoph Bruder[3], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Faculty of Physics, University of Warsaw, PL02-093 Warsaw, Poland — [3]Department of Physics, University of Basel, CH-4056 Basel, Switzerland

Generalized quantum measurement schemes are described by positive operator-valued measures that go beyond the projection postulate, i.e., the instantaneous collapse of the systems' wave function by the measurement. They allow to consider the noninvasive limit of so-called weak measurements, and, in particular, to investigate the correlations of several such measurements which permits the tracking of non-commuting observables. We propose a scheme in which the detectors are coupled to the measured system for a finite time which leads to non-Markovian effects [1]. We derive microscopic expressions for the memory functions which are related to the Kubo linear-response formalism. The deviations from the standard Markovian measurement with symmetrized operator order (Keldysh ordering) can be traced back to a detector-detector interaction mediated by the measured system. Finally, we discuss different detector types, and show that an appropriate choice enables e.g. the proof of the non-classical nature of a system by second-order correlation functions.

[1] A. Bednorz, C. Bruder, B. Reulet, and W. Belzig, PRL **110**, 250404 (2013)

DY 20: Chimera State: Symmetry breaking in dynamical networks (joint session DY/SOE accompanying symposium SYCS)

Time: Tuesday 14:00–15:00 Location: H36

DY 20.1 Tue 14:00 H36

Controlling Chimera States - The influence of excitable units — •Philipp Hövel[1,2], Thomas Isele[1], Johanne Hizanidis[3,4], and Astero Provata[3] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, Humboldt Universität zu Berlin, Germany — [3]National Center for Scientific Research "Demokritos", Athen, Greece — [4]Crete Center for Quantum Complexity and Nanotechnology, University of Crete, Heraklion, Greece

We explore the influence of a block of excitable units on the existence and behavior of chimera states in a nonlocally coupled ring-network of FitzHugh-Nagumo elements. The FitzHugh-Nagumo system, a paradigmatic model in many fields from neuroscience to chemical pattern formation and nonlinear electronics, exhibits oscillatory or excitable behavior depending on the values of its parameters. Until now, chimera states have been studied in networks of coupled oscillatory FitzHugh-Nagumo elements. In the present work, we find that introducing a block of excitable units into the network may lead to several interesting effects. It allows for controlling the position of a chimera state as well as for generating a chimera state directly from the synchronous state.

DY 20.2 Tue 14:15 H36

Stability analysis of long-living transient amplitude chimeras — •Liudmila Tumash, Anna Zakharova, Judith Lehnert, and Eckehard Schöll — Institut für Theoretische Physik,TU-Berlin, Hardenbergstr 36, 10623 Berlin, Germany,

Chimera states are characterized by a spontaneous break-up of a network of identical elements into coexisting domains of coherent (synchronized) and incoherent (desynchronized) dynamics. We study networks with coupled phase and amplitude dynamics. In contrast to classical phase chimeras, pure amplitude chimeras exhibit domains of coherent and incoherent dynamics with respect to the amplitude, but the phases are always regular and correlated. These states are long-living transients. In this work we investigate networks of Stuart-Landau oscillators with symmetry-breaking non-local coupling, in which amplitude chimeras can occur [1]. We verify the hypothesis that amplitude chimeras represent saddle-states in a high-dimensional phase space by calculating the Floquet exponents and the corresponding Floquet eigenvectors. In this way we can explain the dependence of the transient times upon coupling strength, coupling range and network size.

[1] A. Zakharova, M. Kapeller, E. Schöll, Phys. Rev. Lett. **112**, 154101 (2014).

DY 20.3 Tue 14:30 H36

Chimera patterns under the impact of noise — •Sarah A. M. Loos[1], Jens Christian Claussen[2], Eckehard Schöll[1], and Anna Zakharova[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany — [2]Computational Systems Biology Lab, Campus Ring 1, Jacobs University Bremen, D- 28759 Bremen, Germany

We investigate two types of chimera states, i.e., patterns consisting of coexisting spatially separated domains with coherent and incoherent dynamics, under the influence of noise [1]. Both chimera states arise in ring networks of Stuart-Landau oscillators with symmetry-breaking coupling [2]. Amplitude chimeras are characterized by temporally periodic dynamics throughout the whole network, but spatially incoherent behavior with respect to the amplitudes in a part of the system. They are long-living transients. Chimera death states generalize chimeras to stationary inhomogeneous patterns (oscillation death), which combine spatially coherent and incoherent domains. We analyze the impact of random perturbations on their occurrence and on their lifetimes, addressing the question of robustness of chimera states in the presence of additive white noise.

[1] S. A. M. Loos et al., arXiv:1508.04010v2, (2015).
[2] A. Zakharova et al., Phys. Rev. Lett. 112, 154101 (2014).

DY 20.4 Tue 14:45 H36

A classification scheme of chimera states — •Felix P. Kemeth[1,2], Sindre W. Haugland[1,2], Lennart Schmidt[1], Ioannis G. Kevrekidis[2,3], and Katharina Krischer[1] — [1]Physik-Department, Nonequilibrium Chemical Physics, Technische Universität München, James-Franck-Str. 1, D-85748 Garching, Germany — [2]TUM Institute for Advanced Study, Lichtenbergstraße 2a, D-85748 Garching, Germany — [3]The Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544, USA

The vast and continuously growing number of chimera or chimera-like states discovered in recent years demands a classification of the various manifestations of these dynamical hybrid states. We propose systematic and reductive approaches to characterize chimera states in systems with and without spatial extent, respectively. For locally and non-locally coupled systems, that is for systems involving a spatial extension, we apply a discrete version of the Laplace operator on spatio-temporal data sets exhibiting coexistence of coherent and incoherent regions. Regarding its statistical properties we introduce a detailed classification of chimera states into groups sharing the same qualitative behavior. For globally coupled systems without a spatial dimension, the statistics of pairwise Euclidean distances between all oscillators allow a similar analysis. This classification helps clarify the different facets of chimera states and broadens our understanding of this peculiar phenomenon.

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

Time: Tuesday 14:00–15:15 Location: H46

DY 21.1 Tue 14:00 H46

Rheo-Chaos of Frictional Grains — •Matthias Grob, Annette Zippelius, and Claus Heussinger — Institut für Theoretische Physik, Georg-August Universität, Göttingen, Deutschland

A two-dimensional dense fluid of frictional grains is shown to exhibit time-chaotic, spatially heterogeneous flow in a range of stress values, σ, chosen in the unstable region of s-shaped flow curves. Stress controlled simulations reveal a phase diagram with reentrant stationary flow for small and large stress σ. In between no steady flow state can be reached, instead the system either jams or displays time dependent heterogeneous strain rates $\dot{\gamma}(\mathbf{r}, t)$. The results of simulations are in agreement with the stability analysis of a simple hydrodynamic model, coupling stress and microstructure which we tentatively associate with the frictional contact network.

DY 21.2 Tue 14:15 H46

From classical to quantum and back: A Hamiltonian scheme for adaptive multi-resolution classical/path integral simulations — •Karsten Kreis[1,2], Mark E. Tuckerman[3,4,5], Davide Donadio[1,6], Kurt Kremer[1], and Raffaello Potestio[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Department of Chemistry, New York University (NYU), New York, NY 10003, USA — [4]Courant Institute of Mathematical Sciences, NYU, New York, NY 10012, USA — [5]NYU-East China Normal University Center for Com-

putational Chemistry at NYU Shanghai, Shanghai 200062, China — [6]Department of Chemistry, University of California Davis, One Shields Ave., Davis, CA 95616, USA

Quantum delocalization of atomic nuclei affects the physical properties of many hydrogen-rich liquids and biological systems. To accurately model these effects, Feynman's path integral formulation of quantum statistical mechanics is typically employed, which implies a substantial increase in computational overhead. By restricting the quantum description to a small spatial region, this cost can be significantly reduced. Herein, we derive and validate a rigorous, Hamiltonian-based scheme that allows molecules to change from quantum to classical and vice versa on the fly as they diffuse through the system, both reducing overhead and making quantum grand-canonical simulations possible. Our adaptive resolution approach paves the way to efficient quantum simulations of biomolecules, membranes, and interfaces.

DY 21.3 Tue 14:30 H46

All-Atom and Coarse-Grained Molecular Dynamics Simulation of Ionic Liquids — •Tamisra Pal and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstrasse 6, 64289 Darmstadt

Room temperature Ionic Liquids (RTILs) have garnered much interest in the last few years as they possess tremendous potential for application in industry as reaction media. The high complexity of these liquids originating from their self-assembly or nano-scale aggregate formation motivates us to understand more on their dynamics. We have employed molecular dynamics simulation for RTILs to connect the length and time scales of simulation models with different levels of molecular resolution provided by the mapping scheme. Specifically, we have investigated a coarse grained (CG) model of 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][PF_6]) and its all-atom (AA) description, at various temperatures. In this way, we unravel the different dynamical modes associated with dynamic heterogeneity and structural relaxation and we quantitatively compare the characteristic time scales from the two model systems to ascertain the effects of coarse graining on the dynamical behavior. The spatial and temporal aspects of molecular dynamics have been studied via calculating non-Gaussian parameters, particle displacement distributions, overlap functions and dynamic susceptibilities. Our simulation results provide a microscopic understanding to the presence of "fast" and "slow" moving particles contributing to dynamic heterogeneity and their relevance for the structural relaxation of ionic liquids.

DY 21.4 Tue 14:45 H46

Equilibrium interfacial free energies and Turnbull coefficient for bcc crystallizing colloidal charged sphere suspensions — •Thomas Palberg[1], Patrick Wette[2,3], and Dieter M. Herlach[2] — [1]Institut f. Physik, Johannes Gutenberg Universität, 55099 Mainz, Germany — [2]Institut f. Materialphysik im Weltraum, DLR, 51147 Köln, Germany — [3]Space Administration, DLR, 53227 Bonn, Germany

The interfacial free energy (IFE) is a central quantity in crystallization from the meta-stable melt. In suspensions of charged colloidal spheres, nucleation and growth kinetics can be accurately measured from optical experiments. We here re-analyze the strictly linear increase of previously reported CNT-effective non-equilibrium IFEs estimated from such experimentsutilizing classical nucleation theory (CNT). For five aqueous suspensions of charged spheres and one binary mixture, we utilize a simple extrapolation scheme and interpret our findings in view of Turnbull's empirical rule. Our first estimates for the reduced equilibrium IFE, $\sigma_{0,bcc}$, between coexisting fluid and bcc-crystal phases are on the order of a few k_BT. Their values are not correlated to any of the electrostatic interaction parameters but rather show a systematic decrease with increasing size polydispersity and a lower value for the mixture as compared to the pure components. At the same time, σ_0 shows an approximately linear correlation to the entropy of freezing. The equilibrium interfacial free energy of strictly monodisperse charged spheres may therefore be still greater.

DY 21.5 Tue 15:00 H46

Size matters: can we use a Hamiltonian adaptive resolution scheme to simulate an open system? — •Robinson Cortes-Huerto, Maziar Heidari, and Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz, Germany

Finite size effects are ubiquitous in molecular dynamics simulations. Apart from the obvious implicit size effects due to periodic boundary conditions, explicit size effects are consequence of simulating a fixed and relatively small number of particles. In particular, measurements of density fluctuations within a sub-domain of a periodic simulation box are strongly dependent on the sub-domain size. These effects can be neglected by carrying out computer simulations for extremely large systems. An alternative solution is to use the Hamiltonian adaptive resolution scheme (H-AdResS), where the computational cost reduces substantially by embedding a relatively small high resolution portion of the system in a larger region at low resolution. Our main goal is to explore the viability to perform grand canonical simulations using this dual-resolution approach. In particular, we propose to use H-AdResS to calculate thermodynamic properties of prototypical molecular liquids in an effective open boundary simulation framework. To this end, we calculate Kirkwood-Buff integrals that connect radial distribution functions, available from molecular dynamics simulations, to thermodynamic properties such as the isothermal compressibility. We compare these results with measurements performed in the fully atomistic case and assess whether an adaptive resolution simulation reproduces the behaviour expected from an open simulation setup.

DY 22: Anomalous Diffusion (joint session DY/BP)

Time: Tuesday 14:00–15:30 Location: H47

DY 22.1 Tue 14:00 H47

Diffusion and subdiffusion of interacting particles on comb-like structures — •Pierre Illien[1], Olivier Bénichou[2], Gleb Oshanin[2], Alessandro Sarracino[2], and Raphaël Voituriez[2] — [1]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK — [2]Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre-et-Marie-Curie, Paris, France

The subdiffusive motion of tracers in crowded media, e.g., biological cells, is widespread, and has motivated a large amount of theoretical work related to diffusion in complex media. Comblike structures have received a particular interest as they constitute minimal models of systems with geometrical constraints. Here, we investigate the effect of excluded-volume interactions on tracer diffusion on such lattices.

We study the dynamics of a tracer particle (TP) on a comb lattice populated by randomly moving hardcore particles. When the TP is constrained to move on the backbone of the comb and in the limit of high density of the particles, we present exact analytical results for the cumulants of the TP position, showing a subdiffusive behavior $t^{3/4}$. At longer times, a second regime is observed where standard diffusion is recovered, with a surprising nonanalytical dependence of the diffusion coefficient on the particle density. When the TP is allowed to visit the teeth of the comb, we unveil a rich and complex scenario with several successive subdiffusive regimes, resulting from the coupling between the geometrical constraints of the lattice and particle interactions. In this case, remarkably, the presence of hard-core interactions asymptotically speeds up the TP motion along the backbone of the structure.

DY 22.2 Tue 14:15 H47

Anomalous transport of circular swimmers in disordered structures: classical edge-state percolation — •Thomas Franosch[1], Walter Schirmacher[2], Benedikt Fuchs[3], and Felix Höfling[4] — [1]UIBK Innsbruck — [2]Universität Mainz — [3]Med.-Uni Wien — [4]FU Berlin

Recently micron-sized self-propelled particles have been realized as model systems [1] for complex living organisms such as bacteria. If the agent is asymmetric a natural circular motion [2] emerges which yields characteristic skipping orbits when interacting with boundaries.

Here, we investigate by molecular dynamics simulations the dynamics of circular swimmers in a two-dimensional model with randomly distributed scatterers. For small radii of the swimming motion the agents orbit only around isolated clusters of scatterers, while at large radii diffusive behavior emerges. A de-localization transition occurs which is generated by percolating skipping orbits along the edges of

obstacle clusters. Directly at the transition the mean-square displacements displays subdiffusive transport. The dynamic exponents differ from those of the conventional transport problem on percolating systems, thus establishing a new dynamic universality class [3]. Last, we draw an analogy to the field-induced localization transition in magnetotransport in 2D electron gases in a disordered array of antidots.

[1] F. Kümmel, et al., Phys. Rev. Lett. **110**, 198302 (2013).

[2] S. van Teeffelen and H. Löwen, Phys. Rev. E **78**, 020101(R) (2008).

[3] W. Schirmacher, B. Fuchs, F. Höfling, and T. Franosch, Phys. Rev. Lett. (2015, in print).

DY 22.3 Tue 14:30 H47

Scales of Function Spaces for Weyl Fractional Calculus — •Tillmann Kleiner and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

Anomalous diffusion models are frequently based on fractional differential equations [1]. Analytical investigations of these mathematical models require suitable function spaces on which the fractional derivatives operate as continuous operators. This contribution introduces function spaces suitable for Weyl fractional calculus. Scales of locally convex spaces with topology generating seminorms are constructed using weighted maximal functions. These scales are sets of spaces partially ordered by inclusion. Minimal and maximal spaces with respect to this ordering are determined such that Weyl fractional derivatives operate on them continuously or isomorphically. Such spaces can also be determined for sets of linear combinations of these operators with orders restricted to some fixed subset of $\mathbb{C}$. Inclusions of spaces within the scale correspond to continuous injections with dense range. As a result the investigated operators and their inverses are continuous extensions from the subspace of test functions for all suitable spaces.

[1] *Applications of Fractional Calculus in Physics*, edited by R. Hilfer (World Scientific, Singapore, 2000).

DY 22.4 Tue 14:45 H47

A simple non-chaotic map generating subdiffusive, diffusive, and superdiffusive dynamics — Lucia Salari[1], Lamberto Rondoni[1,2], Claudio Giberti[3], and •Rainer Klages[4,5] — [1]Dipartimento di Scienze Matematiche, Politecnico di Torino — [2]GraphenePoliTO Lab, Politecnico di Torino and INFN Sezione di Torino — [3]Dipartimento di Scienze e Metodi dell' Ingegneria, Universita di Modena e Reggio E. — [4]Max Planck Institute for the Physics of Complex Systems, Dresden — [5]School of Mathematical Sciences, Queen Mary University of London

Consider equations of motion that generate dispersion of an ensemble of particles in the long time limit. An interesting problem is to predict the diffusive properties of such a dynamical system starting from first principles. Motivated by numerical results on diffusion in polygonal billiards, we introduce an interval exchange transformation lifted onto the whole real line that mimicks deterministic diffusion in these billiards. By definition our simple map model is not chaotic, in the sense of exhibiting a vanishing Lyapunov exponent. We show analytically that it nevertheless displays a whole range of normal and anomalous diffusion under variation of a single control parameter [1].

[1] L. Salari et al., Chaos **25**, 073113 (2015)

DY 22.5 Tue 15:00 H47

Localisation of ballistic tracers in the two-dimensional Lorentz model interpreted as a renormalisation group flow — •Felix Höfling — Fachbereich Mathematik und Informatik, Freie Universität Berlin — Max-Planck-Institut für Intelligente Systeme, Stuttgart, und IV. Institut für Theoretische Physik, Universität Stuttgart

The Lorentz model serves as a minimal model to explain many facets of the rich phenomenology of anomalous transport, as frequently observed in porous materials and cellular transport [1]. Here, I will discuss the localisation transition of "ballistic" tracers (subject to Newton's equations of motion) in the two-dimensional, overlapping Lorentz model. Extensive simulations provide evidence for the universality of the dynamic critical exponent, which has been crucial in the interpretation of recent studies [2,3]. The long-time asymptotes, however, are obscured by non-universal corrections to scaling, explaining the contradicting values for the diffusivity exponent in the literature. A spectral analysis of the obtained correlation functions allows for an interpretation of the dynamics as an renormalisation flow of the transport at long times and gives insight into the fixed point structure of the RG flow.

[1] F. Höfling and T. Franosch, Rep. Prog. Phys. **76**, 046602 (2013).

[2] S. K. Schnyder, M. Spanner, F. Höfling, T. Franosch, and J. Horbach, Soft Matter **11**, 701 (2015).

[3] W. Schirmacher, B. Fuchs, F. Höfling, and T. Franosch, arXiv:1511.05218, Phys. Rev. Lett. in print (2015).

DY 22.6 Tue 15:15 H47

Non-adiabatic quantum pumping by a randomly moving quantum dot [1] — •Daniel Waltner[1] and Stanislav Derevyanko[2] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel

We look at time dependent fluctuations of the electrical charge in an open 1D quantum system represented by a quantum dot experiencing random lateral motion. In essentially non-adiabatic settings we study both diffusive and ballistic (Levy) regimes of the barrier motion where the electric current as well as the net pumped electric charge experience random fluctuations over the static background. We show that in the large-time limit, the wavefunction is naturally separated into the Berry-phase (BP) 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). Based on this separation we report two key results: firstly, the disorder averaged wave function and current are asymptotically mainly determined by the same BP contribution that applies in the case of adiabatic motion. Secondly, after a short transition period the pumped electric charge exhibits fluctuations that grow much faster than predicted by the adiabatic theory. We also derive the exact expressions for the average propagator (in the co-moving basis representation) for the diffusive and ballistic types of motion considered.

[1] S. Derevyanko, D. Waltner, J. Phys. A **48** (2015) 305302

DY 23: Quantum Dynamics, Decoherence and Quanten Information

Time: Tuesday 14:00–15:15 Location: H48

DY 23.1 Tue 14:00 H48

Distortion of a reduced equilibrium density matrix — •Iris Schwenk and Michael Marthaler — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie

We study a system coupled to external degrees of freedom, called bath, where we assume that the total system, consisting of system and bath is in equilibrium. An expansion in the coupling between system and bath leads to a general form of the reduced density matrix of the system as a function of the bath selfenergy. The coupling to the bath results in a renormalization of the energies of the system and in a change of the eigenbasis. We study the influence of bosonic degrees of freedom on the state of a six qubit system similar to the eight qubit unit cell of a quantum annealing processor examined by Lanting et al.[1].

[1] T. Lanting et al., Phys. Rev. X 4, 021041 (2014).

DY 23.2 Tue 14:15 H48

Diagrammatic description of a quantum system coupled to strong noise — •Michael Marthaler and Juha Leppäkangas — Karlsruhe Institute of Technology

We study a system-bath description in the strong coupling regime, where it is not possible to derive a master equation for the reduced density matrix by a direct expansion in the system-bath coupling. A particular example is a bath with significant spectral weight at low frequencies. Through a unitary transformation it can be possible to find a more suitable small expansion parameter. Within this approach we construct a formally exact expansion of the master equation on the Keldysh contour. The lowest-order expansion is similar to the so-called P(E)-theory or non-interacting blip approximation (NIBA). The analysis of the higher-order contributions shows that there are two different classes of higher-order diagrams. We study how the form of the spectral function affects their convergence.

DY 23.3 Tue 14:30 H48

Lindblad dynamics of Gaussian states in the semiclassical limit — •Bradley Longstaff[1], Eva-Maria Graefe[1], and Roman Schubert[2] — [1]Imperial College London, UK — [2]University of Bristol, UK

The time evolution of wave packets forms the basis of many semiclassical methods for closed systems. An important ingredient is Heller's method in which the centre of a wave packet moves along a classical trajectory and the width follows a linearised classical flow. Here this method is extended to open systems described by the Lindblad equation. By considering Gaussian Wigner functions, semiclassical equations of motion are derived for both the centre of the wave packet and the covariance matrix. The approximation is exact for maximally quadratic Hamiltonians and linear Lindblad operators. As an illustration, the Gross-Pitaevskii equation for a Bose-Einstein condensate in an optical lattice with particle losses is derived.

DY 23.4 Tue 14:45 H48

A positive tensor network approach for simulating open quantum many-body systems — •Albert H. Werner[1], Daniel Jaschke[2], Pietro Silvi[3], Martin Kliesch[1], Tommaso Calarco[3], Jens Eisert[1], and Simone Montangero[3] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [2]Department of Physics, Colorado School of Mines, Golden, Colorado 80401, USA — [3]Institute for Complex Quantum systems (ICQ), Universität Ulm, 89069 Ulm, Germany

Open many-body quantum systems play an important role in quantum optics and condensed-matter physics, and capture phenomena like transport, interplay between Hamiltonian and incoherent dynamics, and topological order generated by dissipation. We introduce a versatile and practical method to numerically simulate one-dimensional open quantum many-body dynamics using tensor networks. It is based on representing mixed quantum states in a locally purified form, which guarantees that positivity is preserved at all times. Moreover, the approximation error is controlled with respect to the trace norm. Hence, this scheme overcomes various obstacles of the known numerical open-system evolution schemes.

DY 23.5 Tue 15:00 H48

Simulation of Heat Transfer in Quantum Chains Far From Equilibrium — •Thomas Motz, Joachim Ankerhold, and Jürgen T. Stockburger — Institute for Complex Quantum Systems, Ulm University, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

We study heat exchange in open harmonic quantum chains by means of a scalable method also for large system sizes and long relaxation times. Starting from a stochastic Liouville-von Neumann equation that models the coupling of systems to quantum reservoirs by an exact c-number representation [1], we turn this approach to a deterministic set of equations correctly accounting for system-bath correlations for any combinations of harmonic systems arbitrarily strong coupled to ohmic reservoirs [2].

We investigate the time-dependence of the energy fluxes and the corresponding steady-states for various couplings, dampings and temperatures [3,4]. A distinct sensitivity of the fluxes with respect to couplings and impurities is found while correlations reveal a ballistic behavior and recurrence effects for a mismatch of coupling strengths and damping.

[1] J. T. Stockburger and H. Grabert, PRL 88, 170407 (2002).
[2] J. Ankerhold and J. P. Pekola, PRB 90, 075421 (2014).
[3] R. Schmidt et al., PRL 107, 130404 (2011).
[4] R. Schmidt et al., PRA 88, 052321 (2013).

DY 24: Networks: From Topology to Dynamics II (joint session SOE / DY / BP)

Time: Tuesday 15:00–15:45 Location: H36

DY 24.1 Tue 15:00 H36

Collective Failure due to Multistability in Oscillator Networks and Power Grid — •Debsankha Manik[1], Dirk Witthaut[2], and Marc Timme[1] — [1]Network Dynamics Group, Max Planck Institute for Dynamics anf self-Organization, 37077 Göttingen — [2]Forschungszentrum Jülich, Institute of Energy and Climate Research Systems Analysis and Technology Evaluation (IEK-STE), 52425 Jülich

Networks of phase oscillators model the collective dynamics of various interacting physical and biological systems, ranging from electric power grid operation to neuronal rhythms. Here we show that the number of stable steady states in phase oscillator systems scales with the length of the topological cycles in the network such that for non-global coupling, multistable steady states may emerge. The clustering of similar natural frequencies favour fewer stable states, whereas homogeneous frequency distributions favour more. Intriguingly, multistability prevails even under conditions for which stable states have been claimed to be unique. This multistability may have significant impact on the collective dynamics of such networks: for example, in power grids where the transmission lines have structural limitations on the maximum load they can safely carry, perturbations may induce switching to different steady states, strongly alter the flow patterns, and in turn yield a collective failure of the grid.

Supported by the BMBF under grant no. 03SF0472E.

DY 24.2 Tue 15:15 H36

Geometric organization of real multiplex networks — •Kaj Kolja Kleineberg[1], Marian Boguna[1], M. Angeles Serrano[1], and Fragkiskos Papadopoulos[2] — [1]Departament de Fisica Fonamental, Universitat de Barcelona, Marti i Franques 1, 08028 Barcelona, Spain — [2]Department of Electrical Engineering, Computer Engineering and Informatics, Cyprus University of Technology

Real complex networks are organized to perform certain functions, among which targeted transport is important in a broad range of real systems, such as the Internet, social networks, or transportation networks. In reality, networks are not isolated entities but instead form interacting parts of larger and more complex systems. These systems are not a random combination of single networks, but instead are organized in a certain way. We investigate the geometric organization of multilayer networks and its implications. We find significant metric correlations between different layers. These correlations are key to answer many important questions concerning real multilayer systems. Metric correlations allow for inter-layer link prediction and the definition and detection of multidimensional communities. Metric correlations improve mutual greedy routing, that is targeted navigation in the whole multilayer system. Interestingly, only in the presence of metric correlations does the whole system outperform its single layers. We find that optimal correlations make multilayer systems perfectly navigable. Finally, we show how correlations present in the real Internet multiplex help navigating the digital world. Our findings have important implications for the design of real multilayer systems.

DY 24.3 Tue 15:30 H36

Interplay of shape and degree distribution in complex networks — •Robin de Regt and Christian von Ferber — Applied Mathematics Research Centre, Coventry University, UK

Complex networks are often described without geometry. Here, we explore possibilities of how an embedding of such networks in real space (e.g. 2D or 3D) may reveal interesting correlations between standard measures such as degree distributions and the shapes these structures may attain when embedded in a given space.

DY 25: Poster: Soft Matter Dynamics / Glasses

Time: Tuesday 18:15–21:00 Location: Poster B2

DY 25.1 Tue 18:15 Poster B2

Fragile-to-strong transition in liquid silica — •Julian Geske, Barbara Drossel, and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt

We investigate anomalies in liquid silica with molecular dynamics simulations and present evidence for a fragile-to-strong transition at around 3000K. To this purpose, we studied the structure and dynamical properties of silica over a wide temperature range, finding three indicators of the fragile-to-strong transition. First, there is a density minimum at around 3000K and a density maximum at 3400K. Second, the local structure characterized by the tetrahedral order parameter changes dramatically around 3000K and changes from a higher-ordered, lower-density phase to a less ordered, higher-density phase. Third, the correlation time τ changes from an Arrhenius behaviour below 3000K to a Vogel-Fulcher behaviour at higher temperatures.

DY 25.2 Tue 18:15 Poster B2

Molecular Mobility and Gas Transport Properties of PIM-1 and Nano composites based on PIM-1 and PhenethylPOSS — Nora Konnertz, Yi Ding, Martin Böhning, and •Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin

Polymers with intrinsic microporosity are of highly interest in the field of gas separation membranes. Especially the first synthesized PIM-1 shows extraordinary permeabilities and selectivities. Unfortunately, PIM-1 tends to physical aging and loses its good properties. Physical aging is related to the molecular mobility of PIM-1 which was here investigated by broadband dielectric spectroscopy (BDS). Besides the studies on pure PIM-1 a polyhedral oligomeric silsesquioxane with phenethyl substituents (PhenethylPOSS) was used as nanofiller (0 - 40 wt-%) in the PIM-1 matrix to improve the gas transport properties and prevent physical aging. The molecular mobility of the solution casted nano composite films was analyzed by BDS as well. Furthermore, gas transport properties were determined with the time lag method (0 - 20 bar) in a temperature range of 35°C to 65°C with N2, O2, CH4 and CO2.

DY 25.3 Tue 18:15 Poster B2

Dynamical coexistence in polydisperse hard spheres — •Matteo Campo and Thomas Speck — Institut für Physik, JGU Mainz, Germany

We investigate the slow dynamics of a model glass former, the polydisperse hard-sphere liquid, using a combination of molecular dynamics and importance sampling in the trajectory ensemble. According to dynamical facilitation theory, the glass transition takes place as a consequence of dynamical heterogeneity which develops as the liquid is quenched. We characterize dynamical heterogeneity by a parameter, the mobility, which quantifies how far particles move in the supercooled liquid. By studying trajectories longer than the structural relaxation time, we observe exponential tails in the probability distribution of mobility, which indicate phase coexistence of normal and exceptionally slow trajectories.

DY 25.4 Tue 18:15 Poster B2

Time needed to form stable glasses is comparable to β-relaxation time — •Yeong Zen Chua, Mathias Ahrenberg, and Christoph Schick — Institute of Physics, University of Rostock, Rostock 18051 Germany

Glasses produced by physical vapor deposition (PVD) exhibit different properties, depending on the deposition conditions. Consistent with previous works, glasses of ethylcyclohexane (ECH) vapor-deposited at temperature of about 0.85 of glass transition temperature, T_g observed to be the most stable glasses with low enthalpy, low heat capacity, high kinetic stability and high density. Isothermal transformation of the as-deposited glasses into the supercooled state is investigated for the deposition rate dependency, covering four orders of magnitude, at different substrate temperatures. The kinetic stability of the glasses (transformation time at 103 K) shows strong deposition rate dependency for lower substrate temperatures. The data provide an estimate for the substrate temperature dependent free surface residence time needed for the molecules in the assumed mobile surface layer to promote stable glass formation. Stable glasses are formed if this time is of the order of the β-relaxation time, many orders of magnitude faster than the α-relaxation at the substrate temperature. Stable glasses are observed even for substrate temperatures below the Vogel and the Kauzmann temperatures, indicating a full decoupling of the process of stable glass formation from the α-relaxation.

DY 25.5 Tue 18:15 Poster B2

Diffusion of PMMA: microgels and linear polymer — •Bastian Pur[1], Werner Köhler[1], Klaus Huber[2] und Martin Schneider[2] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Physikalische Chemie, Universität Paderborn, 33098 Paderborn, Germany

In present theories for polymer thermophoresis in dilute solutions there are two theoretical models under discussion: draining coil and nondraining coil, corresponding to the Rouse and the Zimm picture, respectively. In order to discriminate between these models we have started a comparative investigation of a linear chain polymer and cross-linked microgels. The linear polymer sample used is poly(methylmethacrylate) (PMMA) and the micro-gel samples are PMMA cross-linked with different amounts of ethylen-di-methacrylate (EGMA). In either case toluene is used as solvent. By means of transient holographic grating technique we obtained the thermal diffusion coefficient D_T , the Fickian diffusion coefficient D and the Soret coefficient S_T as functions of the polymer concentration c. We have found out that for $c \to 0$ the hermophoretic mobility of the linear polymer and the microgel with 3.5% EGMA are identical within experimental accuracy. In addition we performed dynamic light scattering experiments to characterize the different microgel samples. Thereby we obtained that the diffusion coefficient is independent of the amount of cross-linker and so are (by using Stokes-Einstein equation) the hydrodynamic radii of the microgels.

DY 25.6 Tue 18:15 Poster B2

Diffusion of PMMA: microgels and linear polymer — •Bastian Pur[1], Werner Köhler[1], Klaus Huber[2] und Martin Schneider[2] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Physikalische Chemie, Universität Paderborn, 33098 Paderborn, Germany

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DY 25.7 Tue 18:15 Poster B2

Extracting material net properties of monomolecular coverages from broadband dielectric spectroscopy measurements with nano-structured electrode arrangements — •Martin Tress[1,2], Nils Neibauer[2], Rene Winkler[3], Petra Uhlmann[3], Emmanuel Mapesa[2], Manfred Reiche[4], and Friedrich Kremer[2] — [1]Max Planck Institute for Polymer Research, Mainz — [2]University of Leipzig — [3]Leibniz-Institut für Polymerforschung Dresden e.V. — [4]Max Planck Institute of Microstructure Physics, Halle (Saale)

Recently, Broadband Dielectric Spectroscopy (BDS) has been combined with a nano-structured electrode arrangement to investigate glassy dynamics in monomolecular layers and isolated polymer chains [1]. Thereby, insulating nano-structures serve as spacers between the silicon electrodes enabling an electrode separation of only 40 nm. Since

this is still larger than the height of the actual sample material, a major fraction of the capacitor volume is empty. Consequently, the measured signal is an average of several contributions, including the dielectric properties of the sample itself, the spacer material and the gap between the electrodes. Due to the particular geometry, the composition of these contributions is not straight-forward. To unravel the individual dielectric functions of all components an equivalent circuit model is employed. Using BDS spectra of poly(2-vinylpyridine) (P2VP) brushes and condensed isolated P2VP chains as examples it is demonstrated how to unravel molecular relaxations, polarization effects and charge transport as well as the extraction of their net properties.

[1] M. Tress et al. Science 341 (2013) 1371

DY 25.8 Tue 18:15 Poster B2

Molecular Dynamic Simulation and forcefield creation of Poly(3-hexylthiophene) for aggregation investigations — •Marie Kathrin Tritschel and Stephan Gekle — Universität Bayreuth

Poly(3-hexylthiophene) is a widely investigated polymer for light harvesting devices as it possesses comparably good performances due to its high charge carrier mobility.

Using molecular dynamics simulation we show that there is a temperature dependent aggregation between different polymer chains in agreement with corresponding spectroscopic experiments.

Additionally investigations of the ordering and the packing behaviour of the chains are performed in atomistic and coarse grained representations of the system.

DY 26: Poster - Quanten Systems

Time: Tuesday 18:15–21:00 Location: Poster C

DY 26.1 Tue 18:15 Poster C

What is the origin of power-law trapping in 4D maps? — •Steffen Lange[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

While power-law trapping in 2D maps can be explained by a hierarchy of partial transport barriers, its origin in higher dimensional maps is still an open question. We study 4D symplectic maps with a regular region embedded in a large chaotic sea. Chaotic orbits are trapped in the vicinity of the regular region and show a power-law decay of trapping times. We search for the trapping mechanism by visualizing the trapped orbits in 3D phase-space slices [1] and by analyzing their time-dependent frequencies. While a hierarchy of regular regions similar to 2D maps is known to be present [2] and surprisingly also signatures of partial barriers are detected, these do not explain the observed trapping in 4D maps. Instead, a stochastic process including a drift along the resonance channels is conjectured to be the origin of the power-law trapping.

[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 26.2 Tue 18:15 Poster C

Phase-space structure of van der Waals dissociation — •Tom Schilling[1] and Arnd Bäcker[1,2] — [1]Institut für Theoretische Physik, TU Dresden, Dresden, Germany — [2]MPI für Physik komplexer Systeme, Dresden, Germany

An effective description of the dissociation of van der Waals complexes, such as $He{-}I_2$, can be obtained in terms of 4D symplectic maps. The escape dynamics is governed by a mixed phase space where in particular normally hyperbolic invariant manifolds are of importance. We use frequency space plots, escape time plots, and 3D phase-space slices [1] to visualize the dynamics. This allows for an understanding of the chaotic transport leading to dissociation.

[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 26.3 Tue 18:15 Poster C

Visualization of regular phase-space structures of the spatial circular restricted three-body problem — •Martin Langer[1] and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden, Germany — [2]MPI für Physik komplexer Systeme, Dresden, Germany

The spatial circular restricted three-body problem is a Hamiltonian system with three degrees of freedom, describing for example the dynamics of an astroid in the field of two heavy masses moving on circular orbits. By a Poincaré section this can be reduced to a 4D symplectic map. To visualize the dynamics in phase space, in particular around the Lagrangian triangular equilibria $\mathcal{L}_{4,5}$, we use the recently introduced 3D phase space slices [1]. We relate regular phase-space structures with those in frequency space and explain the organization of phase space using lower-dimensional tori.

[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 26.4 Tue 18:15 Poster C

Resonance–assisted tunneling in 4D symplectic maps — •Markus Firmbach[1], Felix Fritzsch[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

Dynamical tunneling allows wave functions to penetrate into regions of phase space which are strictly separated by classical dynamics. Nonlinear resonances can enhance tunneling rates by several orders of magnitude due to resonance–assisted tunneling. While this is both qualitatively and quantitatively well understood for 2D systems, this is not the case for higher–dimensional systems. As a first step we introduce a class of 4D symplectic maps with just a single resonance and determine the tunneling rates numerically. In order to obtain a theoretical prediction we employ quantum perturbation theory and a suitable integrable approximation. We find good agreement with numerical data.

DY 26.5 Tue 18:15 Poster C

Distance dependence of fluctuations in mesoscopic transport: From branched flow to UCFs — •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 two dimensional random potential with spatial Gaussian correlation. We calculate the density of classical trajectories and find the well-known branching pattern near the source. However, we observe its gradual disappearance into a homogeneously fluctuating pattern at larger distances away from the source. This is accompanied by a continuous change in the trajectory-density probability distribution from lognormal-like to Gaussian-like, which is suggestive of change of the transport dynamics from ballistic to diffusive. We present the distribution of momenta, and confirm that, for shorter distances, a certain direction corresponding to the branched flow is properly preferred, while there is no such a direction at larger distances. Also, we show that the intensity distribution of each trajectory at a given distance can be obtained by correctly taking into account the distribution of travelling times to points at a certain distance from the source. These results are compared with those of the quasi one-dimensional (i.e. one of space coordinates is proportional to time) case to clarify the dependence on the degree of freedom.

DY 26.6 Tue 18:15 Poster C

Localization of Chaotic Resonance States due to a Partial Transport Barrier — •Martin Körber[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

Chaotic eigenstates of quantum systems are known to localize on either side of a classical partial transport barrier if the flux connecting the two sides is quantum mechanically not resolved due to Heisenberg's uncertainty. Surprisingly, in open systems with escape chaotic resonance states can localize even if the flux is quantum mechanically resolved [1]. We explain this using the concept of conditionally invariant measures by introducing a new quantum mechanically relevant

class of such fractal measures [2]. We numerically find quantum-to-classical correspondence for localization transitions depending on the openness of the system and on the decay rate of resonance states.
[1] Phys. Rev. Lett. **111**, 114102 (2013)
[2] Phys. Rev. Lett. (accepted); arXiv:1509.00665

DY 26.7 Tue 18:15 Poster C

Whispering Gallery Modes in Graphene Billiards — •Guido Natura — Institut für Physik, Technische Universität Ilmenau. 98693 Ilmenau

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

[1] Yue Zhao, Jonathan Wyrick, Fabian D. Natterer, Joaquin F. Rodriguez-Nieva, Cyprian Lewandowski, Kenji Watanabe, Takashi Taniguchi, Leonid S. Levitov, Nikolai B. Zhitenev, and Joseph A. Stroscio. Creating and probing electron whispering-gallery modes in graphene. *Science*, 348(6235):672-675, 2015.

[2] M. V. Berry and R. J. Mondragon. Neutrino billiards: Time-reversal symmetry-breaking without magnetic fields. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 412(1842):53-74, 1987.

DY 26.8 Tue 18:15 Poster C

Semiclassical Theory for Interacting Many-Body Scattering of Bosons Through Mesoscopic Chaotic Cavities — •Josef Michl, Fabian Stöger, Juan-Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We report our progress in constructing a theory for mesoscopic scattering of identical particles through open chaotic cavities suitable for studying the interplay between three physical effects: universality of single-particle transport, many-body correlations due to quantum indistinguishability, and the presence of interparticle interactions.

Already at the level of non-interacting particles, indistinguishability alone produces non-trivial combinations of single-particle scattering matrices in the transport of many particles through mesoscopic chaotic cavities, which result in a mesoscopic version of the Hong-Ou-Mandel effect known from quantum optics[1]. Going beyond non-interacting systems, the study of interaction effects requires a proper choice of the underlying single-particle basis for the Fock space. We show, that in the basis of chaotic single-particle scattering states, the many-body Hamiltonian takes a universal form, which is ready to be used within a non-perturbative semiclassical approach based on solutions of mean-field equations, similar to that for Bose-Hubbard systems[2]. We present analytical and numerical results at the level of the diagonal approximation and discuss how to go beyond.

[1] Hong, C. K., Ou, Z. Y., Mandel, L., PRL 18, 2044 (1987)
[2] Engl, T. et al., PRL 112, 140403 (2014)

DY 26.9 Tue 18:15 Poster C

Stationary waves on nonlinear quantum graphs — Sven Gnutzmann[1] and •Daniel Waltner[2] — [1]School of Mathematical Sciences, University of Nottingham, Nottingham NG7 2RD, UK — [2]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany

We present a general framework for solving the stationary nonlinear Schrödinger equation (NLSE) on a network of one-dimensional wires modelled by a metric graph with suitable matching conditions at the vertices. For the cubic NLSE the solutions are given by Jacobi elliptic functions. For sufficiently small amplitudes we use canonical perturbation theory that allows to extract the leading nonlinear corrections over large distances. Simple closed and scattering graphs serve as examples.

DY 26.10 Tue 18:15 Poster C

Nonthermal Fixed Points and Superfluid Turbulence in Ultracold Bose Gases — Halil Cakir[1], Stefanie Czischek[1], •Markus Karl[1,2], Eike Nicklas[1], Thomas Gasenzer[1,2], and Markus K. Oberthaler[1] — [1]Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg — [2]Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg

Ultracold quantum gases provide various means to probe universal many-body dynamics far from equilibrium. Here, we focus on the non-linear dynamical evolution induced in an ultra cold Bose gas by a sudden initial parameter quench. Considering one- or multi-component (spin) systems, various types of spatial and wavenumber- space patterns emerge, being characterized by universal scaling functions associated with non-thermal fixed points. Such fixed points can be observed in existing experiments and are closely related to quantum turbulence usually discussed in systems of more than one spatial dimension. While these situations are associated with quenches to a symmetry-broken state, quenches within the symmetric phase offer a way to probe the properties of universal dynamics similar to those near a quantum critical point in equilibrium. Scaling properties have been found which indicate the importance of pre-thermalisation temperatures long before dephasing has occurred in the nearly gapless system. We discuss the theoretical results in the light of and illustrated by recent experimental measurements.

DY 26.11 Tue 18:15 Poster C

Self-localization of Bose-Einstein condensates in leaking optical lattices — •Johannes Kruse and Ragnar Fleischmann — Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen, Germany

Mean field and beyond mean field model calculations of Bose-Einstein condensates trapped in optical lattices have shown that initially homogeneous condensates can evolve into self-trapped, strongly localized states in the presence of weak boundary dissipation, a phenomenon called self-localization. A phase transition from extended to localized states has been observed when the effective nonlinearity exceeds a critical threshold Λ^b_{eff}.
We investigate the phase transition to self-localization in the mean field approximation of the discrete nonlinear Schrödinger equation. Earlier, based on the concept of the Peierls-Nabarro barrier an analytical upper bound for Λ^b_{eff} as a function of the system size had been found. We now propose and numerically verify an analytical lower bound for Λ^b_{eff}, linking it to the phenomenon of Anderson localization. Moreover we quantitatively characterize the properties of the nonlinear localized solutions, so called *discrete breathers*, directly after the phase transition. The results strongly suggest that in the thermodynamic limit the average shape of the solutions at the transition approaches a fixed limiting profile located in the center of the lattice.

DY 26.12 Tue 18:15 Poster C

DMRG simulations of relaxation dynamics of interacting electrons in a disordered quantum wire — •Felix Weiner[1], Peter Schmitteckert[2], and Ferdinand Evers[1] — [1]Institut I - Theoretische Physik, Universität Regensburg — [2]Institut für Theoretische Physik IV, Heinrich-Heine-Universität Düsseldorf

We study high temperature relaxation dynamics of electrons with short range interaction in a disordered quantum wire. Such systems are believed to exhibit many-body localisation, which has attracted considerable attention in recent thereotical investigations. Our simulations are performed by means of time-dependent density matrix renormalization group (DMRG) with the standard extension to mixed state evolution via purification. Accessible time scales in this approach are known to be limited by the fast growth of entanglement with time. Nevertheless, we are able to demonstrate results for time traces that are converged in a systematic way for a given disorder realisation. Charge relaxation is investigated via a wave-packet propagation. Besides the variance also higher moments of the distribution are investigated because one would expect a non-Gaussian broadening. The goal of the project is to obtain, eventually, the time evolution of the entire (non-Gaussian) distribution function in the localised and delocalised phase.

DY 26.13 Tue 18:15 Poster C

Thermalization in Two Uncoupled Wires of Interacting Luttinger Liquids — •Sebastian Huber[1,2,3], Michael Buchhold[2,3] und Sebastian Diehl[2,3] — [1]Physics Department, Ludwig-Maximilians-Universität München, 80333 Munich, Germany — [2]Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden, Germany — [3]Institute of Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria

Coherently splitting a one-dimensional Bose gas provides an attractive, experimentally established platform to investigate thermalization dynamics. After the split, the two wires are in a strongly entangled non-equilibrium state with equal longitudinal phase profiles. The dynamics is generated by interactions within the two uncoupled Luttinger Liquids.

In order to find signatures of thermalization and to calculate the non-equilibrium dynamics of this system, we derive the kinetic equations for the time dependent normal and anomalous phonon densities in a Keldysh framework. We determine the spatial expansion of the relative phase correlation function numerically at each time step, which is experimentally detectable by means of matter-wave interferometry.

The time evolution of the relative phase correlation function has two distinct regimes: At early times the system evolves to a prethermal state characterized by a light-cone behaviour and described by a GGE state. However, the presence of phonon scattering induces late time dynamics, during which the relative phase correlation function shows clear signatures of thermalization.

DY 27: Poster - Statistical Physics, Critical Phenomena, Brownian motion

Time: Tuesday 18:15–21:00 Location: Poster C

DY 27.1 Tue 18:15 Poster C

Phase separation in mixtures of soft particles in 2D: A dynamical DFT study — •Alexander Kraft and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

We investigate binary mixtures of soft particles (e.g. of Gaussian core type) in a two-dimensional system within the framework of density functional theory and dynamical density functional theory. Depending on system parameters, we observe homogeneous mixing or a phase separation of both species. In order to classify the system behaviour, we calculate the phase diagram, i.e. the spinodal and binodal lines, based on thermodynamic stability conditions. Furthermore, we compare the regions of thermodynamic stability with estimates based on linear stability analysis of the homogeneously mixed system. In contrast to previous studies [1,2], in this work, we focus on a two-dimensional system, in order to gain access to the behaviour in flat geometries or on surfaces. We also discuss possible control strategies for the manipulation of the phase separation process.

[1] A. A. Louis, P. G. Bolhuis, and J. P. Hansen, Phys. Rev. E **62**, 7961 (2000)

[2] A. J. Archer and R. Evans, Phys. Rev. E **64** (2001)

DY 27.2 Tue 18:15 Poster C

P-T-V equations of state for III-V compound semiconductors — •Alrik Stegmaier, Ulrich Vetter, and Hans Hofsäss — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Equations of state (EoS) for solids are necessary for relating the state variables to each other and an important application is the description of the technologically important III-V compound semiconductors at different temperatures and pressures.

While many general EoS for solids exist, the introduction of a temperature dependence is not unique [1] and the materials considered here have negative thermal expansion coefficients at low temperatures [2], hampering a simple but accurate description. Further more, EoS are often not easily invertible [3] and several constraints have been suggested for isothermal EoS for solids that are not fullfilled by all formulations [4].

Here several EoS for III-V compound semiconductors are compared against experimental data and the results of ab-initio calculations. As a result a general P-T-V equation of state is proposed that is relatively accurate, simple, invertible and approximately fullfills the constraints reported in the literature for such an equation.

[1] R. E. Cohen et al., Am. Mineral., 85(4), 338-344, 2000
[2] G. Dolling and R. A. Cowley, Proc. Phys. Soc., 88, 463, 1965
[3] M. Etter and R. E. Dinnebier, J. Appl. Cryst., 47, 384-390, 2014
[4] P. K. Singh and A. Dwivedi, Indian J. Pure & Appl. Phys., 50, 734-738, 2012

DY 27.3 Tue 18:15 Poster C

Bi-stable state on the prestructured surface: Free energy calculation — •Oleg Buller, Lisa Götte, and Andreas Heuer — Institut für Physikalische Chemie, WWU, Münster

Attachment of molecules on a prepatterned surface by vapor deposition displays a wide variety of resulting structures. We are interested in the single stripe and double stripe prepattern. For the case of a single stripe geometry an instability is observed forming a bulge. A second stripe close-by can destabilize the bulge leading to the agglomeration of the molecules in-between the stripes. We model this system by a kinetic Monte Carlo model and calculate the relative free energies by using Markov State sampling techniques. We analyze the influence on the stripe distance and the amount of particles forming a bulge.

DY 27.4 Tue 18:15 Poster C

The Voronoi liquid — •Céline Ruscher, Jörg Baschnagel, and Jean Farago — Institut Charles Sadron, Strasbourg, France

Voronoi tessellations are defined as a mathematical partition of the space where a cell containing the point of interest is defined through the points of space which are the closest from this point than from any other. In soft matter physics Voronoi tessellations are widely used to probe the local environnement of particles.

We describe here a new model of fluid called the Voronoi fluid where the force field is directly expressed through the intrinsic properties of the Voronoi tessellations. Due to its definition this monodisperse fluid presents many-body interactions and there is no excluded volume. Moreover the force field derives from a potential energy which exhibits scaling properties.

Thermodynamics and microscopic observables of the Voronoi fluid are both investigated through numerical simulations. Similarities with simple liquids have been observed however some differences occur. For instance an unexpected relation between the pair correlation function and the chemical potential has been found and the dynamic structure factor exhibits an unusual behavior in the hydrodynamic regime.

Finally we observed that when the Voronoi fluid crystallizes into a BCC an atypical behavior appears. Below the melting point particles move leaving the whole structure unchanged. As the motion seems to be a collective phenomenon these rearrangements appear to be a good indicator that the model can be extended to probe glass-forming systems.

DY 27.5 Tue 18:15 Poster C

Behavior of electronic states on random Voronoi-Delaunay lattices in the orthogonal and the unitary universality class — •Martin Puschmann[1], Philipp Cain[1], Michael Schreiber[1], and Thomas Vojta[2] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Department of Physics, Missouri University of Science and Technology, Rolla, Missouri, USA

The random Voronoi-Delaunay lattice (VDL) is defined as a set of bonds between randomly positioned sites. The bonds connect neighboring Voronoi cells and are obtained by the Delaunay triangulation. The resulting topologically disordered lattice features strong anticorrelations between the coordination numbers of neighboring sites. The disorder fluctuations therefore decay qualitatively faster with increasing length scale than those of generic random systems. A recent study showed that this modifies the Harris and Imry-Ma criteria and leads to qualitatively changes of the scaling behavior at magnetic phase transitions [1]. We consider the transport of non-interacting electrons on two- and three dimensional random VDLs without and with magnetic fields. The electronic wave functions are analyzed by multifractal analysis. Without magnetic fields, we obtain results in accordance to the orthogonal universality class [2]. Applying magnetic fields introduces a phase shift to the local wave function. This shift is proportional to the area of the local Delaunay triangle. We show how the topological aspect affects the behavior of the wave functions in magnetic VDLs and whether this is compatible with unitary universality class.

[1] PRL 113, 120602 (2014) [2] EPJ B 88, 314 (2015)

DY 27.6 Tue 18:15 Poster C

Spin glasses with variable frustration — •Ravinder Kumar[1,2], Martin Weigel[1], and Wolfhard Janke[2] — [1]Applied Mathematics

Research Centre, Coventry University, Coventry, UK. — [2]Institut für Theoretische Physik, Leipzig University, Leipzig, Germany.

Together with randomness, frustration is believed to be a crucial prerequisite for the occurrence of glassy behavior in spin systems. The degree of frustration is normally the result of a chosen distribution of exchange couplings in combination with the structure of the lattice under consideration. Here, however, we discuss a process for tuning the frustration content of the Edwards-Anderson model on arbitrary lattices. With the help of extensive parallel-tempering Monte Carlo simulations we study such systems on the square lattice and compare the outcomes to the predictions of a recent study employing the Migdal-Kadanoff real-space renormalization procedure [1].

[1] Efe Ilker and A. Nihat Berker, Phys. Rev. E 89, 042139 (2014).

DY 27.7 Tue 18:15 Poster C

Using entanglement to discern phases in the disordered one-dimensional Bose-Hubbard model — Andrew M. Goldsborough[1,2] and •Rudolf A. Römer[2] — [1]JARA Institute for Quantum Information, RWTH Aachen University - D-52056 Aachen, Germany — [2]University of Warwick, Coventry CV4 7AL, UK

We perform a matrix-product-state based density matrix renormalisation group analysis of the phases for the disordered one-dimensional Bose-Hubbard model. For particle densities $N/L = 1$, $1/2$ and 2 we show that it is possible to obtain a full phase diagram using only the entanglement properties, which come for free when performing an update. We confirm the presence of Mott insulating, superfluid and Bose glass phases when $N/L = 1$ and $1/2$ (without the Mott insulator) as found in previous studies. For the $N/L = 2$ system we find a double-lobed superfluid phase with possible re-entrance.

DY 27.8 Tue 18:15 Poster C

Characterization of multifractality at the Anderson transition from wavefunction dynamics — Chi-Hung Weng, Andreas Buchleitner, and •Alberto Rodriguez — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg

While stationary numerical techniques to obtain the multifractal spectrum from eigenstates close to the Anderson transition have been extensively studied, the implications of multifractality on the dynamics close to the critical point, and in particular the validation of the different proposed dynamical scaling laws involving multifractal exponents have not received comparable attention. The dynamical approach may however be crucial for the characterization of multifractality from experimental data of the expansion of wave packets in disordered potentials. For this task, we consider several scaling laws: the scaling of the return probability with time, the decaying profile of the time-dependent wavefunction with distance, and the scaling of the long-time return probability with system size. We present a thorough analysis of the regimes of validity of these scaling laws and their suitability to obtain a reliable estimate of the multifractal exponent D_2 from the dynamics of a localized initial excitation in a critical power-law random banded matrix model.

DY 27.9 Tue 18:15 Poster C

Optimal performance under limited control of periodically driven, stochastic heat engines — •Michael Bauer[1], Kay Brandner[1,2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Department of Applied Physics, Aalto University, 00076 Aalto, Finland

We investigate the performance of periodically driven, stochastic heat engines under optimal driving in the linear response regime. The Onsager coefficients for such machines obeying Fokker-Planck dynamics have recently been developed and illustrated with an overdamped Brownian particle, where the driving protocol allows full control on the particle [1].

Here, we are interested in the performance of such heat engines if only a limited number of degrees of freedom can be externally controlled. In a case study, we examine a heat engine consisting of an underdamped Brownian particle in a magnetic field, where the kinetic degrees of freedom cannot be controlled. We find expressions for the efficiency in analogy to the performance of thermoelectric devices and define an adequate figure of merit. In the absence of a magnetic field, more general results are obtained if the control functions are assumed to be given by the eigenfunctions of the adjoint Fokker-Planck operator. We recover the expressions of the case study and obtain a condition for the attainability of Carnot efficiency.

[1] K. Brandner, K. Saito, and U. Seifert, Phys. Rev. X 5, 031019 (2015)

DY 27.10 Tue 18:15 Poster C

Aging Universality Classes in Surface Growth Models — •Jeffrey Kelling[1], Geza Odor[2], and Sibylle Gemming[1,3] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]MTA-EK-MFA Institute of Technical Physics and Materials Science, Budapest, Hungary — [3]Institute of Physics, TU-Chemnitz, Germany

Extensive dynamical simluations of a 2 dimensional driven dimer lattice gas are presented, which can be mapped to (2+1) dimensional surface growth in the Kardar-Parisi-Zhang (KPZ) or Edwards-Wilkinson unversality classes. From this autocorrelation and autoresponse functions have been determined for the KPZ universality class and the underlying lattice gas. Studying the effects of different dimer lattice gas dynamics revealed strong differences in the aging behavior of the stochastic cellular automaton (SCA) and the random sequential update models. We show numerical evidence for nontrivial corrections as well as different universal scaling behaviors.

DY 27.11 Tue 18:15 Poster C

Transport of colloidal particles under the impact of time-delayed feedback control — •Sarah A. M. Loos and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We explore possibilities to analytically investigate the influence of time-delayed feedback control on transport and diffusion of overdamped Brownian particles in one dimension [1]. In particular, we consider particles in static external potentials supplemented by linear feedback forces, where the delayed particle position serves as control target. We use both, the equation of motion which is given by a non-Markovian Langevin equation, and the equation of the temporal evolution of the corresponding probability density field, i.e., the delayed Fokker-Planck equation [2,3]. We have thus access to the fluctuating trajectories as well as to the deterministic evolution of the density field. We focus on theoretical predictions of transport and diffusion properties such as the mean particle position and the mean squared displacement. In order to validate our analytical findings, we compare them with numerical results obtained by Brownian dynamics simulations. We further discuss possible applications to the case of interacting particles.

[1] R. Gernert, et al., arXiv:1511.00413 (2015).
[2] S. Guillouzic et al., Phys. Rev. E 59, 3970 (1999).
[3] T. D. Frank, Phys. Rev. E 71, 031106 (2005).

DY 27.12 Tue 18:15 Poster C

Effective Perrin Theory for a Liquid of Infinitely Thin Brownian Needles — •Sebastian Leitmann[1], Felix Höfling[2], and Thomas Franosch[1] — [1]Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria — [2]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany, and Institut für Theoretische Physik IV, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Liquids of infinitely thin Brownian needles of length L are considered up to reduced densities of $n^* = nL^3 > 10^3$ deep in the semidilute regime $n^* > 1$. By a stochastic simulation of a liquid of subsequent moving particles, we corroborate the scaling behavior n^{*-2} of the diffusion coefficients of a needle liquid. We find excellent agreement between the intermediate scattering function in the semidilute regime and a full analytic solution for a freely moving rod with the transport coefficients obtained from stochastic simulation as input parameters. We argue, that the single-needle dynamics in the liquid is asymptotically insensitive to the dynamic rearrangement of the surroundings. Therefore, we map the problem to the movement of a single needle in a frozen disordered array of needles, which enables us to characterize the dynamics in a considerably wider time window.

DY 27.13 Tue 18:15 Poster C

Random matrices and condensation into multiple states — •Sina Sadeghi and Andreas Engel — Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, Oldenburg, Germany

Condensation is a collective phenomenon that ubiquitously occurs in nature. A well-known example in physics is the Bose-Einstein condensation of a bosonic gas in equilibrium into its ground state at low tem-

perature. Recently, it has been shown that a driven-dissipative bosonic gas may condensate into multiple states rather than into a single one [Phys. Rev. Let. 111, 240405 (2014)] and a connection between such non-equilibrium condensation and evolutionary game theory has been established [Nat. Comm. 6, 6977 (2015)]. In the present work we employ statistical mechanics methods from disordered systems to investigate static properties of condensation in a general framework. We aim at showing how typical properties of random interaction matrices play a vital role in manifesting the statistics of condensate states. To this end we study the interplay between the condensation problem and zero-sum games with random pay-off matrices. We show for the game theoretical problem that as far as static quantities are concerned spherical and simplex constraints for the degrees of freedom are equivalent. This is advantageous also in the case of condensation since the number of order parameters is reduced which simplifies the analysis.

DY 28: Poster - Complex Fluids, Granular Matter, Glasses

Time: Tuesday 18:15–21:00 Location: Poster C

DY 28.1 Tue 18:15 Poster C

Simple and efficient implementation of the Hamiltonian Adaptive Resolution Simulation (H-AdResS) scheme in LAMMPS — •Maziar Heidari, Robinson Cortes-Huerto, and Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz, Germany

Computational studies of complex molecular systems often require the usage of multiscale strategies that access simultaneously various time and length scales. The Hamiltonian adaptive resolution simulation scheme (H-AdResS) is a dual-resolution simulation method that joins models with different levels of complexity for the same system within a global Hamiltonian framework. In the past, this method has been implemented in several specific-purpose softwares, in-house modifications of the GROMACS package, and, most notably, the ESPResSo++ platform.

Here we present an efficient implementation of the H-AdResS scheme in the LAMMPS simulation package. The latter is provided with simple extensions of the available potential energy functions and simulation algorithms. Minimal additions in the input files are sufficient to set up a dual-resolution simulation. The algorithmic workflow and the practical usage are explicitly discussed. This implementation is validated by studying thermodynamic properties of prototypical molecular liquids.

DY 28.2 Tue 18:15 Poster C

Thin film model of drops on soft substrates — •Johannes Kemper and Uwe Thiele — Institut für Theoretische Physik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 9, 48149 Münster

For drops of liquid on a rigid substrate the force balance that gives the contact angle at the three phase contact line is given by the Young condition that only captures forces parallel to the substrate. However, for liquid drops on viscous soft substrates the balance is given by the Neumann condition that has a vertical and a horizontal component. For a soft substrate with elastic properties, elastic stresses (in general, non-local) have to be accounted for. Here, we present a local approximation of elastic influences that can be incorporated in a long-wave evolution equation for thin viscoelastic films and small-contact angle drops when written in gradient dynamics form. First we use the static limit of the model to determine drop profiles and analyse how the equilibrium contact angles depend on the softness of the substrate. Ridge profiles and radially symmetric drops are analysed employing numerical continuation techniques. It is shown that the simplified model reproduces experimentally observed phenomena like the formation of a wedge-shaped protrusion that is drawn out of the elastic substrate at the contact line [1]. Moreover, the dependence of the contact angle on substrate softness reproduces results of the full elastic model in [2]. These static results give a validity range of parameters for which the elastic long-wave model can be employed in time simulations. [1] T. Kajiya et al., Soft Matter, 9:454-461, 2013; [2] L.A. Lubbers et al., J. Fluid Mech., 747:R1, 2014.

DY 28.3 Tue 18:15 Poster C

Long wave modelling of osmotic spreading of biofilms — •Sarah Trinschek[1,2], Uwe Thiele[1,2], and Karin John[3] — [1]Institut für Theoretische Physik, WWU, Münster, Germany — [2]Center of Nonlinear Science (CeNoS), WWU, Münster, Germany — [3]Laboratoire Interdisciplinaire de Physique, CNRS / Université Grenoble-Alpes, Saint-Martin-d'Hères, France

Biofilms are ubiquitous macrocolonies of bacteria that develop at interfaces. Their widespread occurrence and either detrimental or beneficial function implies that it is highly important to understand the principles underlying their development. Biofilm formation starts with the attachment of individual bacteria to a surface, which then proliferate and produce a slimy polymeric matrix - two processes that result in colony growth and spreading.

Our model is based on thermodynamically consitent gradient dynamics developed for passive thin liquid mixtures. We supplement this approach by active processes (i.e. proliferation of bacteria and the secretion of polymeric matrix) that cause volume growth. Osmotic pressure gradients are generated as cells consume water and nutrient to produce biomass. This osmotic imbalance causes swelling and spreading of the biofilm through uptake of water from the moist agar substrate. We treat the system within a coarse-grained long-wave approach assuming that the thickness of the biofilm is small as compared to the typical length scale of lateral variations in film height and composition. This allows us to study the dynamics of swelling droplets with direct time simulations and analyse the front velocity of spreading biofilms.

DY 28.4 Tue 18:15 Poster C

Studying the The dynamics of polymeric liquids under time-delayed feedback — •Peter Kalle and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Soft materials or complex fluids strongly respond to external fields and thereby show prominent non-equilibrium structure formation. Applying control strategies to shape and engineer the flow of liquids on the micron scale virtually is an unexplored field.

We study the dynamics of the Oldroyd B model, a nonlinear model to treat the dynamics of polymeric liquids, under the influence of time-delayed feedback schemes in the limit of low Reynolds numbers.

Experiments with polymeric liquids in channel flows at low Reynolds numbers have recently demonstrated that a nonlinear bifurcation towards a fluctuating flow field occurs [1]. Hence, we study the impact of time-delayed feedback schemes on a channel flow. Furthermore, as the curvature of a geometry is linked to linear elastic instabilities [2], we present first results for controlling Taylor-Couette flow as in [3] and also address the circular geometry of [4] without inner cylinder.

[1] L. Pan, A. Morozov, C. Wagner, P.E. Arratia, Phys. Rev. Lett. 110, 174502 (2013).
[2] G. H. McKinley, P. Pakdel and A. Öztekin, J. Non-Newt. Fluid Mech. 67, 19 (1996).
[3] R. G. Larson, S. G. Shaqfeh and S. J. Muller, J. Fluid Mech. 218, 573-600 (1990).
[4] M. Zeitz, P. Gurevich and H. Stark, Eur. Phys. J. E 38, 22 (2015).

DY 28.5 Tue 18:15 Poster C

Many-body critical Casimir interactions in colloidal suspensions — Hendrik Hobrecht and •Alfred Hucht — Fakultät für Physik and CENIDE, Universität Duisburg-Essen, 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. To simulate these systems, we present a highly efficient cluster Monte Carlo algorithm based on geometric symmetries of the Hamiltonian. Utilizing the principle of universality, the medium 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 at the critical point in two dimensions perfectly agree with the exact predictions. However, we find that in finite systems the behavior strongly depends on whether the Z_2 symmetry of the system is broken by the particles. We present Monte Carlo results for the three-body Casimir interaction potential and take a close look onto the case of one particle in the vicinity of

two adjacent particles, which can be calculated from the two-particle interaction by a conformal mapping. These results emphasize the failure of the common decomposition approach for many-particle critical Casimir interactions.
Hendrik Hobrecht and Alfred Hucht, Phys. Rev. E 92, 042315 (2015), http://dx.doi.org/10.1103/PhysRevE.92.042315

DY 28.6 Tue 18:15 Poster C

Dissipation in sheared frictional granular media near the jamming transition — •Florian Spreckelsen, Matthias Grob, Claus Heussinger, and Anette Zippelius — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Dense assemblies of frictional grains show reentrant flow when sheared, i.e., the system flows for high and low shear stress and jams in between. This behavior is absent in frictionless systems and signals the importance of dissipation mechanisms emerging from frictional particle interaction. We deploy molecular dynamics simulations in order to investigate the dominant contributions to dissipation near the jamming transition in two-dimensional systems.

DY 28.7 Tue 18:15 Poster C

Fracturing of a model cohesive porous medium — •Alexander Schmeink, Arnaud Hemmerle, and Lucas Goehring — Max-Planck-Institiute for Dynamics and Self-Organisation (MPIDS), 37077 Göttingen. Germany

Understanding the way cohesive porous materials fracture is essential in quantifying the mechanical contributions to phenomena like the deterioration of man-made structures, biogenic fracture of rocks, hydraulic fracture, and CO_2-Sequestration. Our goal is to characterize the fracture toughness of a cohesive porous medium in order to analyse the initiation of cracks in such situations. We designed a model porous medium made of glass beads held together by polydimethylsiloxane (PDMS). The cohesion of this medium can be controlled by curing conditions and crosslinking of the PDMS. In addition, the shape of bridges can be tuned by varying the amount of PDMS added to the beads. One advantage of this material is the fact that it can be molded into any desired shape. In order to analyze the initiation and propagation of cracks, we are conducting standard fracture toughness tests which have high requirements on the geometry of a tested specimen. We observe the fracture toughness of our material in dependence of parameters of its composition, such as polymer content, polymer composition, packing fraction, and bead diameter.

DY 28.8 Tue 18:15 Poster C

Measuring the buckling of a chain of permanent magnets under load — •Lucas Bartosch and Reinhard Richter — Experimentalphysik 5, Universität Bayreuth

A one-dimensional chain of spherical neodymium-iron-boron magnets responds to mechanical loadings in a manner reminiscent of an elastic rod, which was recently described by introducing an effective magnetic bending stiffness [1]. We are investigating the deformation of such a chain resting on a plain by means of images recorded by a digital camera. The positions of the magnets are extracted utilizing OpenCV for image processing. The distance between the two endpoints of the chain is manipulated via a computer controlled stepper motor. Moreover, the lateral force is recorded with a magnetic insensitive force gauge. We compare our quantitative results with the model proposed in [1].

[1] D. Vella, E. du Pontavice, C. L. Hall and A. Goriely, *Proc. R. Soc. A* **470**, 20130609 (2013).

DY 28.9 Tue 18:15 Poster C

The densest packing of ellipsoids — Fabian M. Schaller, •Robert F. B. Weigel, and Sebastian C. Kapfer — Theoretische Physik 1, FAU Erlangen, Germany

The relationship between local structure and macroscopic properties is a current research focus in granular matter. We study the distribution of local packing fractions (or Voronoi volumina) as a sensitive observable in order to test theoretical descriptions of such systems. Previously, mainly packings of spherical particles were considered. Here, we focus on packings of uniaxial ellipsoids as an instance of aspherical particles. In particular, we report numerical results on the locally densest packings of ellipsoids with aspect ratio between 0.7 and 1.4, generalizing the famous "kissing problem". Like in the spherical case, these packings locally exceed the density of known crystal structures. In low concentrations, distorted variations of some of these packing motifs can be found embedded in dense random packings of ellipsoids. Moreover, we find that the volume and packing fraction distributions in dense random ellipsoid packings deviate from theoretical predictions in the literature.

DY 28.10 Tue 18:15 Poster C

Flow and clogging of shape-anisotropic grains in a silo — Sandra Wegner[1], •Ahmed Ashour[1], Ralf Stannarius[1], Balázs Szabó[2], and Tamás Börzsönyi[2] — [1]Otto von Guericke University, Magdeburg, Germany — [2]Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary

Storage of granular materials is of considerable importance in many branches of agriculture, pharmaceutics and other industrial branches. It is often realized with silos or hoppers. When grains flow out of a hopper outlet, clogging is a frequently encountered problem. We investigate such clogging events in laboratory experiments by means of 3D imaging and optical characterization techniques, and extract the structure of the dome of grains blocking outflow. Particular emphasize is laid on influences of the geometry of the grains: spherical, prolate and oblate shapes are compared. X-ray computed tomography allows the identification of positions and orientations of all individual particles in the volume. With the complete 3D information of grain positions and orientations, packing fractions and orientational ordering of the systems are calculated and compared.

DY 28.11 Tue 18:15 Poster C

Mechanical properties of sheared wet granular piles — •Anna-Lena Hippler[1], Marc Schaber[1], Somnath Karmakar[1], Mario Scheel[3], Marco DiMichiel[3], Martin Brinkmann[2], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, 66041 Saarbruecken, Germany — [2]MPI for Dynamics and Self-Organization, Am Faßberg 17, 37077 Goettingen, Germany — [3]European 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 analyzing the corresponding liquid bridge volumes.

DY 28.12 Tue 18:15 Poster C

Thermal conductivity and geometric cohesion in aspherical granular materials — •Katharina Staudt[1] and Thomas Grillenbeck[1,2] — [1]Ignaz-Günther-Gymnasium Rosenheim, Germany — [2]Fachhochschule Rosenheim University of Applied Sciences, Germany

Aspherical granular materials show the phenomenon of geometric cohesion, i.e. cohesion due to particle geometry. Geometric cohesion is influenced by the contacts between particles - as is the thermal conductivity of any granular material. In my study, I examined the thermal conductivity of various package fractions of U-shaped staples as radically aspherical granular material. The experiments showed an increasing thermal conductivity with increasing package fraction, without evidence for an influence of geometric cohesion on thermal conductivity. Therefore, the (trivial) positive correlation between package fraction and thermal conductivity apparently applies also to radically aspherical granular materials like U-shaped staples.

DY 28.13 Tue 18:15 Poster C

Novel readout system and online analysis of dielectric two-pulse echoes — •Andreas Schaller, Sergey Tsurkan, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg

The low temperature properties of glasses are governed by atomic tunneling systems. These tunneling systems can couple resonantly to

electric fields and can be studied by phase coherent methods such as two-pulse polarization echo measurements using a reentrant cavity microwave resonator with a resonance frequency of approximately 1 GHz.

We built up a new fully automated data acquisition and analyzing system for the measurement of two-pulse polarization echoes with high accuracy. The new setup allows for measurements at shorter pulse separation-times and for a real-time frequency domain data analysis, which allows us to reject unwanted contributions to the integrated echo amplitude stemming from external disturbances. We will discuss the new setup and data acquisition system. In addition we will show results obtained for BK7 glass.

DY 28.14 Tue 18:15 Poster C

Novel LC-resonator techniques for measurements of MHz dielectric properties of glasses at very low temperatures — •Benedikt Frey, Wiebke Scholz, Guido Homann, Anne Zeissner, Annina Luck, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

Many properties of amorphous solids at low temperatures can be explained with the standard tunneling model, which is based on two level-tunneling systems. Significant deviations from the standard tunneling model were observed in dielectric measurements, both in the kHz and in the GHz regime. Moreover these measurements show a strongly frequency dependent behaviour that indicate a non-phonon based thermal relaxation process.
For further investigations of the crossover into this relaxation process, we have developed novel LC-resonator based measurement setups for the MHz regime. Our current setup operating at 30 MHz allows measurements with both very low field strengths and ultra low input power, while its high quality factor also permits a determination of the dielectric loss factor.
Measurements performed on the samples HY-1, N-BK7, Herasil and PVAc show the influence of nuclear quadrupoles and long range interactions on dielectric properties of glasses in this frequency regime.

DY 28.15 Tue 18:15 Poster C

Confinement effects on binary mixtures of water and glycerol investigated by 1H and 2H NMR — •Max Schaefer, Edda Klotz, and Wida Kohshekan — Institut für Festkörperphysik, Tu Darmstadt, 64289 Darmstadt, Hochschulstraße 6, Germany

Dynamics in binary mixtures of water and glycerol with various concentrations was investigated by NMR. Applying different NMR technics the dynamics was studied in a broad temperature range down to very low temperatures. As a confinement effect the freezing point of water can be suppressed. Using 2H spin-lattice relaxation and stimulated-echo experiments we determined the rotational correlation function. By 1H diffusion measurements in an ultra high static field gradient the confinement effect on the translational motion caused by geometric restrictions as well as by surface interactions was studied. The dynamical properties were investigated within different types of confinement having various solidities. By comparison to the dynamics of their bulk systems, the influence of "soft confinement" (proteins) and "hard confinements" (MCM 41 with various pore diameters) was ascertained. A possible microphase separation of glycerol and water initiated by the confinement, is also of great interest.

DY 28.16 Tue 18:15 Poster C

Molecular dynamcis study of modified SPC/e water in neutral confinements — •Robin Horstmann, Michael Vogel, and Felix Klameth — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

Liquids either supercooled close to the glass transition temperature or inside nanoscopic confinements exhibit a slowdown of dynamics of several orders of magnitude. While a full explanation is still missing the ECNLE (elastic collective nonlinear Langevin equation) theory proposed by Mirigian and Schweizer et al. [1] shows promising features explaning the α relaxation as a combination of a local hopping motion and the elastic distortion of the environment.

Recent molecular dynamics simulations [2] showed that the ECNLE theory, proposed for supercooled vdW-like systems, well describes the dynamcis of interfacial water. In this simulation work, neutral pores were used, i.e., a fraction of the bulk water was pinned leaving a nanoscopic pore of selectable geometry. Here, we reduce the partial charges of SPC/e water to systematically study the role of hydrogen bonds and to move in the direction of vdW-like behavior. Using the advantages of trajectories from molecular dynamics simulations we perform spatially resolved calculations of correlations, e.g., of the incoherent scattering functions, near the pore wall.
[1] Mirigan & Schweizer et al., J. Phys. Chem. Lett., 2013, 4 (21), pp 3648-3653
[2] Klameth et al., J. Phys. Chem. Lett., 2015, 6(21), pp 4385-4389

DY 28.17 Tue 18:15 Poster C

Spherical core-shell colloids with multiple cores as probes for rotational dynamics — Stefan Schütter[1], •Nicolai Sänger[1], Jörg Roller[2], and Patrick Pfleiderer[2] — [1]Universität Konstanz Fachbereich Chemie — [2]Universität Konstanz Fachbereich Physik

We introduce two new types of spherical probe particles for investigating rotational dynamics in colloidal fluids and solid states. The particles are tailormade for confocal fluorescence microscopy and coherent anti-Stokes Raman scattering (CARS) microscopy in three dimensions. CARS microscopy is a non-linear technique for tracking non-labeled colloids by generating signal of different polymer materials.[1,2] CARS methods, on the one hand, do not suffer from photobleaching and are attractive alternatives for longterm observations. On the other hand, two-color fluorescence of the cores provides robust access to the rapid determination of the particles* orientation. The two-color labeling strategy is beneficial to be able to observe the full 360 degree rotational movement of single colloidal clusters in contrast to other core-shell geometries where only angles of 180 degrees are accessible. It has already been shown for non-spherical single-color clusters that coupling effects for translational as well as rotational diffusion for different particle volume fractions are of high interest.[3] The choice of materials permits specific experiments for addressing diverse phenomena where rotation plays an important role.

[1] M. Müller and A. Zumbusch, ChemPhysChem, 2007, 8, 2156-2170. [2] M. K. Klein et al., Langmuir, 2014. [3] G. L. Hunter et al. Opt. Express, 2011, 19, 17189-17202.

DY 29: Poster - Active Matter, Microswimmers and -fluidics, Statistical Physics Biosystems

Time: Tuesday 18:15–21:00 Location: Poster C

DY 29.1 Tue 18:15 Poster C

Stability and bifurcations in a model for active crystals — •Lukas Ophaus[1,2], Alexander Chervanyov[1,2], and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, WWU, Münster, Germany — [2]Center of Nonlinear Science (CeNoS), WWU, Münster, Germany

The conserved Swift-Hohenberg equation [or Phase-Field-Crystal (PFC) model] provides a simple microscopic description of the thermodynamic transition from a fluid to a crystalline state [1,2]. The model can be combined with the Toner-Tu theory [3] for self-propelled particles to obtain a model for crystallization (swarm formation) in active systems [4]. Within the resulting active PFC model, resting and travelling crystals can be identified. The moving states migrate with a well-defined velocity while keeping their periodicity. These ordered swarms start to move at a critical value of an activity parameter.

We investigate the influence of this parameter on the linear stability of the homogeneous, fluid state. In addition, we use a one-dimensional version to explore the bifurcation structure at the onset of motion. Numerical continuation is applied to follow steady and travelling states to construct the bifurcation diagram.

[1] H. Emmerich, H. Löwen, R. Wittkowski, T. Gruhn, G. I. Tóth, G. Tegze and L. Gránásy, 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)
[3] J. Toner and Y. Tu, Phys. Rev. E 58, 4828 (1998)
[4] A. M. Menzel and H. Löwen, Phys. Rev. Lett. 110, 055702 (2013)

DY 29.2 Tue 18:15 Poster C

Large deviation statistics for self-propelled particles — •Kevin Kleinbeck, Patrick Pietzonka, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

For a self-propelled particle, e.g., a Janus particle, we calculate the probability of fluctuations in the displacement during long time intervals. The particle is modeled with a translational and a rotational degree of freedom, with the latter affecting the direction of the constant self-propelling force. Moreover, we assume that the particle has a permanent magnetic moment that interacts with an external magnetic field. This symmetry breaking leads to a non-vanishing average velocity. We apply large deviation theory to calculate extreme fluctuations beyond the Gaussian regime.

For externally driven particles, the displacement along individual trajectories is proportional to the entropy production. As a central result of stochastic thermodynamics, the probability distribution of such an observable satisfies a fluctuation theorem relating the left and the right wing of the distribution. We show how the lack of the proportionality to entropy production for the displacement of self-driven particles affects the characteristic shape of the probability distribution. Moreover, we prove that the distribution satisfies a symmetry that is similar to the fluctuation theorem, but contains an additional term that depends only on the ratio between the field strength and the propulsion force.

DY 29.3 Tue 18:15 Poster C

Fluctuating Lattice Boltzmann simulations of microswimmers — •Felix Winterhalter, Matthieu Marechal, and Klaus Mecke — Friedrich-Alexander-Universität, Erlangen, Germany

During the last years the interest in microswimmers has steadily increased. To gauge the effect of hydrodynamical interactions between the microswimmers and to include the flow of the solvent around the swimmer, a simulation technique with a good model for the solvent is required. Our method of choice is fluctuating Lattice Boltzmann simulations that includes thermal fluctuations, which are often important for synthetic swimmers. The currently existing particle simulation using the software WaLBerla is expanded to encompass self-propelled microswimmers to study their behavior in a variety of confining geometries and external fields. We are currently looking at ferromagnetic beads in an oscillating magnetic field and the flow field which is developing as a result of the collective motion.

DY 29.4 Tue 18:15 Poster C

Bead-spring microswimmers in a MPCD fluid — •Hendrik Ender and Jan Kierfeld — Theoretische Physik I, Technische Universität Dortmund, Germany

Bead-spring structures undergoing cyclic shape changes in a viscous liquid can serve as model systems for artifical 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 different swimmer shapes and show that cyclic changes of linker lengths can give rise to a net swimming motion. The model can be generalized by including more beads and represents a step towards the simulation of bigger capsule-like swimmers, which propel by cyclic swelling and shrinking.

DY 29.5 Tue 18:15 Poster C

Turbulence driven clustering in nematic active particles — Devin Waas, •Rebekka E. Breier, and Marco G. Mazza — MPI for Dynamics and Self-Organization, Göttingen

Many active swimmers are, especially in biological applications, exposed to a surrounding turbulent field. We assume the active particles to be self-propelled and to interact nematically with each other as well as with the turbulent field. We present a numerical study in terms of time-driven molecular dynamics simulations. The turbulent field is calculated via the so-called "Kraichnan model" which mimics the correct scaling behavior as given by the Kolmogorov law. We find that the turbulent field causes the active particles to cluster and investigate the clustering in detail. Moreover, the global alignment is destroyed by the turbulence.

DY 29.6 Tue 18:15 Poster C

The influence of intrinsic stochasticity on the stability and bifurcations of few-species networks — •Johannes Falk and Barbara Drossel — TU Darmstadt, Germany

Intrinsic stochasticity in biological networks arises due to the limited number of individuals, which have stochastic birth and death rates. These individuals can be the biomolecules of gene regulation networks or the number of animals of an ecological population in foodwebs. Understanding the influence of stochasticity is important for assessing the stability of a system or for suppressing fluctuations in synthetic networks. Two important effects of intrinsic stochasticity are the shift of bifurcation points and of the eigenvalues of the stability matrix. Since explicit stochastic simulation is very time-consuming, analytical approaches for evaluating these effects were developed by various groups. We will apply these approaches to small reaction networks consisting of 2-4 nodes, which can be interpreted as foodweb modules or small chemical reaction networks.

DY 29.7 Tue 18:15 Poster C

The effect of small population sizes on the dynamics of biological networks with few nodes — •Marc Mendler, Johannes Falk, and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt

Often, biological networks such as food webs or chemical reaction networks are described by deterministic coupled differential equations. However, in systems of only few individuals stochastic birth and death rates can modify the dynamics considerably, giving rise to macroscopic effects that cannot be explained by deterministic equations. When the intrinsic noise does not drive the system too far away from the deterministic limit, van Kampen's system-size expansion is a useful tool to calculate analytically the effects of stochasticity. Different groups have suggested different ways of applying the system-size expansion to small networks. We will compare these methods, determine their underlying assumptions and ranges of applicability, and compare analytical calculations to stochastic simulations.

DY 29.8 Tue 18:15 Poster C

Complex Polymers: DNA denaturation transitions — Yurij Holovatch[1,4] and •Christian von Ferber[2,3,4] — [1]Institute for Condensed Matter Physics, NAS Ukraine, Lviv — [2]Applied Mathematics Research Centre, Coventry University, Coventry, UK — [3]Heinrich-Heine University, Dusseldorf — [4]Doctoral College, Statistical Physics of Complex Systems, Leipzig-Lorraine-Lviv-Coventry (L4)

We reconsider the Poland and Scheraga model for the DNA denaturation transition taking into account environmental effects. Here, 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 influence 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 combinations of these. We show that all of these have significant effects on the transition.

DY 29.9 Tue 18:15 Poster C

The evolution of network structure in an evolutionary foodweb model without explicit population dynamics — •Tobias Rogge[1], Korinna T. Allhoff[2], and Barbara Drossel[1] — [1]TU Darmstadt, Germany — [2]UPMC Paris, France

Evolutionary foodweb models provide important insights into the stability and the functioning of ecosystems, since the network structure is a highly nontrivial outcome of the ongoing processes of species addition and species deletion. Here, we introduce and investigate an evolutionary food web model that includes no population dynamics but generates nevertheless a large variety of complex, multi-trophic networks. In this model, species are characterized by a few traits that are based on their body mass and that determine the connections to other species in the network. Starting from a simple initial network, the system evolves due to the addition of new species, which are modifications of existing species. Whether a new species can survive in the network depends on a criterion that takes into account the predators, the prey, and the competitors of the new species. When the new species survives, it changes the environment for other species, which will die out if they do not fulfil any longer the survival criterion.

Depending on the parameters, the long-term dynamics of the network can show layered structures, highly dynamical configurations with frequent extinctions, or frozen configurations that allow no mutant to survive. Using computer simulations and analytical calculations, we identify the conditions under which the different types of dynamical and structural patterns emerge.

DY 29.10 Tue 18:15 Poster C

Probing defects and correlations in the hydrogen-bond network of ab initio water — •Piero Gasparotto and Michele Ceriotti — Laboratory of Computational Science and Modeling, IMX, EPFL, 1015 Lausanne, Switzerland

Water is an unusual liquid and many of its unique properties are due to the presence of an highly-structured hydrogen-bond (HB) network that is populated by a wide variety of different coordination defects. Due to the structural constraints imposed by the HB network, coordination defects do not come alone, but clustered together. Here, we compute defect-resolved distribution functions from ab initio molecular dynamics to probe the radial and angular correlation between defects. In doing this, we shed light on how fluctuations from the ideal tetrahedral structure contribute to the total radial distribution function of liquid water. We also present a systematic comparison of the concentration of different defects and the structural correlations between them, with a variety of simulation protocols. For instance, we considered different temperature, system size, basis set, integrator timestep, cutoff for the plane waves, the modeling of van-der-Waals corrections, nuclear quantum effects or exact exchange. We also compare these results with those coming from empirical force field simulations. These comparisons show that regardless of the details of the choice of the water potential, the qualitative predictions of the defect distributions are very similar. The most significant effect can be attributed to dispersion interactions, that impact the most on the relative populations of the various defects.

DY 29.11 Tue 18:15 Poster C

Lateral migration of soft microparticles in wavy microchannels — •Matthias Laumann[1], Badr Kaoui[1], Georg Freund[1], Alexander Farutin[2], Chaouqi Misbah[2], Diego Kienle[1], and Walter Zimmermann[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]LiPhy, CNRS-Universite Joseph Fourier, F-28402 Saint-Martin d'Heres Cedex, France

We study the cross-streamline migration (CSM) of deformable particles in the limit of vanishing Reynold number in Poiseuille channel flow, which boundaries are spatially modulated. Using 1D dumbbells, 2D ring polymers, and 3D capsules, we demonstrate how the CSM can be modified when the waviness of the micro-channel is varied. Starting with the case of flat boundaries, these particles perform a CSM that is always directed towards the channel center. In the case of wavy boundaries, this centric motion may be reversed once the modulation amplitude exceeds a threshold, in which case the particles migrate off-center and approach a stationary trajectory, located between the walls and the channel center. The distance between such a trajectory and center can be increased by turning up the modulation amplitude, but depends also on other parameters such as the particle elasticity. The results shown are obtained via a perturbation calculation of the wavy Poiseuille flow in the limit of small modulation amplitudes, and is compared with those from Stokesian particle dynamics for arbitrary modulation amplitudes, showing good agreement. Out study suggests that the flow in wavy microfluidic channels may be exploited for the separation of particles.

DY 29.12 Tue 18:15 Poster C

Migration of soft particles in a modulated microchannel with flow along the grooves — •Winfried Schmidt, Matthias Laumann, and Walter Zimmermann — Theoretische Physik, Universitaet Bayreuth, Bayreuth, Germany

We find cross-streamline migration (CSM) of deformable particles in the low Reynold number limit in a plane Poiseuille flow with modulated boundaries and the flow along the grooves. CSM is studied for elastic 2D ring polymers, tetrahedrons and 3D capsules. We find two directions of cross-stream migration of particles. 3D particles migrate to the midplane between the two boundaries, similar as in the case of Poiseuille flow with plane boundaries [1]. In the case of modulated boundaries, the particles migrate in addition to the maxima and the minima of the distance between the two modulated boundaries. The migration velocity can be tuned by the amplitude of the boundary modulations. The migration velocity depends also on elasticity and size of the particles as well on the flow velocity. Our study suggests that the flow generated between wavy boundaries may be exploited for the separation of particles in modulated microfluidic channels.

[1] B. Kaoui, G. H. Ristow, I. Cantat, C. Misbah, W. Zimmermann, Phys. Rev. E 77 , 021903 (2008)

DY 29.13 Tue 18:15 Poster C

Phase-field model for phagocytosis — Kornelius Sücker[1], •Christian König[1], Walter Zimmermann[1], and Falko Ziebert[1,2] — [1]Theoretische Physik, Universität Bayreuth, Bayreuth, Germany — [2]Physikalisches Institut, Universität Freiburg, Freiburg, Germany

Phagocytosis is the process of engulfment of small (typically micron sized) particles by cells. It is used by unicellular organisms to take up nutrients, but also essential for the immune response in higher organisms. In contrast to the so-called endocytosis of nanoscale particles, which are taken up mainly by particle-induced membrane curvature, phagocytosis relies on active processes in the cytoskeleton. We here model the particle engulfment by a cell via a two-dimensional phase-field approach that allows to elegantly describe the moving cell boundary. The main mechanisms taken into account so far are the stimulation of actin polymerization and its associated propulsion force, as well as of motor contraction, by the presence of the particle.

DY 30: Poster - Complex nonlinear systems

Time: Tuesday 18:15–21:00 Location: Poster C

DY 30.1 Tue 18:15 Poster C

A stochastic individual-based model of the progression of atrial fibrillation — Eugene Chang[1], •Yen Ting Lin[2], Tobias Galla[2], Richard Clayton[1], and Julie Eatock[3] — [1]The University of Sheffield, Sheffield, UK — [2]The University of Manchester, Manchester, UK — [3]Brunel University London, Uxbridge, Middlesex, UK

Atrial fibrillation (AF) is one of the most common rhythm disorders in the heart, and it progresses through several stages. While mechanistic models of AF exist at cellular level, there is no systematic framework with which to connect these to population-level models of AF progression. In this work we propose a stochastic individual-based model of the progression of AF. The outputs of the model are times when the patient is in normal rhythm and AF. We carry out a population-level analysis of the statistics of disease progression. While the model is stylised at present and not directly predictive, future improvements are proposed to tighten the gap between existing mechanistic models of AF, and epidemiological data, with a view towards model-based personalised medicine.

DY 30.2 Tue 18:15 Poster C

From Number Theory to dynamics of ac+dc driven Frenkel-Kontorova model — •Jovan Odavic — Aachen University

The Frenkel - Kontorova (FK) model is widely used to describe systems where competition between length scales determines the ground state energy. Dissipative FK model has been often used as one of the most suitable models for description of different kinds of phenomena in many fields of physics, such as charge or spin density wave systems, vortex lattices, Josephson-junction arrays biased by external currents and in recent years even superconducting nanowires. Main feature of the model is the appearance of a step-like (or staircase) behaviour in the response function which are due to dynamical mode-locking (synchronization) of the internal frequency with the applied external one. We will explore these step-like features and their connection to some number theory results.

Key reference: - J. Odavic, P. Mali, J. Tekic, Farey sequence in the appearance of subharmonic Shapiro steps, Phys. Rev. E 91, 052904 - J. Odavic, P. Mali, J. Tekic, M. Pantic, M. Pavkov Hrvojevic, Application of largest Lyapunov exponent analysis on the studies of dynamics under external forces, pre-print: http://arxiv.org/abs/1510.07267

DY 30.3 Tue 18:15 Poster C

Frustrated magnetic clutches – do they really work? — •Simeon Völkel and Ingo Rehberg — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

It has been proposed to construct new types of couplings and gears

based on the interaction of magnetic multipoles. These couplings exploit a continuous degenerate ground state for the chosen arrangement of the multipoles.[1]

We study experimentally the structural stability of the most basic realization of such a coupling consisting in two magnetic dipoles, where each of them is mounted perpendicularly to its dipole moment on a shaft that allows for rotation around this fixed axis. While the first magnet is driven by a motor, the second magnet rotates freely. Depending on the relative arrangement, co-rotating, counterrotating and chaotic regimes are found.

[1] Johannes Schönke, Smooth teeth: Why multipoles are perfect gears, to be published in Phys. Rev. Appl.

DY 30.4 Tue 18:15 Poster C

A novel measure to distinguish limit cycles and chaotic attractors — •Hendrik Wernecke, Bulcsú Sándor, and Claudius Gros — Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main, Germany

In many dissipative dynamical systems exhibiting chaos there are parameter regions, where it is hard to distinguish between regular and chaotic motion. Then the attractors do not 'fill-up' the phase space, but the motion is bound to narrow areas. Furthermore, the maximum Lyapunov exponent can become arbitrary small in these regions, so that the standard classification can be difficult to interpret.

In the present work we describe a novel method that is able to draw a discrete distinction between limit cycles and chaotic attractors. Therefore we use the long-term distance between two trajectories starting close-by in the vicinity of the attractor and how this distance scales with the initial distance of trajectories. For the regular motion of a limit cycle one finds a linear scaling, while for the chaotic attractor the long-term distance is only correlated to the size of the attractor and therefore constant.

Furthermore, we propose a new classification of chaotic states in dissipative systems. We introduce the term 'weak dissipative chaos' for those chaotic attractors that can be distinguished from others by there topology. This classification is also indicated by the order of magnitude of the maximum Lyapunov exponent.

DY 30.5 Tue 18:15 Poster C

Nonlinear waves in biological membranes — •Julian Kappler and Roland R. Netz — Institut für Theoretische Physik, Freie Universität Berlin, 14195 Berlin, Germany

We present a theory for nonlinear waves in biological membranes. We compare predictions of this theory to recent measurements and find that our model is able to reproduce key experimental features, such as an abrupt increase in both range and velocity as the external driving amplitude is increased.

DY 30.6 Tue 18:15 Poster C

Evolution of random Boolean networks by a hill-climbing process under selection for robust functioning — •Lara Becker, Isabella-Hilda Bodea, and Barbara Drossel — TU Darmstadt, Germany

Gene regulatory networks (GRNs) play a vital role in the control of cellular processes, including differentiation, the cell cycle and metabolism. Like other biological systems, they are subject to noise, which can manifest itself e.g. as thermodynamic fluctuations. In order to maintain their functioning under stochastic influences, GRNs need to be robust, i.e. they must tolerate perturbations that would otherwise impair their funcionality.

We use Boolean threshold networks as a simple model for GRNs and subject individual networks to an evolutionary process, accepting only those mutations that do not reduce the fitness of the network. The fitness is evaluated based on the ability to display a predetermined dynamical behavior in the presence of noise. Stochastic influences are implemented through random changes in the state of nodes. A mutation modifies either the connections or update functions. We examine the change in structural as well as dynamical properties of the networks during the evolutionary process in dependence of the model parameters, and we relate them to the developing functional robustness.

DY 30.7 Tue 18:15 Poster C

Evolution of a population of Boolean threshold networks for a targeted expression pattern — •Isabella-Hilda Bodea, Lara Becker, and Barbara Drossel — TU Darmstadt, Germany

We study the evolution of a population of Boolean threshold networks under selection for dynamical robustness of a predefined expression pattern to noise.

Random Boolean networks were introduced in 1969 by S. Kauffman as a simple model for gene regulatory networks. The nodes of these networks represent genes that can only be in two different states, "on" (expressed) or "off" (not expressed). In spite of their simplicity, Boolean models are able to reproduce the essential dynamical steps of real developmental processes, where the network switches from one expression pattern to another one. Such switching processes must function reliably in the presence of mutations and dynamical noise.

In order to investigate the evolution of such gene regulatory networks in the presence of noise, we introduce stochasticity by perturbing the states of randomly chosen nodes. The evolutionary process proceeds with discrete generations, where the fitter part of the population become the parents of the next generation. While mutations act on the genotype, i.e. the connections between the nodes and the update functions, selection is based on the phenotype, i.e. the dynamical behaviour of a network. We investigate the mutational and dynamical robustness of the population as a function of time for different noise levels and mutation rates, as well as the dynamical properties of the evolved networks.

DY 30.8 Tue 18:15 Poster C

Leaf-to-leaf distances in ordered Catalan tree graphs — Andrew M. Goldsborough, John M. Fellows, Matthew Bates, S. Alex Rautu, George Rowlands, and •Rudolf A. Römer — University of Warwick, Coventry, CV4 7AL, UK

We study the average leaf-to-leaf path lengths on ordered Catalan tree graphs with n nodes and show that these are equivalent to the average length of paths starting from the root node. We give an explicit analytic formula for the average leaf-to-leaf path length as a function of separation of the leaves and study its asymptotic properties. At the heart of our method is a strategy based on an abstract graph representation of generating functions which we hope can be useful also in other contexts.

DY 30.9 Tue 18:15 Poster C

Autonomous learning in networks of heterogeneous relaxation oscillators — •Enrico Fengler, Jan F. Totz, and Harald Engel — Institut für Theoretische Physik, TU-Berlin, Berlin

Recently, networks of coupled phase oscillators with intrinsic time-delayed feedback have been trained to exhibit a desired level of partial synchronization adjusting their adjacency matrix accordingly [1]. We extend this model in two directions. First, we replace a single by a multi-valued target state. Second, instead of adapting the connection weights between the links in one network, we introduce linking probabilities between two nodes and study the performance of an ensemble of networks. Finally, in numerical simulations with a modified ZBKE model [2], we analyze numerically synchronization patterns in a network of heterogeneous Belousov-Zhabotinsky chemical oscillators [3].

[1] P. Kaluza, A.S. Mikhailov, Autonomous learning by simple dynamical systems with delayed feedback, Phys. Rev. E 90(R), 030901 (2014). [2] A. M. Zhabotinsky, F. Buchholtz, A. B. Kiyatkin, and I. R. Epstein, Oscillations and waves in metal-ion-catalyzed bromate oscillating reactions in highly oxidized states, J. Phys. Chem. 97, 7578 (1993). [3] J. F. Totz, R. Snari, D. Yengi, M. R. Tinsley, H. Engel, and K. Showalter, Phase-lag synchronization in networks of coupled chemical oscillators, Phys. Rev. E 92, 022819 (2015).

DY 30.10 Tue 18:15 Poster C

Feedback control in evolutionary dynamics: controlling the coexistence state — •Jens Christian Claussen — Computational Systems Biology, Jacobs University Bremen

Evolutionary dynamics in the frameworks of Lotka-Volterra systems and replicator equations in evolutionary game theory can include fixed points and cycles which can be neutrally stable, repelling or attracting. Of particular interest is the case where a coexistence state loses stability due to non-zero-sum payoffs, corresponding to dissipative interactions. Here I introduce a general ansatz of feedback control where an additive control term is implemented in the payoff matrix which is chosen proportional to an observable of the system which is suitably chosen to reflect the distance from the fixed point. This feedback control is implemented for the Rock-Paper-Scissors system which has applications in biology and in socio-economic systems, and for which the loss of stability depending on payoffs and population size has been recently discussed [J. Claussen and A. Traulsen, PRL 100, 058104 (2008)]. As the discretization stochasticity in a finite popula-

tion additionally destabilizes coexistence, here I discuss also an implementation by a pairwise comparison process to demonstrate that the control scheme is applicable in a finite population.

DY 30.11 Tue 18:15 Poster C

Reservoir computing simulated by using the Lang Kobayashi laser equations with time delayed feedback — •David Schicke, André Röhm, and Kathy Lüdge — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623Berlin, Germany

Reservoir computing has the potential to outperform traditional van-Neumann architectures in terms of swiftness as well as accuracy. Traditionally achieved by a system consisting of about 200-1000 physical nodes which are connected to each other, reservoir computing can also be performed by a single node with time delayed self feedback. Physical nodes are simulated as virtual nodes along the delay line. To achieve different coupling strength between virtual nodes, the input also has to be masked. Two different non-linearities are compared, one being the Ikeda nonlinearity, already discussed in e.g. [1], [2] and the other the Lang Kobayashi differential equation describing laser dynamics with linewidth enhancement and optical feedback. Their computing capability will be tested with the NARMA10 task, their performance expressed by the normalized root mean square error.

[1] Larger, L. et al., Photonic information processing beyond turing: an optoelectronic implementation of reservoir computing, *Optics Express* **20**, 3241-3249 (2012).

[2] Hermans, M. et al., Photonic Delay Systems as Machine Learning Implementations, *arXiv:* 1501.02592v1 [cs.NE] (2015)

DY 30.12 Tue 18:15 Poster C

Optimal demand control in a decentralized smart grid — •Sabine Auer[1,2], Kirsten Kleis[3], Paul Schulzu[1,2], Frank Hellmann[1], Jobst Heitzig[1], and Jürgen Kurths[1,2,4,5] — [1]Potsdam Institute for Climate Impact Research, 14412 Potsdam, Germany — [2]Department of Physics, Humboldt University Berlin, 12489 Berlin, Germany — [3]Oldenburg University, Germany — [4]Institute of Complex Systems and Mathematical Biology, University of Aberdeen, Aberdeen AB24 3FX, UK — [5]Department of Control Theory, Nizhny Novgorod State University, 606950 Nizhny Novgorod, Russia

The questions to what extent increasing shares in variable renewable energy sources influence power grid stability and whether additional costs will accrue at power markets are subject to a controversial public debate. Due to the broad scope of these questions, we show how conceptional models are built to test for the necessary model features for such a power system. To investigate grid stability, we test for the necessary model details for power grids [1] and the corresponding resilience measures. As a concept of cost efficient power balancing, we propose the optimal control of distributed generators and consumers based on a novel decentral smart grid approach [2]. Attempts how to incorporate market dynamics into such power grid models will be discussed [3, 4].

[1] S. Auer et al. arXiv:1510.05640 (2015). Submitted to EPJ. [2] B. Schäfer et al. arXiv:1508.02217 (2015). Submitted to EPJ. [3] M. Mureddu et al. Green power grids (2015). arXiv:1503.02957. [4] AH Mohsenian-Rad et al., IEEE Transactions on 1.2 (2010).

DY 30.13 Tue 18:15 Poster C

Dynamical Systems Based Modeling — •Bastian Seifert and Christian Uhl — University of Applied Sciences, Ansbach, Germany

Most approaches to the analysis of multi-variate time-series either reduce the dimensionality of the embedding or try to recognize the underlying dynamics. We present with Dynamical Systems Based Modeling an approach, which does both simultaneously. Consider a multivariate time-series q, which is subject to dynamics described by a (unknown) set of ordinary differential-equations

$$\dot{x_i} = d_i(x_1, \ldots, x_N),$$

with d_i a set of e.g. polynomial functions. We show how to define a cost-function, whose global minimum yields a low-dimensional embedding of the signal q and the corresponding dynamics in form of the coefficients for the differential equation d_i.

DY 30.14 Tue 18:15 Poster C

Survivability: How Dangerous Transients Affect the Stability of Dynamical Systems — •Paul Schultz[1,2], Frank Hellmann[1], Carsten Grabow[1], Jobst Heitzig[1], and Jürgen Kurths[1,2,3,4] — [1]Potsdam Institute for Climate Impact Research, P.O. Box 60 12 03, 14412 Potsdam, Germany — [2]Department of Physics, Humboldt University of Berlin, Newtonstr. 15, 12489 Berlin, Germany — [3]nstitute for Complex Systems and Mathematical Biology, University of Aberdeen, Aberdeen AB24 3UE, United Kingdom — [4]Department of Control Theory, Nizhny Novgorod State University, Gagarin Avenue 23, 606950 Nizhny Novgorod, Russia

The notion of a part of phase space containing desired/allowed states of a dynamical system is important in a wide range of complex systems research. It has been called safe operating space, viability kernel or sunny region. Here we define *survivability*: Given a random initial condition, what is the likelihood that the transient behaviour of a deterministic system leaves the region of desirable states? In conceptual examples we show that this basic measure captures notions of fundamental for interest various systems, e.g. climate models or power grids. We also derive a semi-analytic lower bound for the survivability of linear systems with polygonal safe operating space. We then apply the concept in the case the power grid model in realistic operating regimes to assess our analytic bound. Here, the kind of stability measured by survivability is of great practical interest. Furthermore, it is not captured by stability measures based on asymptotic trajectories.

DY 30.15 Tue 18:15 Poster C

Application of reduced-order model based on cluster analysis in numerical simulation of low permeability reservoir — •Weiwei Li[1,2], Yanyu Zhang[1], and Jianghai Lv[3] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]College of Petroleum Engineering, China University of Petroleum, 266580, Qingdao, China — [3]PetroChina ChangQing Oilfield Company Oil Production No.5, 710200, Xi'an, China

A mathematical model for a two dimensional reservoir considering the influence of start-up pressure gradients is solved based on a fully implicit finite difference scheme. The reduced-order model is established by projecting the original model on the low dimension which is formed by the basis function produced from the collected snapshots. The Lloyd algorithm for centroidal Voronoi tessellation is employed for cluster analysis to tackle the potential shortcomings from collecting snapshots with same time intervals. The computational results show that the used reduced-order model based on proper orthogonal decomposition is able to effectively approximate the results of the original model. With the help of the cluster analysis, data reduction is achieved on one hand, which could create uniform snapshots in space resulting to the enhanced accuracy of reduce-order model. On the other hand, extremely limited clustering groups might lead to loss of information and thus impairing the accuracy of the final reduced-order model.

DY 30.16 Tue 18:15 Poster C

Chimera states in chemical relaxation oscillators — •Julian Rode, Jan Totz, and Harald Engel — Technische Universität Berlin, Berlin

A system of identical oscillators with an identical coupling can differentiate in a synchronized and a desynchronized part, the so called chimera state [1]. Experiments on various chemical and physical systems have confirmed its existence [2]. We study the simplest scenario first: Ideal phase oscillators on a ring network. Inspired by real world oscillators like nerve cells, we take one further step and numerically explore chimera states on relaxation oscillators, which we compare with our experimental findings.

[1] Y. Kuramoto and D. Battogtokh, "Coexistence of coherence and incoherence in nonlocally coupled phase oscillators," Nonlin. Phenom. in Complex Syst. 5, 380 (2002)

[2] M. R. Tinsley, S. Nkomo, and K. Showalte, "Chimera and phase-cluster states in populations of coupled chemical oscillators." Nat. Phys. 8, 662 (2012) ; A. M. Hagerstrom et al. "Experimental observation of chimeras in coupled-map lattices." Nat. Phys. 8, 658 (2012)

DY 31: Poster - Pattern Formation

Time: Tuesday 18:15–21:00 Location: Poster C

DY 31.1 Tue 18:15 Poster C

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 stability properties of localized structures subjected to time-delayed feedback in systems with spatial inhomogeneities. Therefore, a Swift-Hohenberg model that describes the behaviour of transversal patterns in a passive cavity in two spatial dimensions is combined with an additional time-delayed feedback term and an inhomogeneous gaussian injection beam.

We show that varying the delay strength, the delay time and the shape of the injection beam leads to various dynamical solutions including drifting solutions, pinned oscillatory structures and the formation of spirals. The onset of these different instabilities can be predicted analytically in terms of a linear stability analysis of the delayed systems.

A special focus lies on the competing effects of the symmetry breaking inhomogeneity, which has a pinning effect on the localized structure, and the drift-inducing modes, which can be destabilized by time delayed feedback. The interplay of these competing effects leads to an oscillatory motion of the structure which is studied both numerically and analytically.

DY 31.2 Tue 18:15 Poster C

Patterns in a Flat Rotating Box — •Adrian Ebert[1], Anna Treffurth[1], and Thomas Grillenbeck[1,2] — [1]Ignaz-Günther Gymnasium Rosenheim, Germany — [2]Rosenheim University of Applied Sciences, Germany

If two granulates of different size and texture are filled into a flat container rotating along its horizontal axis, patterns form inside. At lower fill levels, vertical stripes develop; at higher ones, convection occurs reminiscent of rolls in the granular structure. This is astonishing, because, depending on the fill level, nearly no movement is possible and the rolls' rotating sense cannot be caused by the cell rotation. It has to be pointed out that the box must rotate over a long period, ca.10 hours at approximately 20 rotations per minute, in order to get the best results. We examine the various mechanisms which lead to the development of so-called "convection rolls", enabling us to clarify ample connections on the one hand and, on the other, generating completely new observations partially complying with the results of the research at Magdeburg University, but sometimes also raising new questions.

DY 31.3 Tue 18:15 Poster C

Sensitive Flames — •Adrian Ebert[1] and Thomas Grillenbeck[1,2] — [1]Ignaz-Günther-Gymnasium Rosenheim, Germany — [2]Rosenheim University of Applied Sciences, Germany

A combustible gas streams out of a fine nozzle and is lit above a copper mesh at a distance of ca. 5cm. The copper conducts away the heat, thus the flame only burns above the mesh and leaves a space of air underneath it. When an acoustic signal meets the resonance of the flame, delivering a certain amount of energy, the flame reacts very sensitively and changes its shape and size. A fishtail nozzle creates a membrane of fire which, in theory, allows an even easier influence. We examine this phenomenon, in order to spot the influence of various parameters.

DY 31.4 Tue 18:15 Poster C

Crystal growth in a channel: effects of the crystalline anisotropy — •Klaus Kassner[1], Jean-Marc Debierre[2], and Rahma Guérin[2] — [1]Otto-von-Guericke Universität Magdeburg, PF 4120, 39016 Magdeburg — [2]Laboratoire Matériaux et Microélectronique de Provence, Aix-Marseille Université, Case 142, F-13397 Marseille Cedex 20, France

Phase-field simulations are performed to explore the thermal solidification of a pure melt in three-dimensional capillaries. Following our previous work for isotropic or slightly anisotropic materials, we now focus on the more general case of anisotropic materials. Different channel cross-sections are compared (square, hexagonal, circular) to reveal the influence of the confining geometry and the effects of a competition between the crystal and the channel symmetries. In particular, the compass effect toward growth directions favored by surface tension is considered. At given undercooling and anisotropy, the simulations generally show the coexistence of several growth modes. The relative stability of these growth modes is tested by submitting them to a strong spatiotemporal noise for a short time. Similarities and differences with experimental growth modes in confined geometry are discussed qualitatively.

DY 31.5 Tue 18:15 Poster C

Measuring the stable range of localised patches of ferrofluidic spikes — •Robin Maretzki, Ingo Rehberg, and Reinhard Richter — Experimentalphysik 5, Universität Bayreuth

Spatial localisation has been predicted for many physical systems, however a comparison of experiment and theory is sparse - see [1] for a review. A convenient experiment is a layer of ferrofluid subjected to a homogeneous magnetic induction B. By applying local magnetic pulses localised radially symmetric spikes [2] have been generated in the bistable regime of the Rosensweig instability. Moreover, utilizing a pulse sequence in B, different localised hexagon patches have been uncovered in experiment [3]. Similar patches have been found as well by applying numerical continuation techniques to the Young-Laplace- and coupled Maxwell equations [3]. They undergo a 'homoclinic snaking' scenario, where each alternating turn of a 'snake' in control parameter phase space is correlated with a discontinuous jump of the topography of the localized pattern. In our contribution we investigate for the first time the range of stability of a patch under continuous variation of B, and the effects of magnetophoresis and magnetoviscosity.

[1] E. Knobloch, *Annu. Rev. Condens. Matter Phys.* **6**, 325 (2015).

[2] R. Richter, I. Barashenkov, *Phys. Rev. Lett.* **94**, 184503 (2005).

[3] D. B. Lloyd, C. Gollwitzer, I. Rehberg, R. Richter, *J. Fluid. Mech.* **783**, 283 (2015).

DY 31.6 Tue 18:15 Poster C

Modelling growth-induced wrinkling of elastic biofilms — •Horst-Holger Boltz and Stefan Klumpp — Faculty of Physics, Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Microbial biofilms have been an important subject of study in the recent years due to their biological, medical and technolog- ical relevance. Biofilms are large multicellular structures of microorganisms adherent to a substrate. The formation of these structures is usually accompanied by the production of an extracellular matrix formed by so-called extra-cellular polymeric substances (EPS). Thus, an elastic film is created that is growing due to the ongoing cell growth and division as well as the continued production of EPS. This growth leads to residual and dynamic stresses that are relieved by a non-planar pattern-formation (wrinkling). We study the mechanics of this morphoelastic problem.

DY 31.7 Tue 18:15 Poster C

Lattice model of 'sticky' hard rods: Bulk equilibrium and layer growth at a substrate — •Miriam Klopotek[1], Martin Oettel[1], Hendrik Hansen-Goos[2], Yuding Ai[3], Eelco Empting[1], and Frank Schreiber[1] — [1]Institute for Applied Physics, University of Tübingen — [2]Institute for Theoretical Physics, University of Tübingen — [3]Hanover College, IN, USA

We model 3D hard rods in the vicinity of a substrate in a lattice model that includes 'sticky' interactions between the rods and/or with the substrate. This study continues a previous lattice-model study of purely hard-core rods forming a monolayer. Rods in bulk are investigated in equilibrium via grand canonical Monte Carlo (GCMC) methods and rods on a substrate out-of-equilibrium via kinetic Monte Carlo (KMC). Specifically, successive umbrella sampling was employed for bulk-GCMC [1].

We seek to understand the origin of structures that form during growth, i.e. if they stem from equilibrium phases or are the products of kinetic effects. Thin film growth is a topic of fundamental experimental research, in particular for organic molecules with semiconducting properties. Organic molecules are typically highly anisotropic, showing intricate ordering not seen in the case of isotropic molecular/atomistic films [2]. Our models explore the effect of particle anisotropy plus interactions with each other and the substrate.

[1] R.L.C. Vink, S. Wolfsheimer, and T. Schilling, *J. Chem. Phys.*

123(7):074901, 2005.
[2] S. Kowarik et al., *Phys. Rev. Lett.* **96**:125504, 2006.

DY 31.8 Tue 18:15 Poster C

Thin film and kinetic Monte Carlo modeling of Rayleigh-Plateau instabilities of ridges on substrates — Walter Tewes[1], •Oleg Buller[2], Svetlana Gurevich[1], Andreas Heuer[2], and Uwe Thiele[1] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster — [2]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149 Münster

The Rayleigh-Plateau-like instability of ridges formed by molecules on prepatterned substrates is studied by means of Kinetic Monte Carlo (KMC) simulations and a thin film continuum model. We show systematically the qualitative agreement of the occurring instability in both models. In particular, we demonstrate that in the KMC model the transversal instability of ridges occurs on well defined scales which are significantly larger than the intrinsic scales of thermodynamical fluctuations. In the thin film model, the transversal instabilty for a single ridge and two weakly interacting ridges is investigated through a transversal linear stability analysis. We show the dispersion relations for transversal modulations and investigate their dependency on the system parameters. In regimes accessible to direct simulations, similar results are obtained for the KMC model. Finally a mapping of the two model approaches in terms of energetics and statics is discussed for the case of homogeneous substrates.

DY 31.9 Tue 18:15 Poster C

Network properties of mitochondria in mammalian cells — •Lorenz Stadler, Sven Bauernfeind, and Matthias Weiss — Experimental Physics I, University of Bayreuth

Mitochondria are the power plants of eukaryotic cells. Besides being the production site for ATP, they are involved in many other vital cellular functions, e.g. apoptosis and Ca2+ homoiostasis. In contrast to textbook illustrations, mitochondria typically form extensive networks throughout mammalian cells rather than being individual granule-like organelles. Mitochondrial networks are subject to constant remodeling, i.e. mitochondrial tubes undergo continuous fission and fusion cycles. To gain insights into the network dynamics, we have analyzed mitochondrial phenotypes in untreated and drug-treated HeLa cells by confocal live cell imaging. Using a custom-made analysis tool, we have determined topological, geometrical, and polymeric parameters of the mitochondrial network. As a result, we observed that the overwhelming majority of nontrivial network nodes are three-way junctions with an exponential distribution of connecting link lengths. Moreover, our data suggest an immediate reaction of the mitochondrial network phenotype to a drug-induced breakdown of the cytoskeleton, whereas stabilization of microtubules had little effect.

DY 31.10 Tue 18:15 Poster C

Particle-based computer simulations of the Min-system — •Nikolas D. Schnellbächer[1,2], Artemij Amiranashvili[1,2], and Ulrich S. Schwarz[1,2] — [1]BioQuant, Heidelberg, Germany — [2]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

E. Coli and similar bacteria use a system of so-called Min-proteins to find the middle for cell division. The Min-system can also be reconstituted outside the cellular context and then leads to a variety of dynamic oscillatory patterns whose details depend both on global compartment geometry and local binding kinetics. We use three-dimensional and stochastic particle-based computer simulations to predict pattern formation as a function of geometry. We investigate the stability of different oscillation modes on the same pattern and the stochastic switching between them. We find that the number of membrane bound molecules is independent of the volume to area ratio and establish requirements for a sharp MinE-ring formation, depending on different MinE-binding modes.

DY 31.11 Tue 18:15 Poster C

Membrane instability driven by an ac electric field — •Mirko Ruppert[1], Walter Zimmermann[1], and Falko Ziebert[1,2] — [1]Theoretische Physik, Universität Bayreuth, Bayreuth, Germany — [2]Physikalisches Institut, Universität Freiburg, Freiburg, Germany

Unilamellar vesicles are important model systems in biophysics. They are typically created by applying a voltage on a stack of membrane bilayers, but this so-called electroformation process is still poorly understood. Models exist for the case of a static (dc) electric field, but experimentally typically ac fields of about 10 Hz have to be used. We therefore study the ac field-induced instability of a capacitive membrane, using an effective zero-thickness model developed previously in the dc case. The instability of the membrane is driven by the charge accumulation in the Debye layers. Increasing the driving frequency reduces this effect. A full Floquet analysis of the coupled Poisson-Nernst-Planck-Stokes boundary value problem is under way.

DY 31.12 Tue 18:15 Poster C

Wavenumber restriction in narrow anisotropic pattern forming systems — •Konstantin Speckner, Fabian Bergmann, Lisa Rapp, and Walter Zimmermann — Theoretische Physik, Universität Bayreuth, Bayreuth, Germany

We investigate stripe patterns in anisotropic pattern forming systems, wherein stripes orient perpendicular (y-direction) to the preferred x-direction. In such systems supercritically bifurcating stripes are stable within a finite range of wavenumbers, the so-called Eckhaus stability band. We study for this class, how spatial variations of the control parameter along the y-direction restrict the band of stable wave numbers? We use simulations of a 2d anisotropic Swift-Hohenberg model where the control parameter is supercritical in a narrow subdomain along the y-axis and then drops down to subcritical values outside that y-domain. The wavenumber range of stable periodic patterns is restricted when the control parameter drops down to subcritical values outside a finite y-domain. We also show that this wavenumber restriction depends on the steepness of such control parameter drops. As a result, the number of defects in stripe patterns evolving from random initial conditions is reduced. Furthermore, we discuss possible applications to wrinkle forming systems.

DY 31.13 Tue 18:15 Poster C

Branched-wrinkles in inhomogeneous film-on-substrate systems — •Roland Aichele[1], Badr Kaoui[1,2], Falko Ziebert[1,3], and Walter Zimmermann[1] — [1]Theoretische Physik, Universitaet Bayreuth, Bayreuth, Germany — [2]Biomechanics and Bioengineering, Universite de Technlogie de Compiegne, Compiegne, France — [3]Physikalisches Institut, Albert-Ludwigs-Universitaet Freiburg, Freiburg, Germany

We model wrinkle formation in thin-solid films supported by soft substrates and subjected to axial compression. Spatial variations of the elasticity of the substrate or of the thin film lead effectively to a spatial variation of the range of accessible wavle-lengths of wrinkle's, and beyond a critical amplitude of the wave-length modulation stable branched wrinkles may emerge. The branching points of the wirnkles are located along step like parameter changes. For a given parameter set, one finds a whole familiy of stable branched periodic pattern and it depends on the initial conditions which of the stable pattern is reached. If parameters change smoothly, the branching points connecting the wrinkles of different wavelength show complex orderings. Smooth parameter variations reduce the stability domains of branched pattern and may lead to complex ordering of the branching points.

B. Kaoui, A. Guckenberger, A. Krekhov, F. Ziebert, W. Zimmermann, New J. Phys. 17, 103015 (2015);B. A. Glatz, M. Tebbe, B. Kaoui, R. Aichele, C. Kuttner, A. E. Schedl, H.-W. Schmidt, W. Zimmermann, A. Fery, Soft Matter 11, 3332 (2015)

DY 32: Poster - Turbulence

Time: Tuesday 18:15–21:00 Location: Poster C

DY 32.1 Tue 18:15 Poster C

Advanced stochastic methods for description of wind gusts — •Christian Behnken[1,2], Ali Hadjihosseini[1,2], Matthias Wächter[1,2], and Joachim Peinke[1,2] — [1]ForWind — [2]Institute of Physics, Carl von Ossietzky University of Oldenburg, 26111 Oldenburg, Germany

Since the share of wind energy in the global energy production is increasing, there is a demand for methods able to capture short time dynamics of wind speeds, which are of great importance for load situations and energy conversion of wind turbines. Firstly, a stochastic analysis of measured wind speed increments has been performed, showing pronouncedly heavy-tailed distributions of wind speed increments for different time scales. Secondly, setting up a coupled system of Langevin equations for these increments, we can estimate drift and diffusion coefficients directly from data which allow for a quantification of the dynamics of increments along the wind profile. Furthermore a stochastic method based on multi-point statistics of increments, joint probabilities and the Markov property is introduced as a tool to reconstruct and model time series of complex systems containing extreme events for a range of scales. It has been shown that the underlying stochastic processes of such time series are governed by a Fokker-Planck-Equation which enables one to statistically capture extreme events accurately. Particularly because there is still no widely accepted definition of wind gusts this might turn out as a promising approach not only for grasping wind gusts, but as well for forecasting of such.

DY 32.2 Tue 18:15 Poster C

Rotation rate of particle pairs in turbulent flow — •Ali Ghaemi and Abdallah Daddi-Moussa-Ider — Biofluid Simulation and Modeling, University of Bayreuth, Germany

The dynamics of solid particles in turbulent flow plays a key role in many environmental phenomena. For instance, the eruption of volcanoes releases particles with different sizes into the atmosphere which then are transported with turbulent currents. In this work, the statistics of particle pair orientation is numerically studied in homogeneous isotropic turbulent flow. We show that the Kolmogorov picture fails to predict the observed probability density functions (PDFs) of the pair rotation rate and the higher order moments accurately. Therefore, a multifractal formalism is derived in order to include the intermittent behavior that is neglected in the Kolmogorov phenomenology. The PDFs of finding the pairs at a given angular velocity for small relative separations reveals extreme events with stretched tails and high kurtosis values. Furthermore, The PDFs are found to be less intermittent and follow a complementary error function distribution for larger separations.

DY 32.3 Tue 18:15 Poster C

Modelling of a coupled mechanical-hydrodynamic system for flow control — •Max Huber[1,3], Andreas Zienert[2], Hans-Reinhard Berger[1], and Jörg Schuster[3] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Reduction of drag and noise as well as lift enhancement for airplane wings can be achieved with actice flow control, using synthetic jet actuators (SJA). These devices consist of a closed cavity with a small orifice and a movable piezoelectric diaphragm. The oscillation of the diaphragm generates the synthetic (i.e. zero net mass flux) jet that transfers momentum to the surrounding medium.

The present work introduces an analytical model to study the interaction between the driving force of the SJA, the pressure inside the cavity and the flow velocity through the orifice. For this purpose, the oscillating diaphragm is treated as a spring pendulum. Fundamental equations from hydrodynamics describe the flow of the fluid.

Besides, simulations based on finite element method (FEM) were carried out to solve the Navier-Stokes equations. While the straightforward analytical approach describes pressure and flow velocitiy in the SJA and its orifice, FEM shows the train of vortices outside the SJA which is the cause of the momentum flux.

DY 33: Transport: Graphene (Joint session of DS, DY, HL, MA, O and TT organized by TT)

Time: Wednesday 9:30–13:15 Location: H22

Invited Talk DY 33.1 Wed 9:30 H22

Ultrafast photo-thermoelectric currents in graphene — •Alexander Holleitner — Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany.

We show that photo-thermoelectric currents occur on a picosecond time-scale in graphene [1]. To this end, we apply an on-chip pump/probe photocurrent spectroscopy [2,3] to double-gated junctions of graphene. Our experiments reveal the interplay of photogenerated hot electrons with so-called photovoltaic currents. Moreover, we demonstrate that hot electrons allow to read-out an ultrafast non-radiative energy transfer from fluorescent emitters, namely nitrogen-vacancy centers in nano-diamonds. The non-radiative energy transfer can be exploited as an ultrafast, electronic read-out process of the electron spin in nitrogen vacancy centers in the diamond nanocrystals. The detection gives access to fast energy transfer processes, which have not yet been observed by fluorescence measurements because of quenching of the optical signal for short transfer distances [4].

We thank A. Brenneis, F. Schade, L. Gaudreau, M. Seifert, H. Karl, M.S. Brandt, H. Huebl, J.A. Garrido, F.H.L. Koppens, for a very fruitful collaboration, and the ERC-grant 'NanoREAL' for financial support.

[1] A. Brenneis et al., (2016)
[2] L. Prechtel et al., Nature Comm. **3**, 646 (2012)
[3] C. Kastl et al. Nature Comm. **6**, 6617 (2015)
[4] A. Brenneis et al. Nature Nanotech. **10**, 135 (2015)

DY 33.2 Wed 10:00 H22

Double-logarithmic velocity renormalization at the Dirac points of graphene — •Peter Kopietz, Anand Sharma, and Carsten Bauer — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Str. 1, 60438 Frankfurt

Using a functional renormalization group approach with partial bosonization in the forward scattering channel we reconsider the effect of long-range Coulomb interactions on the quasi-particle velocity v_k close to the Dirac points of graphene. In contrast to calculations based on perturbation theory and field theoretical renormalization group methods, we find that v_k is proportional to $\ln[\kappa_k/k]$ where k is the deviation of the quasiparticle momentum from the Dirac points and the cutoff scale κ_k vanishes logarithmically for small k. We show that this double-logarithmic singularity is compatible with experiments and with the known three-loop expansion of v_k which contains terms of order $\ln k$ and $\ln^2 k$.

DY 33.3 Wed 10:15 H22

Dirac fermion wave packets in oscillating potential barriers — Walter Pötz[1], Sergey E. Savel'ev[2], Peter Hänggi[3], and •Wolfgang Häusler[3] — [1]Karl Franzens Univ. Graz, Inst. Phys., A-8010 Graz, Austria — [2]Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom — [3]Institut für Physik, Univ. Augsburg, 86135 Augsburg, Germany

We integrate the time-dependent (2+1)D Dirac equation for massless fermions in graphene or topological insulator surfaces. A recently developed staggered-grid leap-frog scheme is employed [1,2]. We consider an initial Gaussian wave packet which moves in the x-direction towards a potential barrier that is homogeneous along y and oscillates periodically in time. As for the x-dependence, we investigate square-

well, sinusoidal, and linear-ramp potential profiles. Small transversal momentum components k_y of the wave packet were analyzed analytically [3] and predicted to generate non-zero current densities j_y, even at normal incidence $k_y = 0$ [4]. These findings are consistent with the present numerical studies of particle-, current-, and spin-density. We also investigate massive fermions: regarding some properties they resemble massless fermions, regarding other properties, however, peculiar intrinsic oscillations, reminiscent of Zitterbewegung, appear.

[1] R. Hammer and W. Pötz, PRB **88**, 235119 (2013)
[2] R. Hammer *et al.*, J. Comp. Phys. **265**, 50 – 70 (2014)
[3] S.E. Savel'ev, W. Häusler, and P. Hänggi, PRL **109**, 226602 (2012)
[4] S.E. Savel'ev, W. Häusler, and P. Hänggi, EPJB **86**, 433 (2013).

DY 33.4 Wed 10:30 H22

Electric and magnetic control of electron guiding in graphene — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

Electrons in graphene are known to behave like massless Dirac fermions, whose transport properties can be best revealed by experiments using ultra-clean graphene. Reliable quantum transport simulations for ballistic graphene is naturally a powerful tool for understanding and predicting high-quality transport experiments. In this talk we show gate-controlled electron guiding along electrically confined channels in suspended graphene, which is a combined work of our transport simulations and the experiment done by the Schönenberger group [1]. We have recently further applied our simulation (Green's function method within the scalable tight-binding model [2]) to revisit the transverse magnetic focusing experiment [3], where the guiding of the electrons is controlled by an external magnetic field, instead of electrical gates. Besides good agreement with the experiments [1,3], our simulations further allow for probing charge flow through an additional scanning probe tip.

[1] P. Rickhaus *et al.*, Nano Lett. **15**, 5819 (2015).
[2] M.-H. Liu *et al.*, Phys. Rev. Lett. **114**, 036601 (2015).
[3] T. Taychatanapat *et al.*, Nat. Phys. **9**, 225 (2013).

DY 33.5 Wed 10:45 H22

Current flow paths in deformed graphene: from quantum transport to classical trajectories in curved space — •Nikodem Szpak[1] and Thomas Stegmann[1,2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca

We compare two contrasting approaches to the electronic transport in deformed graphene: a) the condensed matter approach in which current flow paths are obtained by applying the non-equilibrium Green's function (NEGF) method to the tight-binding model with local strain, b) the general relativistic approach in which classical trajectories of relativistic point particles moving in a curved surface with a pseudomagnetic field are calculated. The connection between the two is established in the long-wave limit via an effective Dirac Hamiltonian in curved space. Geometrical optics approximation, applied to focused current beams, allows us to directly compare the wave and the particle pictures. We obtain very good numerical agreement between the quantum and the classical approaches for a fairly wide set of parameters. The presented method offers an enormous reduction of complexity from irregular tight-binding Hamiltonians defined on large lattices to geometric language for curved continuous surfaces. It facilitates a comfortable and efficient tool for predicting electronic transport properties in graphene nanostructures with complicated geometries, paving the way to new interesting transport phenomena such as bending or focusing (lensing) of currents depending on the shape of the deformation. It can be applied in designing ultrasensitive sensors or in nanoelectronics.

DY 33.6 Wed 11:00 H22

Trigonal Warping in Bilayer Graphene: Energy versus Entanglement Spectrum — •Sonja Predin, Paul Wenk, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We present a mainly analytical study of the entanglement spectrum of Bernal-stacked graphene bilayers in the presence of trigonal warping in the energy spectrum. Upon tracing out one layer, the entanglement spectrum shows qualitative geometric differences to the energy spectrum of a graphene monolayer. However, topological quantities such as Berry phase type contributions to Chern numbers agree. The latter analysis involves not only the eigenvalues of the entanglement Hamiltonian but also its eigenvectors. We also discuss the entanglement spectra resulting from tracing out other sublattices.

15 min. break

DY 33.7 Wed 11:30 H22

Valley-based Cooper pair splitting via topologically confined channels in bilayer graphene — •Alexander Schroer[1], Peter G. Silvestrov[1], and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology Braunschweig, D-38106 Braunschweig, Germany

Bilayer graphene hosts valley-chiral one-dimensional modes at domain walls between regions of different interlayer potential or stacking order. When such a channel is close to a superconductor, the two electrons of a Cooper pair, which tunnel into it, move in opposite directions because they belong to different valleys related by the time-reversal symmetry. This kinetic variant of Cooper pair splitting requires neither Coulomb repulsion nor energy filtering but is enforced by the robustness of the valley isospin in the absence of atomic-scale defects. We derive an effective normal/superconducting/normal (NSN) model of the channel in proximity to an *s*-wave superconductor, calculate the conductance of split and spin-entangled pairs, and interpret it as a result of *local* Andreev reflection, in contrast to the widespread identification of Cooper pair splitting with crossed Andreev reflection in an NSN geometry.

DY 33.8 Wed 11:45 H22

The decisive role of stacking faults for understanding transport in bilayer graphene — •Heiko B. Weber[1], Ferdinand Kisslinger[1], Christian Ott[1], and Sam Shallcross[2] — [1]Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany — [2]Lehrstuhl für Theoretische Festkörperphysik, FAU Erlangen-Nürnberg (FAU)

Charge transport in bilayer graphene provides rich low-temperature phenomena, often assigned to interaction-driven phase transitions. We will discuss charge transport in bilayer graphene in a single-particle picture, but including stacking faults. Such partial dislocations are unavoidable in bilayer graphene and were recently imaged [1]. Depending on details, partial dislocations can introduce improved conductance, fully insulating behaviour or linear magnetoresistance. The latter is reliably found in transport experiments at elevated temperatures [2].

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature **505**, 533 (2014)
[2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Phys. **11**, 650 (2015).

DY 33.9 Wed 12:00 H22

Linear magnetoresistance in two-dimensional disordered conductors — •Ferdinand Kisslinger[1], Christian Ott[1], Erik Kampert[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany. — [2]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.

The recent observation of linear magnetoresistance (MR) in large-area bilayer graphene gives a key to the understanding of this old and barely understood phenomenon [1]. In bilayer graphene, it can be traced back to mosaic-like pattern of a partial dislocation network [2]. In this talk we discuss how linear MR evolves in disordered samples, using a two dimensional resistor network model conceptually introduced by Parish and Littlewood [3]. This model is in the weak disorder regime dominated by boundary effects. We identified a new regime representing the bulk situation in a disordered conductor. We investigated different possible sources of disorder: mobility, charge carrier density and network structure. The slope of the MR turned out to be simply governed by the Hall resistance and therefore by the inverse of the charge carrier density. An equivalent circuit model finally gives a consistent explanation as to why the magnetoresistance is linear in mosaic like samples.

[1] F. Kisslinger et al., Nature Physics **11**, 650 (2015)
[2] B. Butz et al., Nature **505**, 533 (2014).
[3] M. M. Parish & P. B. Littlewood, Nature **426**, 162 (2003)

DY 33.10 Wed 12:15 H22

Mechanically strained graphene nanojunctions — •Seddigheh Nikipar[1], Dmitry Ryndyk[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Germany

It has been demonstrated recently that mechanically strained graphene presents interesting electrical properties, which have great potential for novel applications in electronic devices. In particular, the strain in graphene nanoribbons can lead to substantial changes in its electronic properties. Besides, it provides a possibility to develop atomic point contacts and break junctions. The main purpose of this work is to investigate theoretically the influence of uniaxial mechanical strains on graphene nanojunctions in order to design graphene point contact.

To this aim, we developed the computational model by combining density functional theory and molecular dynamics methods. First, we investigated the change of the junction shape with increasing strain and the breaking with the formation of the nanogap. As expected, our theoretical model predicts the deformation of the break junction bottleneck into carbon chains before the rupture of the structure. we evaluated the electronic transmission function of graphene quantum junction by employing a coupled tight bonding and nonequilibrium green function methods. Interestingly it is found that graphene point contact can present resonance transmission in contrast to the conventional metallic point contacts with quantized conductance. This might be originated from influence of other parameters on transmission.

DY 33.11 Wed 12:30 H22

Graphene nanoribbons as effective spin ladders — •Cornelie Koop, Manuel J. Schmidt, and Stefan Wessel — Institut für Theoretische Festkörperphysik, RWTH Aachen University

Zigzag edges of graphene nanoribbons host particular, localized edge states. Since the density of states is strongly enhanced near the edges in graphene, interaction effects between the spins of these edge states become important. We can significantly simplify the analysis of such systems by means of an effective model that separates the edge and bulk states. Treating the effective interactions to first order proves sufficient in most cases, while second order corrections do not dramatically change the results. In many cases, the edge system can be reduced to a general spin ladder model, where the decay of the spin-spin interaction is determined by the shape of the edges. We examine these effective spin ladders at finite temperatures by means of quantum Monte Carlo simulations, using the stochastic series expansion method. Thereby, correlation functions and spin structure factors can be determined for realistically large graphene nanoribbons.

DY 33.12 Wed 12:45 H22

Edge State Structure of the $\nu = 0$ quantum Hall State in monolayer Graphene — •Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Université Paris 11, CNRS, LPTMS, UMR 8626, Orsay 91405 France

Single-layer graphene at neutrality under a magnetic field is a many-body insulator whose phase structure is under intense scrutiny. When tilting the applied magnetic field, there is a phase transition towards a conducting state [1]. A plausible description is to start from a SU(4) spin-valley symmetric quantum Hall ferromagnet and add some lattice-scale anisotropies in valley space [2]. In the manifold of ground states captured by this approach, it has been proposed that graphene undergoes a transition between a canted antiferromagnetic state and a ferromagnetic state. While this picture is clear in the bulk of the system, it remains to understand the effect of this phase change on the current-carrying edge states that are formed a the physical boundaries of a real sample [3]. We use an extended Hartree-Fock approach to describe a finite-size system with a simple model for the edge and extract the one-body spectrum. We then describe the current-carrying edge textures.

[1] A. F. Young et al., Nature (London) 505, 528 (2014) [2] M. Kharitonov, Phys. Rev. B 85, 155439 (2012) [3] M. Kharitonov, Phys. Rev. B 86, 075450 (2012); G. Murthy et al., Phys. Rev. B 90, 241410 (2014) and arXiv:1510.04255; A. Knothe and T. Jolicoeur, Phys. Rev. B 92, 165110 (2015)

DY 33.13 Wed 13:00 H22

Spin lifetimes exceeding 12 ns in graphene non-local spin valves at room temperature — •Christopher Franzen[1], Marc Drögeler[1], Frank Volmer[1], Tobias Pohlmann[1], Maik Wolter[1], Kenji Watanabe[2], Takashi Taniguchi[2], Christoph Stampfer[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

We present spin transport measurements on graphene non-local spin transport devices by fabricating the electrodes first and subsequently transfer graphene with hexagonal boron nitride on top [1]. We achieve spin lifetimes of 12.6 ns and a spin diffusion length as high as 30 μm at room temperature.

This improvement exceeds all current models for contact-induced spin dephasing which paves the way towards probing intrinsic spin properties of graphene. Furthermore, we investigate the contact properties of our devices using scanning force microscopy (SFM) and conductive SFM. We discuss the importance of using large area hexagonal boron nitride for the transfer process and for achieving such high spin lifetimes and spin diffusion lengths.

[1] M. Drögeler *et al.* Nano Letters **14**, 6050 (2014).

DY 34: Crystallization, Nucleation, Self Assembly I (joint session CPP/DY, organized by CPP)

Time: Wednesday 9:30–12:15 Location: H42

Invited Talk DY 34.1 Wed 9:30 H42

Polymer crystallization and nucleation: New insights from fast scanning calorimetry — •Christoph Schick[1], Evgeny Zhuravlev[1], and René Androsch[2] — [1]University of Rostock, Institute of Physics, 18051 Rostock — [2]Martin-Luther-University Halle-Wittenberg, Center of Engineering Sciences, 06099 Halle/Saale

Crystallization commonly starts from a (sub)nanoscale nuclei which eventually growth to a crystal. Classical nucleation theory (CNT) provides a qualitative description of these processes. Nevertheless, CNT often fails to predict nucleation and crystallization on a quantitative level. Differential scanning calorimetry (DSC) is often employed to probe such complex phase transitions. The traditional DSC is limited in its cooling capability to cooling rates below 10 K/s. However, many materials are crystallizing, e.g. during processing, at much faster cooling rates (100 to a few 1000 K/s). Knowledge about the phase transitions on fast cooling is therefore required. Chip based calorimeters cover this range but so far they do not allow to obtain the full information for fast crystallizing materials like PE or PTFE. Faster controlled cooling and heating rates above 106 K/s are therefore required. These novel fast scanning calorimeters were used in combination with conventional DSC to study crystallization of polymers on fast cooling, isothermal crystallization after fast quenches, the efficiency of nucleating agents, the kinetics of crystal nucleation and the kinetics of the glass transition. The basic principle of the new technique and applications to polymeric and non-polymeric materials will be presented.

DY 34.2 Wed 10:00 H42

Elementary steps of chain folding in a melt of linear polyethylene * a proposal for discussion. — •Heinz H. W. Preuss — Sedanstr. 6, 31785 Hameln

As far as lamellae of crystalline polyethylene from solution or melt consist of close folded molecular chains (Preuss DPG Spring Meeting 2015, CPP 6.7), one has to find out how the folding can occur. The answer is in the understanding of the limited mobility and flexibility of polymer molecules in a melt. If the molecules are with a large portion nearly close and parallel packed, they can move freely in the direction of their backbone by *worming*(Faraday Discussion 1979, F. C. Frank, p 7 ff., A. Keller, p.146 ff.).In the direction perpendicular to the backbone, molecules have 8,5 % (1/12)of their diameter as average room of move for isomeric exchange of the place of C and H atomes. By simultaneous exchange of some C-H-pairs one can get pairs of folds in an extended chain keeping its general orientation. This would be possible with small molecules neighbouring only and should occur already during polymerization in solution or gas. The expression *adjacent reentry* is in this context a source of missunderstandig, for it provokes the meaning, molecules would move out of the place of junktion in a lamella and would reenter nearby after returning, a probably impossible motion.

DY 34.3 Wed 10:15 H42

How realistic are *random coils* in HD-PE? Analysis of the closeness of the packing. — •Heinz H. W. Preuss — Hameln

In a previous talk (CPP 6.7 Spring Meeting 2015) was demonstrated evidence of chain folding in HD-PE after slow cooling from the melt. With an analysis of the density and closeness of Packing including a model experiment with balls close wound with a clothes line one can learn that the density of the melt can be reached only with a high portion (at 80 %) of chain segments beeing nearly close and parallel neigbouring but not with *random coils* understood as balls packed with an entangeled molecular chain. The conformation in the melt should be near to the conformation in the crystal what is easy to be understood with the existence of folded chains in the melt. Compared with the crystal structure in the melt the molecules have 27,6 % more volume and 8,5 % more average distance available for mobility and flexibility. The random coil remains an important abstract mathematical tool, but should not be missinterpreted as if an arbitrarily coiled line could be a correct model of polymer molecules in a melt.

DY 34.4 Wed 10:30 H42

Wang-Landau simulation of short single polyethylene chain's "crystallization" — •Timur Shakirov and Wolfgang Paul — University of Halle, Halle, Germany

The phase behaviour of polyethylene has been under wide investigation during the last 6 decades. But investigation of single chain crystallization is a technically difficult problem. In the case of molecular dynamics simulations, it is not so easy to distinguish kinetic and thermodynamic effects on chain folding. We present results of a Wang-Landau type Monte Carlo study at thermodynamical equilibrium of folding of a single polymer chain. Our simulations are based on a chemically realistic united atom model [1].

[1] W. Paul, D.Y. Yoon, G.D. Smith. An optimized united atom model for simulations of polymethylene melts. The Journal of chemical physics, 103(4), 1702-1709. (1995)

15 min. break

DY 34.5 Wed 11:00 H42

Control of homogeneous crystal nucleation in polymers — •Evgeny Zhuravlev[1], Jürn Schmelzer[1], René Androsch[2], and Christoph Schick[1] — [1]University of Rostock, Institute of Pysics, Wismarsche Str, 43-45, 18057 Rostock — [2]Martin-Luther-University Halle-Wittenberg, Center for Engineering Sciences, 06099 Halle/S., Germany

A summary of recent application of Tammann's nuclei development method [1] to fast crystallizing polymers has been laid out to further address the role of pre-formed homogeneous nuclei on crystallization kinetics as well as semi-crystalline morphology. Making use of the separation in time of homogeneous nucleation and growth in the vicinity of glass transition temperature, the nuclei can be pre-formed using the precision and fast temperature control of a fast scanning calorimeter [2]. Further non-isothermal and isothermal heat treatments of these nuclei largely affects on crystallization kinetics and morphology. Combination of these studies contributes to a better understanding of homogeneous nuclei volume density, thermal stability and reordering kinetics. [1] Tammann, G., Number of nuclei in supercooled liquids. Zeitschrift für Physikalische Chemie 1898, 25, 441-479; [2] Zhuravlev, E., et al., Experimental test of Tammann's nuclei development approach in crystallization of macromolecules. Crystal Growth & Design, 2015. 15(2): p. 786-798.

DY 34.6 Wed 11:15 H42

Crystallization behavior of nanocomposites based on Polylactide - Rigid Amorphous Phase due to the Nanofiller — •Jing Leng[1], De-Yi Wang[2], Andreas Wurm[3], Christoph Schick[3], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und prüfung — [2]IMDEA Materials Institute — [3]University of Rostock, Institute of Physics

Two kinds of synthesized NiAl (NiAl-LDH) and MgAl (MgAl-LDH) layered double hydroxides were melt blended with commercial polylactide to prepare different polymer based nanocomposites. The MgAl-LDH based nanocomposites and NiAl-LDH based nanocomposites have a different but mixed intercalated / exfoliated structure. Based on the different structures, the crystallization behaviors of polymer based nanocomposites were investigated by differential scanning calorimetry (DSC) and temperature modulated differential scanning calorimetry (TMDSC) specificly where the heating and cooling rates were varied in a considerably wide range. In a first step, the cooling rate where crystallization can be completely surpressed is estimated. In a second step, based on a specified temperature program the crystalline fraction (CF), the rigid amorphous fraction (RAF) and the mobile amorphous fraction (MAF) were calculated from the the enthalpy and specific heat capacity in dependence on the concentration of the nanofiller. The rigid amorphous fraction was considered as resulting from the the crystallites and the nanofiller. For the first time both fractions were calculated quantitatively without any additional assumption.

DY 34.7 Wed 11:30 H42

Improved Transferability of Coarse Grained Models for Polymer Crystallization Using Machine Learning — •Chan Liu[1], Christine Peter[2], Kurt Kremer[1], and Tristan Bereau[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Theoretical Chemistry, University of Konstanz, Konstanz, Germany

Coarse-grained (CG) models, which combine a number of atoms into superatoms or beads, can significantly speed up the simulations and provide reasonable resolution for studying polymer crystallization. One of the major challenges in CG modeling is that the reduction of the number of degrees of freedom makes the resulting coarse models state point dependent; that is, most CG force fields developed from the structures of an atomistic melt are not guaranteed to be transferred to crystalline structures. Thus deriving a transferable CG potential across different thermodynamic states is rather crucial if one want to study the phase behavior of polymeric systems. In this work, we introduce a Machine Learning approach to improve an existing CG model parametrized for a different phase by predicting the deviation between CG and atomistic forces, which can be seen as an external force added on the original CG force field. This model predicts a force on each bead based on the surrounding geometry without projecting it onto pairwise potentials such that it can potentially reproduce many-body contributions. This approach opens the perspective to modeling many-body interactions in CG simulations and thus improve the transferability and accuracy of its force field.

DY 34.8 Wed 11:45 H42

Double-Crystalline Diblock Copolymer Nanostructures by Crystal Thickening — •Robert Stössel, Tobias 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

Nanostructures of semi-crystalline diblock copolymers (DBCP) can be tailored by controlled crystal thickening. In double-crystalline DBCP, both blocks have the ability to crystallize and, thus, can be used for crystal thickening which was not investigated so far. The aim of the study was to test the hypothesis that the lamellar long period of a linear double crystalline polyethylene-block-poly(ethylene oxide) (PE-b-PEO) can be increased by stepwise annealing of both crystalline phases. Using differential scanning calorimetry, one-step annealing experiments revealed crystal thickening of both crystalline phases, PE and PEO, separately. X-ray scattering experiments showed that PEO crystal thickening did not affect the PE-b-PEOs morphology while PE crystal thickening increased the lamellar long period. Crystal thickening of both phases together was realized by two-step annealing which further increased the lamellar long period as compared to the sole PE crystal thickening. This observation was attributed to a stretching of PEO-blocks triggered by the initial PE crystal thickening that enabled the formation of thicker PEO crystals compared to the one-step annealing of PEO. The defined crystal thickening of double-crystalline DBCP can be used to fabricate tailorable nanopatterns for materials science applications in photonics or the biomedical field.

DY 34.9 Wed 12:00 H42

Interface & confinement induced order and orientation in thin films of Poly-Caprolactone — •Wilhelm Kossack[1], Anne Seidlitz[2], Thomas Thurn-Albrecht[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Institute for exp. physics 1,04103 Leipzig — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06120 Halle/Saale

Infrared-transition moment orientational analysis (IR-TMOA), X-ray Diffraction (XRD) measurements and model calculations are combined to study interface and confinement induced order and orientation in thin ($h \approx 11 \times 10^{-6}$ m) films of Poly-caprolactone (PCL) prepared by drop-casting on silicon wafers. Depending on the crystallization tem-

perature, 303 K $\leq T_x \leq$ 333 K, spherulites with a diameter of 1×10^{-6} m $\leq d_S \leq 500 \times 10^{-6}$ m form. Macroscopic order of the crystalline lamellae is imposed by spatial ($d_S > h$) and interfacial interactions and quantified IR-TMOA and XRD pole figures. Both techniques rely on the relative orientation of sample and incident radiation, and measure, in case of PCL, the orientation distribution of *complementary* crystal directions. This allows to (1) correlate the directions of the transition moments with the crystal axes; and (2) estimate the volume fractions of flat- or edge on lamellae as induced by the different interfaces, as well as the fractions of surface-induced- or bulk-nucleated spherulites in dependence on T_x. The contribution of substrate induced spherulitic structures rises with $T_x = 323$ K up to ~ 12 vol%, whereas no indications of edge on lamellae at the free surface are found. The bulk phase, on the other hand, dominates at $T_x \leq 313$ K.

DY 35: Active Matter (joint session DY/BP)

Time: Wednesday 9:30–12:45 Location: H46

Invited Talk DY 35.1 Wed 9:30 H46

Nonreciprocal forces in soft matter systems: passive particles become active — •Hartmut Löwen — Institute of Theoretical Physics: Soft Matter, Heinrich-Heine University Duesseldorf,

There is a variety of situations in which Newton's third law is violated. Generally, the action-reaction symmetry can be broken for mesoscopic colloidal particles, when their effective interactions are mediated by a nonequilibrium environment. Here, we investigate different classes of nonreciprocal interactions relevant to real experimental situations and present their basic statistical mechanics analysis verify the principal theoretical predictions in experimental tests performed with two-dimensional binary complex plasmas [1]. For underlying Brownian dynamics [2], nonreciprocal forces result in active particle pairs thus linking nonreciprocal interactions to the field of microswimmers.

References:

[1] A. V. Ivlev, J. Bartnick, M. Heinen, C.-R. Du, V. Nosenko, H. Löwen, Physical Review X **5**, 011035 (2015).

[2] J. Bartnick, M. Heinen, A. V. Ivlev, H. Löwen, J. Phys.: Condensed Matter **28**, 025102 (2016).

DY 35.2 Wed 10:00 H46

Kinetic theory of self-driven particles: Invasion waves and correlation effects — •Thomas Ihle — Institute for Physics, Ernst-Moritz-Arndt University Greifswald, Germany

Models of self-driven agents similar to the Vicsek model are studied by means of kinetic theory. In these models, particles try to align their travel directions with the average direction of their neighbors. At strong alignment a globally ordered state of collective motion forms. An Enskog-like kinetic theory is derived from the exact equation for a Markov chain in phase space using Boltzmann's mean-field approximation of molecular chaos. The kinetic equation is solved numerically by a nonlocal Lattice- Boltzmann-like algorithm. Steep soliton-like waves are observed that lead to an abrupt jump of the global order parameter if the noise level is changed. The shape of the wave is shown to quantitatively agree within 3% with agent-based simulations at large particle speeds. This provides a mean-field mechanism to change the second-order character of the flocking transition to first order. At small densities and realistic particle speeds, the mean-field assumption of Molecular Chaos is invalid near the onset of collective motion, and correlation effects become relevant.

I will show how to self-consistently include correlation effects at the level of ring-kinetic theory. Instead of just one kinetic equation, an additional equation for the time evolution of two-particle correlations will be derived. This equation is solved numerically for a homogeneous system and shown to be in excellent agreement with agent-based simulations in certain parameter ranges.

DY 35.3 Wed 10:15 H46

Model of aerotactic bands — •Marco Giacomo Mazza — Max Planck Institute for Dynamics and Self-Organization, Göttingen

Some bacteria exhibit surprising behavior in the presence of an oxygen concentration. They perform an aerotactic motion along the gradient until they reach their optimal oxygen concentration. And they often organize collectively by forming dense regions, called 'bands', that travel towards the oxygen source. We have developed a model of swimmers with stochastic interaction rules moving in proximity of an air bubble. We perform MD simulations that reproduce the aerotactic behavior of bacteria. If the oxygen concentration in the system sinks locally below a threshold value, the formation of a migrating aerotactic band toward the bubble can be observed. We reproduce quantitatively the experimental observations on the aerotactic band.

DY 35.4 Wed 10:30 H46

Phase Behavior of Active Particles — •Jonathan Tammo Siebert[1], Janina Carmen Letz[1,2], and Peter Virnau[1] — [1]Johannes Gutenberg University Mainz, Department of Physics, Staudingerweg 7, 55128 Mainz, Germany — [2]University of Utah, Department of Mathematics, Salt Lake City, UT 84112-0090, USA

We have studied the phase behavior of active colloidal particles. Such systems undergo phase separation into a dense liquid-like and a dilute gas-like phase due to self trapping when a certain critical activity is exceeded both in experiment and simulation (Buttinoni et al., Phys. Rev. Lett., 110 (2013)). Starting point of our studies are the well known two dimensional active brownian particles. Further investigations were done on three dimensional as well as systems of active dimers. For all systems the phase diagrams were computed by extensive brownian dynamics simulations. Employing methods from equilibrium statistical physics we have aimed for an accurate estimate of the binodal line in a bulk system. Starting from a simple model system has allowed us to separate the influence of dimensionality and bonding of particles. In agreement with earlier studies we have found that active velocities needed for phase separation are much larger in the three dimensional system. Also active dimers only phase separate at higher activities than active disks.

DY 35.5 Wed 10:45 H46

Active Brownian particles at interfaces: An effective equilibrium approach — •René Wittmann and Joseph Brader — Departement für Physik, Universität Fribourg, 1700 Fribourg, Schweiz

Understanding self-organization in active Brownian systems is a subject of increasing theoretical interest. Recently, a microscopic equilibrium theory was developed from first principles [1], which accounts for the motility-induced phase separation (MIPS) observed in numerous experiments. This is achieved by mapping the active system onto an effective (static) interaction potential.

So far, experimental studies of active systems have focused on bulk properties. We apply our effective equilibrium theory [1] to inhomogeneous systems using density functional theory (DFT) with a simple perturbative treatment of the (effective) attractive interaction. In this case, the activity induces an effective external (wall) potential [2,3].

For a passively repulsive active fluid at a passively repulsive wall, the theory predicts motility-induced wetting as the MIPS transition is approached. For a Lennard-Jones interparticle potential the wall first dries with increasing activity, followed by a re-entrant wetting phenomenon. In a slit pore we observe motility-induced capillary condensation or evaporation, depending on the passive potential. These findings [3] constitute a compelling motivation to study such systems experimentally or using Brownian dynamics simulations.

[1] T. F. F. Farage, P. Krinninger and J. M. Brader, Phys. Rev. E **91**, 042310 (2015). [2] A. Pototsky and H. Stark, Europhys. Lett. **98** 50004 (2012). [3] R. Wittmann and J. M. Brader, in preparation.

15 min. break

DY 35.6 Wed 11:15 H46

Using motility patterns to manipulate self-propelled particles — •Celia Lozano[1,2], Borge ten Hagen[3], Hartmut Löwen[3], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universitaet Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [3]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany.

Active colloidal particles capture many aspects of motile microorganisms and are therefore considered to provide a suitable model system

to understand self-organization and pattern formation in living and non-equilibrium systems. Contrary to most experimental situations where the particle motility is position-independent, here we investigate a system where the self-propulsion velocity is spatially modulated. This is achieved by a light-induced propulsion mechanism and a spatially modulated light field [1]. By subjecting a dilute active colloidal suspension to an asymmetric and periodic light field, we demonstrate directed particle motion. In addition, we show, that particle transport is highly sensitive to the particle size and thus acts also as a filtering device for active suspensions [2].

[1] VOLPE G, BUTTINONI I, VOGT D, KÜMMERER H J AND BECHINGER C 2011 MICROSWIMMERS IN PATTERNED ENVIRONMENTS SOFT MATTER 7, 8810 (2011) [2] C. Lozano, B. ten Hagen, H. Löwen, and C. Bechinger. In preparation

DY 35.7 Wed 11:30 H46

Dynamics of self-propelled Janus particles in viscoelastic fluids — •Juan Ruben Gomez-Solano[1] and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universitaet Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-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 media. 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 particles. Although the motion of microswimmers in Newtonian fluids has been extensively studied, so far only few investigations have focused on the swimming of microorganisms in viscoelastic fluids. In this work, we experimentally investigate the dynamics of spherical Janus colloidal particles in a viscoelastic fluid. The particles are self-propelled by local demixing of a critical binary polymer mixture induced by laser illumination. We observe a dramatic enhancement of both translational and rotational diffusion with increasing particle velocity, even at low Weissenberg number, where the drag force on the particle exerted by the fluid obeys the Stokes law. We observe a similar enhancement for passive particles driven by an external constant force, e.g. gravity. Our results suggest that these effects originate from the coupling between the thermal fluctuations of the particle and the surrounding flow field, which displays large relaxation times of several seconds.

DY 35.8 Wed 11:45 H46

Hydrodynamicaly-Tuned Phase Separation of Spherical Micro-Swimmers — •Johannes Blaschke, Karthik Menon, Maurice Maurer, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Active motion of microorganisms and artificial micro-swimmers is relevant both to real world applications, as well as for posing fundamental questions in non-equilibrium statistical physics. A striking feature of their collective behaviour is that, for sufficiently strong self-propulsion dense clusters coexists with a low-density disordered surrounding. Due to the required computational effort, active particles are often modelled by neglecting the full hydrodynamic interactions.

However, real micro-swimmers, such as ciliated microorganisms, catalytic janus particles, or emulsions of active droplets, employ propulsion mechanisms reliant on hydrodynamics.

Here we examine the influence of the full hydrodynamic interactions on the motility-induced phase separation of spherical micro-swimmers in quasi-2D confinement. We follow up on previous work [1] by increasing the total system size allowing us to quantitatively resolve the phase-coexistence regime.

[1] A. Zöttl and H. Stark, PRL **112**, 118101 (2014)

DY 35.9 Wed 12:00 H46

Comparison of external control strategies for optimized payload delivery — •Tobias Bäuerle[1], Jakob Steiner[1], Lena Bremicker[2], Daniel Häufle[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Institut für Sport- und Bewegungswissenschaft, Universität Stuttgart, 70569 Stuttgart, Germany

Synthetic microswimmers, i.e. self-propelled particles, constitute an interesting class of non-equilibrium systems which exhibit structural and dynamical features similar to those observed in assemblies of motile organisms like bacteria or cells. In addition, they may find applications as microrobots which will deliver payloads to specific sites in liquid environments.

In our studies, we addressed the question how the delivery process can be optimized by the choice of the control strategy. Experimentally, this was achieved by light-activated microswimmers, where the propulsion velocity was controlled by the light intensity. Depending on the particle orientation and its distance from the target, the illumination was turned on and off, resulting in an intermittent change between Brownian and active motion. Even for slight variations of control strategies, we find large changes e.g. in the ratio of the delivery time and the total propulsion energy. Our results are in excellent agreement with numerical simulations.

DY 35.10 Wed 12:15 H46

Self-propelled janus droplets for gene extraction and controlled cargo delivery — •Menglin Li[1], Martin Brinkmann[1,2], Ralf Seemann[1,2], and Jean-Baptiste Fleury[1] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

We report the existence of a new type of self-propelled Janus droplets, that are obtained from the spontaneous phase separation between two fully miscible fluids (water/solvent) in the presence of surfactants which are preferentially soluble in the solvent phase. At start, the related self-propulsion mechanism is generated by a Marangoni flow mediated by the solvent dissolution into the oily phase. During this motion, the droplets are absorbing a large amount of surfactant. This dynamic surfactant adsorption leads to spontaneous water/solvent demixing and the formation of Janus droplet. We characterize the hydrodynamics properties of these microwimmers during their different stages of evolution. Interestingly, the squirmer properties evolve in time from a weak pusher to a neutral squirmer and potentially to a dimer of neutral squirmers. Finally, we used this active system as a smart carrier to extract genes in situ and delivering them at a target location. (Submitted)

DY 35.11 Wed 12:30 H46

Pattern Formation and Clustering in Chemorepulsive Active Colloids — •Benno Liebchen[1], Davide Marenduzzo[1], Ignacio Pagonabarraga[2], and Michael E Cates[3] — [1]SUPA, School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3FD, United Kingdom — [2]Departament de Fisica Fonamental, Universitat de Barcelona-Carrer Marti i Franques 1, 08028-Barcelona, Spain — [3]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

Chemotaxis is the directed motion of particles in response to a gradient in a chemical signal. It allows micro-organisms, like bacteria, to find food and to escape from toxins. Some micro-organisms can produce the species to which they respond themselves and use chemotaxis for signalling. This can, in the case of chemoattraction where particles migrate up chemical gradients, induce a clustering-instability of the uniform state. This instability currently attracts renewed attention in artificial Janus colloids that swim by catalysing reactions in a chemical bath and show a similar signalling behaviour as micro-organisms.

Here, we demonstrate that also the previously underappreciated case of chemorepulsion (where particles migrate away from high chemical density) can induce clustering. The underlying instability may either rely on anisotropy in the chemical production at the particle surface or on delay effects. In contrast to chemoattractive clustering our chemorepulsive route predicts clusters of self-limiting size. This size increases with self-propulsion velocity which agrees qualitatively with recent experimental observations of dynamic clustering in active Janus colloids.

DY 36: Complex Fluids and Colloids V (joint session DY/BP/CPP)

Time: Wednesday 10:00–13:00 Location: H47

DY 36.1 Wed 10:00 H47

Self-assembly in binary mixtures of liquid-crystalline rods and dipolar spheres: A free-energy study — •Alice C. von der Heydt, Stavros D. Peroukidis, and Sabine H. L. Klapp — Inst. f. Theoretische Physik, Techn. Univ. Berlin, Hardenbergstr. 36, 10623 Berlin

Mixtures of differently shaped particles with hard-core repulsion only can exhibit a variety of spatially periodic phase-separation patterns combined with liquid-crystalline order [1]. Simulations have revealed an even more complex behavior with uni- or biaxial, smectic and lamellar structures in binary mixtures of rods and soft magnetic spheres of comparable diameter [2]. In this study, we aim at a theoretical description that will allow us to trace phase boundaries and to explain topologies of some of these structures for a model mixture of hard rods with nematic order and dipolar hard spheres. The semi-analytical route we propose starts from a free-energy functional which governs the single-particle component-density distribution functions of position and orientation. This functional is constructed using concepts of classical density functional theory and the modified mean-field approximation for the dipolar interaction [3].

[1] Z. Dogic, D. Frenkel, S. Fraden, Phys. Rev. E **62**, 3925 (2000)
[2] S. D. Peroukidis, K. Lichtner, S. H. L. Klapp, Soft Matter **11**, 5999 (2015)
[3] G. M. Range, S. H. L. Klapp, Phys. Rev. E **69**, 041201 (2004)

DY 36.2 Wed 10:15 H47

Clogging in a microfluidic hourglass — •Alvaro Marin[1], Massimiliano Rossi[1], Henri Lhuissier[2], and Christian J. Kähler[1] — [1]Institut für Strömungsmechanik und Aerodynamik, Universität der Bundeswehr München — [2]IUSTI - Aix-Marseille Université & CNRS

Mass flows through geometric constrictions tend to clog under certain circumstances, it occurs no matter what type of object you consider: sand in an hourglass, particles in a fluid through a porous medium or people leaving a room (Zuriguel et al., Scientific reports 4, 2014). However, it is well-known that hourglasses work optimally when the particle-to-neck ratio is within certain ratio without interruption, while arching occurs for particle-to-neck ratios above. In the case of porous mediums, filters and membranes, these get easily clogged by particles in the fluid and therefore unfunctional after a certain amount of time. Being the only solution the replacement of the membrane/filter. Certainly the adherence of the particles to the walls and to each other is an important parameter, but even in the case without adherence, the clogging probability is far from negligible. To study these regimes, we study microfluidic devices with a bottleneck of squared cross-section through which we force dilute polystyrene particle solutions with diameters comparable to the bottleneck size and down to one tenth its size. The experimental results show that particles flowing through a geometrical constriction in these conditions (as it occurs with the flow in certain filters and membranes) reveals strong statistical similarities with an hourglass, which is explained with a simple statistical model.

DY 36.3 Wed 10:30 H47

Viscoelastic properties of marginal networks in a solvent — •Matthew Dennison and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Elastic networks that are at the margins of mechanical stability are known to exhibit an anomalously large resistance to deformation which is highly sensitive to applied forces and fields. While many previous studies have examined the static properties of such networks, relatively little is known about their dynamical behavior. Using a hybrid molecular dynamics and multi-particle collision dynamics simulation technique, we have studied how hydrodynamic interactions affect the stiffening behavior of marginal networks.

We show how the properties of the filaments making up the network, as well as the properties of the solvent it is immersed in, can affect the response of marginal networks to shear. We find that the network is less stiff when hydrodynamic interactions are present than when they are not. The network shear modulus scales as $G' \sim \omega^{\alpha_c}$, with a critical stiffening exponent α_c that can be controlled by varying the network concentration relative to that of the solvent. Our results show that this behavior arises due to the solvent aiding the relaxation of the network and suppressing the network non-affinity, with the system deforming more affinely when hydrodynamic interactions are maximized. Finally, we show how thermal fluctuations can suppress this observed stiffening behavior.

DY 36.4 Wed 10:45 H47

Rheology of weakly attractive systems: the role of energy dissipation — •Ehsan Irani[1], Pinaki Chaudhuri[2], and Claus Heussinger[1] — [1]Institute for Theoretical Physics, Georg-August University of Göttingen, Göttingen, Germany — [2]Institute of Mathematical Sciences, Tamil Nadu, India

The rheological response of a particulate system with attractive interactions is studied using different models for the dissipation of energy. In systems with the damping force directed normally to the contact point, attractive interactions result in a finite yield stress, and an isostatic structure emerges below the jamming point with shear bands forming as a consequence of non-monotonic flow curves. On the other hand, tangential damping gives rise to the monotonic flow curves and a viscous flow develops in the overdamped regime. However in that case, decreasing the damping factor introduces the inertial time-scale, leading again to non-monotonic flow curves and inertia-induced shear-banding is observed in the underdamped regime. In both cases, the rheology of the system is expressed in terms of relevant damping time-scales and the ratio of dissipative to elastic forces.

DY 36.5 Wed 11:00 H47

Transport properties of correlated fluids in confinement — •Christian Rohwer[1,2] and Matthias Krueger[1,2] — [1]Max Planck Institute for Intelligent Systems, 70569 Stuttgart, Germany — [2]4th Institute for Theoretical Physics, University of Stuttgart, 70569 Stuttgart, Germany

Correlations in confined fluids give rise to a wealth of remarkable phenomena. Several equilibrium phenomena, e.g. the critical (thermal) Casimir forces, have been described theoretically and observed experimentally. However, although certain non-equilibrium aspects of such systems can be probed experimentally or through computer simulations, a clear theoretical understanding for confined, correlated fluids out of equilibrium is still lacking.

In this work we consider a dynamical theoretical model for confined fluids with correlations (e.g. oil-water mixtures near / at the critical point), thereby extending known results for bulk systems. In particular, we investigate the steady state velocity profiles in a sheared near-critical fluid film, in dependence on various parameters (e.g. separation of the plates, bulk correlation length, external fields...). Our approach is based on linear response theory for small shearing velocities, and leads to a self-consistent formulation for the shear rate in the film.

We also address the dependence on the choice of dynamical model, since conservation laws strongly affect dynamical time-scales. Lastly we discuss potential experimental realisations of our model.

15 min. break

DY 36.6 Wed 11:30 H47

The Gyroid phase in a System of Pear-shaped Particles — Philipp Schönhöfer[1], Matthieu Marechal[1], Klaus Mecke[1], Gerd Schröder-Turk[2], and •Douglas Cleaver[3] — [1]Theoretische Physik I, FAU Erlangen, Germany — [2]School of Engineering and IT, Murdoch University, Australia — [3]Materials and Engineering Research Institute, Sheffield Hallam University, UK

It is established that elongated or flattened mesogens like spherocylinders and oblate discs form liquid crystal phases – like the nematic or smectic phase – in addition to the isotropic fluid and crystalline solid states.

A highly complex liquid crystal phase which can be generated by amphiphiles or block co-polymers is the double gyroid Ia3d cubic phase. A promising system which forms this structure consists of hard pear-shaped particles with suitable aspect ratio and degree of tapering.

Using Molecular Dynamics and Monte Carlo simulations with a generalized Gay-Berne potential, the spontaneous formation of the gyroid phase was reproduced. Additionally a defect-free gyroid with the same number of particles per unit cell as the spontaneously formed phase was generated. We calculate the scattering functions and use Voronoi tesselation to study the geometrical properties of both systems.

The next step is to introduce hard spheres which will take up the role of solvent to model mixtures such as the lipid-water system. With an explicit solvent the system should be complex enough to model most common phenomena in cubic phases yet simple enough to allow us to simulate large systems.

DY 36.7 Wed 11:45 H47

Critical three-body Casimir interaction — •Hendrik Hobrecht and Alfred Hucht — Fakultät für Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg

It was shown by Burkhardt and Eisenriegler that the critical Casimir interaction between two colloids at $T = T_c$ can be calculated exactly by a conformal mapping in arbitrary dimension d [1]. For the two-dimensional case $d = 2$ Bimonte et al. extended this calculation to arbitrary shaped objects [2], where the form of the interaction potential between two disks is known exactly. Utilizing those concepts we present a calculation which maps the case of two separated two-dimensional disks onto a limiting case of a three-body system, where two particles are in contact and one is free to move. We compare the results of this calculation to Monte Carlo simulations, using a highly efficient cluster algorithm [3].

[1] T. W. Burkhardt and E. Eisenriegler, Phys. Rev. Lett. 74, 3189 (1995).

[2] G. Bimonte et al., Europhys. Lett. 104, 21001 (2013).

[3] H. Hobrecht and A. Hucht, Phys. Rev. E 92, 042315 (2015)

DY 36.8 Wed 12:00 H47

Defect-mediated melting of two-dimensional colloidal quasicrystals — Miriam Martinsons and •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Quasicrystals are structures that possess long range order but no translational symmetry. Due to additional degrees of freedom in quasicrystals there are properties and phenomena that for quasicrystalline structures significantly differ from their counterpart in periodic crystals.

We study how thermally excited excitations or defects develop in two-dimensional colloidal quasicrystals close to the melting transition. According to an extension of the KTHNY theory [1], the formation and dissociation of pairs of dislocation and disclinations is expected to cause the melting of the quasicrystal. Melting should occur via an intermediate phase termed pentahedratic phase [1].

We use Monte-Carlo and Brownian dynamics simulations to study the melting process of decagonal colloidal quasicrystals. By analyzing the positional and bond-orientational correlation functions during the melting process we reveal an intermediate state with quasi-long ranged orientational order but only short ranged positional order as in the predicted pentahedratic phase. Furthermore, we observe network-like structures composed of defects spanning through defect-free areas as well as a coexistence between the intermediate phase and the fluid.

[1] P. De, R.A. Pelcovits, J. Phys. A 22, 1167 (1989); Phys. Rev. B 38, 5042 (1988).

DY 36.9 Wed 12:15 H47

Protein phase separation controlled by phosphorylation — •David Zwicker[1,2], Oliver Wüseke[3], Jeffrey B. Woodruff[3], Markus Decker[3], Steffen Jaensch[3], Anne Schwager[3], Anthony A. Hyman[3], and Frank Jülicher[2] — [1]School of Engineering and Applied Sciences, Harvard University — [2]Max Planck Institute for the Physics of Complex Systems, Dresden — [3]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden

Biological cells have to organize their proteins in space and time. Membrane-enclosed compartments, like the nucleus, are one solution to this problem. Recent discoveries show that liquid-like droplets are an alternative organization principle. To understand how phase separation can help cells to organize their proteins in space and time, we investigated the formation of the pericentriolar material (PCM), an integral part of the cell scaffold. We combine the theory of phase separation in the presence of chemical reactions with in vivo and in vitro experiments. Our work suggests that the protein responsible for forming the PCM occurs in two different states: one in which it is soluble in the cytosol and one in which it phase separates. The transition between these two states is regulated by chemical reactions that maintain the system away from thermodynamic equilibrium. This allows the cell to control the nucleation process and the growth dynamics, and thus also the droplet count and size. I will discuss the physical principles of this spatial organization, which are likely important for other cellular compartments and might also be used in technological applications.

DY 36.10 Wed 12:30 H47

Two and three dimensional shapes of simple three and four junction comb polymers — Marvin Bishop[1], Adam J. Barillas[1], Tylor Borgeson[1], •Robin de Regt[2], and Christian von Ferber[2] — [1]Departments of Computer Science and Mathematics, Manhattan College, NY, USA — [2]Applied Mathematics Research Centre, Coventry University, UK

We redesign and apply a scheme originally proposed by G. Wei [Physica A **222**, 155 (1995)] to produce numerical shape parameters with high precision for arbitrary tree-branched polymers based on their Kirchhoff matrix eigenvalue spectrum. This algorithm and a Monte Carlo growth method on square and triangular lattices are employed to investigate the shapes of ideal three and four junction two dimensional comb polymers. We find that the extrapolated values obtained by all of these methods are in excellent agreement with each other and the available theory. We confirm that polymers with a complete set of interior branches display a more circular (resp. spherical) shape.

DY 36.11 Wed 12:45 H47

How (classical) density functional theory describes structure in electric double layers — •Andreas Härtel[1], Sela Samin[2], and Rene van Roij[2] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, Germany — [2]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University, The Netherlands

Ongoing scientific interest is aimed on the properties and structure of electric double layers (EDLs), which are crucial for capacitive water treatment and energy harvesting technologies like desalination devices, blue engines, and thermocapacitive heat-to-current converters. A promising tool for their microscopic description is (classical) density functional theory, which we have applied in order to analyze pair correlations and charge ordering in the primitive model of charged hard spheres. Interestingly, this simple model already describes structural in-plane transitions of EDLs, which occur while their corresponding electrodes are charged. Furthermore, our results demonstrate the impact of screening by solvents on the ability of EDLs to adsorb charges. In conclusion, our work points up issues in the theoretical description of EDLs, which finally might lead to a more sophisticated theory for ionic systems.

DY 37: Nonlinear Dynamics, Synchronization and Chaos

Time: Wednesday 10:00–12:00 Location: H48

DY 37.1 Wed 10:00 H48

Synchronization patterns in hierarchical networks — •Sanjukta Krishnagopal[1,2], Judith Lehnert[1], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, TU-Berlin, Hardenbergstr 36, 10623 Berlin, Germany, — [2]Birla Institute of Technology and Science - Pilani K. K. Birla Goa Campus, NH 17B Bypass Road, Zuarinagar, Sancoale, 403726 Goa, India.

We consider Stuart-Landau oscillators, a generic model for systems close to a Hopf bifurcation, coupled in a hierarchical (fractal) topology. We present an analytic study of these networks using an extension of the eigensolution concept first introduced in [1]. The resulting eigensolutions of the network are found to be cluster states, where the nodes in the network are synchronized in clusters with a constant phase shift between the clusters. For hierarchical networks in particular, we study the effect of fractal dimension, base pattern and number of iterations on network dynamics.

[1] W. Poel, A. Zakharova, E. Schöll, Phys. Rev. E 91, 022915 (2015)

DY 37.2 Wed 10:15 H48

Injection Locking in the Quantum Regime — •Steffen Holzinger[1], Elisabeth Schlottmann[1], Benjamin Lingnau[2], Kathy Lüdge[2], Christian Schneider[3], Martin Kamp[3], Sven Höfling[3], Janik Wolters[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [3]Technische Physik, Julius-Maximilians-Universität Würzburg, Würzburg, Germany

The frequency of an oscillator can be controlled by injecting an external signal. This general concept in non-linear dynamics can be applied to plenty of physical and biological systems. In classical systems this control is well understood by Adler's theory and modifications thereof. In the present work we explore the phenomenon of injection locking, widely applied in standard semiconductor lasers, for the first time in quantum-dot microlasers operating in the regime of cavity quantum electrodynamics (cQED) with on average only few tens of photons in the cavity. In contrast to predictions of classical deterministic rate equations, we find the laser in a superposition of oscillating synchronized to the external signal and at its solitary frequency. With semiclassical rate equations based on a quantum Langevin approach we can show that our experimental results on "partial injection locking" are specific to non-linear cQED systems where cavity enhanced spontaneous emission noise plays an important role. As such, our results pave the way for unravelling exciting effects of injection locking and synchronization in the quantum regime.

DY 37.3 Wed 10:30 H48

Synchronization of particle motion in compressed two-dimensional plasma crystals — •Ingo Laut[1], Christoph Räth[1], Sergey Zhdanov[2], Vladimir Nosenko[1], Lénaïc Couëdel[3], and Hubertus M. Thomas[1] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Forschungsgruppe Komplexe Plasmen, Weßling — [2]Max-Planck-Institut für Extraterrestrische Physik, Garching — [3]CNRS, Aix-Marseille Université, Laboratoire de Physique des Interactions Ioniques et Moléculaires, Marseille, France

Two-dimensional complex plasma crystals are an ideal model system to study dynamic processes on the kinetic level. Recently, synchronized motion of alternating in-phase and anti-phase particle lines was observed during the so-called mode-coupling instability (MCI), where the out-of-plane wave mode of the crystal couples to the longitudinal mode. While MCI is equally strong in three directions for an ideal hexagonal lattice, it was observed in only two directions in the experiment.

Here, we demonstrate with molecular dynamics simulations that an asymmetry in the horizontal confinement of the plasma crystal can cause this anisotropic ignition of MCI. The confinement asymmetry leads to a deformation of the hexagonal lattice that is typically observed in experiments. The instability is accompanied by synchronized particle motion that is characterized by a new order parameter. This order parameter is sensitive to the explicit direction-dependency of the synchronization pattern.

DY 37.4 Wed 10:45 H48

A combined time averaging and frequency mixing approach to parameter identification in nonlinear response — •Si Mohamed Sah, Daniel Forchheimer, Riccardo Borgani, and David B. Haviland — Royal Institute of Technology KTH, Applied Physics SE - 106 91 Stockholm Sweden

We present a method for identifying the parameters of a model describing the tip-sample interaction force in Intermodulation Atomic Force Microscopy (ImAFM). The method uses analytic expressions for the slow-time amplitude and phase evolution, obtained from time-averaging over the rapidly oscillating part of the cantilever dynamics. The slow-time behavior can be easily obtained in the experiment by down-shifting the measured intermodulation spectrum that results when a high-Q resonator is perturbed by nonlinearity. A direct fit of the theoretical expressions to the experimental data gives the best-fit parameters for the model. The method combines and complements previous work [1,2] and it allows for computationally more efficient parameter mapping with ImAFM. Results for both simulation and experiment are shown.

References:

1) Platz, D., Forchhheimer, D., Tholen, E. A. & Haviland, D. B., Interaction imaging with amplitude-dependence force spectroscopy. Nat. Commun. 4, 1360 (2013).

2) Forchheimer, D., Platz, D., Tholen, E. A. & Haviland, D., Model-based extraction of material properties in multifrequency atomic force microscopy. Phys. Rev. B 85, 195449 (2012).

DY 37.5 Wed 11:00 H48

Eigenmode decomposition for synchronized solutions in networks with heterogeneous delay coupling — •Andreas Otto[1], Gabor Orosz[2], Daniel Bachrathy[3], and Günter Radons[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA — [3]Department of Applied Mechanics, Budapest University of Technology and Economics , H1111, Budapest, Hungary

Synchronization in networks of delay-coupled nonlinear systems can be found, for example, in social systems, biology, engineering or physics. In technical applications, e.g. in coupled semiconductor lasers, the time-delays can be tuned to be identical, whereas in real world systems, such as neuronal or social networks, the delays are typically heterogeneous. For networks with instantaneous or identical delays the master stability function can be used to analyze the stability of the network eigenmodes. For heterogeneous delays this approach is restricted to the specific case, where the coupling matrices for the different delays commute. A general approach for the decomposition of the network eigenmodes around synchronized equilibria has been proposed in [1]. In this talk, an extension of this general approach for the eigenmode decomposition around synchronized periodic orbits is presented. In this case the master stability function becomes, in general, a periodic delay differential equation with multiple delays. Numerical results on the stability are shown for delay-coupled Hodgkin-Huxley neurons.

[1] R. Szalai and G. Orosz, *Phys. Rev. E* **88**, 040902 (2013).

DY 37.6 Wed 11:15 H48

Periodic sequence of stabilized wave segments in excitable media — Vladimir Zykov and •Eberhard Bodenschatz — MPI of the Dynamics and Self-Organization, Goettingen, Germany

Wave segments represent an interesting and important example of spatio-temporal pattern formation in a broad class of nonlinear dynamic systems, so-called excitable media. For a given excitability a medium supports propagation of a wave segment with a selected size and shape, which is intrinsically unstable, but can be stabilized by an adequate noninvasive feedback control. For the case of a solitary propagating wave segments a universal selection rules have been found by use a free-boundary approach [1,2]. The main aim of our study is to generalize these results on a case of a periodic sequence of wave segments. To this aim a periodic sequence of stabilized wave segments is numerically studied by use of a generic reaction-diffusion model. In addition, the free-boundary approach is applied which allows us to determine the wave segment shape and the speed as functions of the medium parametersa high accuracy.

[1] A. Kothe, V.S. Zykov and H. Engel, Phys. Rev. Lett., 103, 154102 (2009). [2] V.S. Zykov and E. Bodenschatz, New Journal of Physics, 16, 043030 (2014).

DY 37.7 Wed 11:30 H48

Impact of intermittent power fluctuations on the dynamics of power grids — Katrin Schmietendorf[1], Joachim Peinke[1], and •Oliver Kamps[2] — [1]ForWind - Center for Wind Energy Research, Institute of Physics, University of Oldenburg, Germany — [2]Center for Nonlinear Science, University of Münster

The increasing share of fluctuating energy sources like wind energy poses big challenges for the stability of power grids and the resilience of energy supply systems in general. From the physics point of view the phase and voltage dynamics of a power grid can be described by a Kuramoto-like model of coupled oscillators [1]. To investigate the influence of wind energy production, which is known to exhibit strongly non-Gaussian statistics [2], on the phase and voltage stability we use a Langevin type model mimicking the main features of wind power time series. We compare our findings with results obtained for Gaussian noise and real power time series.

[1] K. Schmietendorf, J. Peinke, O. Kamps, and R. Friedrich, EPJ STI 223, p. 2577-2592, 2014

[2] P. Milan, M. Wächter, and J. Peinke, Phys. Rev. Lett., vol. 110, p. 138701, 2013

DY 37.8 Wed 11:45 H48

Collective Failure due to Multistability in Oscillator

Networks and Power Grid — •Debsankha Manik[1], Dirk Witthaut[2], and Marc Timme[1] — [1]Network Dynamics Group, Max Planck Institute for Dynamics anf self-Organization, 37077 Göttingen — [2]Forschungszentrum Jülich, Institute of Energy and Climate Research Systems Analysis and Technology Evaluation (IEK-STE), 52425 Jülich

Networks of phase oscillators model the collective dynamics of various interacting physical and biological systems, ranging from electric power grid operation to neuronal rhythms. Here we show that the number of stable steady states in phase oscillator systems scales with the length of the topological cycles in the network such that for non-global coupling, multistable steady states may emerge. The clustering of similar natural frequencies favour fewer stable states, whereas homogeneous frequency distributions favour more. Intriguingly, multistability prevails even under conditions for which stable states have been claimed to be unique. This multistability may have significant impact on the collective dynamics of such networks: for example, in power grids where the transmission lines have structural limitations on the maximum load they can safely carry, perturbations may induce switching to different steady states, strongly alter the flow patterns, and in turn yield a collective failure of the grid.

Supported by the BMBF under grant no. 03SF0472E.

DY 38: Statistical Physics of Biological Systems II (Joint Session with DY)

Joint session with DY organized by BP.

Time: Wednesday 11:30–12:30 Location: H43

DY 38.1 Wed 11:30 H43

Receptor arrays optimized for sensing natural odors — •David Zwicker[1], Arvind Murugan[1,2], and Michael P. Brenner[1] — [1]School of Engineering and Applied Sciences, Harvard University — [2]Department of Physics and the James Franck Institute, University of Chicago

Natural odors typically consist of many molecules at different concentrations, which together determine the odor identity. This information is encoded in the collective response of olfactory receptors and subsequently interpreted by the brain. However, it is unclear how the receptors can measure both the composition of the odor and the concentrations of its constituents. I will discuss a theoretical model of receptor arrays from which we derive design principles for optimally communicating the odor information. These principles can be summarized as two possibly conflicting goals: (i) each receptor should respond to half of all odor mixtures; (ii) activity patterns of different receptors should be orthogonal. We show that there is a family of receptor arrays that satisfy these conditions and thus transfer the odor information near-optimally. Within this family, we can then discuss additional optimization goals, like the accuracy of concentration measurements and the capability for discriminating mixtures. Taken together, we can predict the performance and properties of receptor arrays based on a few, measurable quantities. Our work can thus be used to infer information about the receptors from physiological measurements. Moreover, we can use our results to improve artificial sensor arrays.

DY 38.2 Wed 11:45 H43

Making a loop - from polymer conformation to single file diffusion and back — •Wenwen Huang[1], Yen Ting Lin[1,2], Daniela Frömberg[1], Frank Jülicher[1], and Vasily Zaburdaev[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]School of Physics and Astronomy, University of Manchester, M139PL, Manchester, United Kingdom.

In this contribution, we show that the conformations of a pinned polymer loop embedded in a heat bath with a constant external force field can be modeled by an asymmetric exclusion process (ASEP) with reflecting boundary conditions. This correspondence allows us to find the exact solution for both systems' equilibrium statistics, which is well approximated by the Fermi–Dirac distribution. Moreover, we can quantify not only the behavior of average positions of the particles of the ASEP and the corresponding monomers of the polymer loop, but also their fluctuations. The condition of forming a loop and the corresponding constraint in the ASEP model lead to explicit dependence of the fluctuations on the position of the particles in ASEP and the monomers of the polymer. To close the loop of analogies we show that the kinetic Monte Carlo simulations, which can be performed for the ASEP with a well defined physical time, can be related to the non-equilibrium dynamics of polymer loops.

DY 38.3 Wed 12:00 H43

Evolutionary emergence of phenotype switching — Pintu Patra[1,2] and •Stefan Klumpp[1,3] — [1]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Germany — [2]Rice University, Houston, Texas, USA — [3]Institut für Nichtlineare Dynamik, Universität Göttingen, Göttingen, Germany

Bacterial persistence (phenotypic tolerance to antibiotics) provides a prime example of bet-hedging, where normally growing cells generate slow-growing but antibiotic-tolerant persister cells to survive through periods of exposure to antibiotics. The population dynamics of persistence is explained by a phenotype switching mechanism that allows individual cells to switch between these different cellular states with different environmental sensitivities. We report a theoretical study based on an exact solution for the case of a periodic variation of the environment to address how phenotype switching emerges and under what conditions switching is or is not beneficial for long-time growth [1]. Specifically we report a bifurcation through which a fitness maximum and minimum emerge above a threshold in the duration of exposure to the antibiotic. Only above this threshold, the optimal phenotype switching rates are adjusted to the time scales of the environment, as emphasized by previous theoretical studies, while below the threshold a non-switching population is fitter than a switching one. Whether the transition is continuous or discontinuous depends on how the phenotype switching rates are allowed to vary. [1] P. Patra and S. Klumpp, Phys. Biol. 12, 046004.

DY 38.4 Wed 12:15 H43

The statistical physics of hematopoiesis: from stem cell engraftment to ageing and disease — •Peter Ashcroft[1], Sebastian Bonhoeffer[1], Philipp Rauch[2], and Markus Manz[2] — [1]ETH Zurich, Zurich, Switzerland — [2]University Hospital Zurich, Zurich, Switzerland

Hematopoietic stem cells (HSCs) maintain blood production. The hematopoietic system has the highest turnover and proliferation rate of cells in the body, however, hematologic malignancies are not the most frequent forms of human cancer. A fine tuned system with many layers of control has evolved that limits and eliminates potentially malignant clones. The overall aim of our research is to obtain a clear, quantitative understanding of the hematopoietic system and the emergence of disease through combined theoretical and experimental work. Here we will describe the theoretical approach. We use techniques from statistical physics and probability theory to analyse the structure of the hematopoietic system at different scales. Experimental investigations of HSCs often involve the transplantation of low numbers of stem cells into a host. We construct and analyse an individual-based model of this process, and determine the probability that donor cells successfully engraft in the host. These donor cells could also represent the invasion of malignant cells and the initiation of blood-based diseases. We also investigate the structure of the hematopoietic tree and the influence this has on the proliferation of diseased cells. Finally, we describe the impact that stem cell ageing has on the hematopoietic system's ability to maintain a healthy supply of blood to the body.

DY 39: Microswimmers II (joint Session BP/DY)

Joint Session with DY organized by BP.

Time: Wednesday 11:30–13:00 Location: H45

DY 39.1 Wed 11:30 H45

Interactions of self-thermophoretic swimmers — •Santiago Muiños Landin, Andreas Bregulla, and Frank Cichos — Molecular Nanophotonics, Universität Leipzig, Institut for Experimental Physics I, Linnéstrasse 5, 04103 Leipzig, Germany

Propulsive mechanisms and collective behavior of self propelled microswimmers are interesting and challenging topics which had been studied in different natural and artificial systems during last years. Given that the collective behavior depends on how do these swimmers interact, and the fact that the aspects of these interactions are directly related to their propulsive mechanisms, we can say that these both aspects are coupled. Here we present an experimental method, based on previous own related work[1,2]. The developed Photon Nudging technique allows us to collect a well defined number of self-thermophoretic Janus particles in a small sample volume. Based on this we show results of a free expansion study of an active particle gas in solution which provides information in the mutual interactions between these photophoretic swimmers

[1] B.Qian, D. Montiel, A. Bregulla, F. Cichos, Chem. Science 4, 1420 (2013) [2] A. Bregulla, H. Yang, and F. Cichos, ACS Nano 8(7), 6542 (2014)

DY 39.2 Wed 11:45 H45

Escaping turbulence? Phytoplankton use active shape control to rapidly adapt swimming strategies — •Anupam Sengupta[1,2], Francesco Carrara[1], and Roman Stocker[2] — [1]Massachusetts Institute of Technology, 15 Vassar Street, Cambridge MA 02139, USA — [2]ETH Zurich, Institute for Environmental Engineering, Stefano-Franscini-Platz 5, 8093 Zurich, Switzerland

Turbulence has long been known to affect phytoplankton fitness and species succession, yet, a mechanistic view of how turbulence affects phytoplankton migration has been lacking. Here we report on the first observations demonstrating that phytoplankton can actively respond to turbulence-like cues. Using the red-tide producing species Heterosigma akashiwo as a model system, we show that hydrodynamic cues mimicking overturning by Kolmogorov-scale turbulent eddies trigger a diversification in the migration behavior. Upon exposure to repeated overturning, an originally upward swimming population robustly splits in two equi-abundant subpopulations, one swimming upward and one swimming downward. Quantitative image analysis at the single-cell level showed that the behavioral switch was accompanied by a rapid morphological change at the sub-micrometer scale, and a mathematical model of the cell's mechanical stability confirms that this shape change can flip the swimming direction and ultimately induce downward migration. The results indicate that certain phytoplankton species may have evolved subtle strategies to actively change their migratory behavior in response to turbulent cues, possibly a bet-hedging strategy to escape from turbulent microzones in the ocean.

DY 39.3 Wed 12:00 H45

Run-reverse-flick strategy of interacting bacteria — •Fabian Schwarzendahl, Stephan Herminghaus, and Marco Giacomo Mazza — Max Planck Institute for Dynamics and Self-Organization, Göttingen Am Fassberg 17, 37077 Göttingen, Germany

Bacteria have different swimming strategies for finding nutrition. *Escherichia coli* follow a run and tumble strategy whereas *Vibrio alginolyticus* have a run-reverse-flick pattern [1]. We simulate the latter using molecular dynamics to integrate the underlying stochastic equations. Without interactions between the bacteria, the analytical result by Theves [2] is recovered. Furthermore, hard-core interactions are used. Here, we study the effect of particle interactions by varying the filling fraction as well as the ratio of mean forward-to-backward run time (biased run). We find that the diffusion-density coupling parameter has a minimum at a forward to backward runtime ratio of 0.6, which is the value that was measured for *Vibrio alginolyticus* by Xie et. al. [1]. Furthermore we present an analytical model based on a Fokker-Planck approach.

[1] Li Xie et. al., Proc. Natl. Acad. Sci. USA **108**, 2246 - 2251 (2010)

[2] Matthias Theves et. al., Biophys. J. **105**, 1915 - 1924 (2013)

DY 39.4 Wed 12:15 H45

Swimming dynamics of a polar multi-flagellated bacterium — •Marius Hintsche[1], Matthias Theves[1], Marco Kühn[2], Kai Thormann[2], and Carsten Beta[1] — [1]Universität Potsdam, Germany — [2]Justus-Liebig-Universität Giessen, Germany

Bacterial motility patterns and chemotaxis strategies are very diverse and depend on factors such as flagellation as well as the typical environment the species encounters. For some bacteria the motility pattern and the underlying flagellar dynamics have already been elucidated – as in the paradigmatic run-and-tumble behavior of *E. coli*. We study the swimming motility and chemotactic behavior of the polar multi-flagellated soil dwelling bacterium *Pseudomonas putida*. Its run-and-reverse motility pattern with many sharp reversal events is reminiscent of the behavior of some monoflagellated species. However, upon a reversal, *P. putida* changes its swimming speed by a factor of two on average. We also analyze the swimming pattern in the presence of chemical gradients. Using benzoate as a chemoattractant, we measure key motility parameters in gradients of different strength in order to quantify the directional bias these conditions introduce in this swimmer's random walk. Our results indicate a change in the reversal frequency depending on changes in the chemoattractant concentration consistent with earlier qualitative reports. Using high-speed fluorescence microscopy, we examine the dynamics of the polar bundle of flagella during smooth swimming and turning and discuss some recent hypotheses concerning the bundle dynamics of these bacteria in the light of our new observations.

DY 39.5 Wed 12:30 H45

Sperm navigation along helical paths in 3D chemoattractant landscapes — •Jan F. Jikeli[1], Luis Alvarez[1], Benjamin Friedrich[2], Laurence G. Wilsion[3], and U.Benjamin Kaupp[1] — [1]research center caesar; Ludwig-Erhard-Allee 2; 53175 Bonn Germany — [2]Biological Physics, Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [3]Department of Physics, University of York, YO10 5DD Heslington, York, UK

Sperm require a sense of direction to locate the egg for fertilization. They follow gradients of chemical and physical cues provided by the egg or the oviduct. However, the principles underlying three-dimensional (3D) navigation in chemical landscapes are unknown. Here using holographic microscopy and optochemical techniques, we track sea urchin sperm navigating in 3D chemoattractant gradients. Sperm sense gradients on two timescales, which produces two different steering responses. A periodic component, resulting from the helical swimming, gradually aligns the helix towards the gradient. When incremental path corrections fail and sperm get off course, a sharp turning manoeuvre puts sperm back on track. Turning results from an "off" Ca2+ response signifying a chemoattractant stimulation decrease and, thereby, a drop in cyclic GMP concentration and membrane voltage. These findings highlight the computational sophistication by which sperm sample gradients for deterministic klinotaxis. We provide a conceptual and technical framework for studying microswimmers in 3D chemical landscapes.

DY 39.6 Wed 12:45 H45

Elastic microswimmers in confined spaces — •Jayant Pande[1], Timm Krüger[2], Jens Harting[3,4], and Ana-Sunčana Smith[1,5] — [1]PULS group, Dept. of Phys. and EAM Cluster of Excellence, Friedrich-Alexander Univ., Erlangen, Germany — [2]School of Engg., Univ. of Edinburgh, Edinburgh, U.K. — [3]Dept. of Appl. Phys., Eindhoven Univ. of Technology, Eindhoven, The Netherlands — [4]Research Centre Jülich, Helmholtz-Inst. Erlangen-Nuremberg, Nuremberg, Germany — [5]Div. of Phys. Chem., Ruđer Bošković Inst., Zagreb, Croatia

Both natural microswimmers such as bacteria and artificial ones such as microscopic drug delivery systems (as currently foreseen) commonly move through constrained spaces such as thin films or biological channels. This constrainment alters their conditions of motion, relative to swimming in an infinite expanse of fluid, due to effects such as fluid reflection from channel walls, heightened drag forces, etc., and is manifested in fundamentally different fluid flow fields. We study these effects by employing the LB3D simulation system, based on the

lattice-Boltzmann and immersed boundary methods, to simulate the three-sphere swimmer of Najafi and Golestanian as it moves through narrow and wide channels. We modify the original three-sphere model to allow different degrees of elasticity in the swimmer, and investigate the interplay of these degrees of elasticity with the channel shapes and dimensions in determining the swimming efficiency. We present ways to take the swimmer elasticity into consideration analytically, and show that motion within channels may be understood in terms of the swimming regimes that depend on the drag force faced by the swimmer.

DY 40: Crystallization, Nucleation, Self Assembly II (joint session CPP/DY, organized by CPP)

Time: Wednesday 16:00–18:30 Location: H42

Invited Talk DY 40.1 Wed 16:00 H42

From holes to drops to toroids: Transcription of surface patterns into 3D-morphologies by dewetting — •Günter Reiter[1], Samer Al Akhrass[2], and Laurant Vonna[3] — [1]Institute of Physics and Freiburg Materials Research Centre, University of Freiburg, 79104 Freiburg, Germany — [2]Université Claude Bernard Lyon 1, Ingénierie des Matèriaux Polymeres (IMP - UMR CNRS 5223), 15 Boulevard Latarjet, 69622 Villeurbanne Cedex, France — [3]Institut de Science des Matériaux de Mulhouse, (IS2M - UMR CNRS 7361), 15, rue Jean Starcky 68057 Mulhouse Cedex, France

Dewetting of thin films is a simple and thus highly convenient process for creating regularly ordered topographical patterns on various lengthscales. Here, we present a general pathway, based on dewetting of a thin polymer film, which allows to convert a chemical surface pattern of hexagonally arranged non-wettable circular patches into a sequence of ordered three-dimensional topographies. With increasing thickness of the dewetting film, cylindrical holes, followed by droplets with the shape of a spherical cap and finally toroids were generated. We identified the width w of the rim, where the dewetted fluid was collected, as the crucial parameter which determined the final three-dimensional morphology. Our experiments demonstrate that for a given surface pattern various three-dimensional morphologies can be obtained by simply varying the initial thickness of the thin film.

DY 40.2 Wed 16:30 H42

Time-resolved characterization of aggregation during printing of thin films — Stephan Pröller[1], Feng Liu[2], Cheng Wang[3], Thomas P. Russell[2], Alexander Hexemer[3], Peter Müller-Buschbaum[4], and •Eva M. Herzig[1] — [1]Technische Universität München, Munich School of Engineering, Lichtenbergstr. 4, 85748 Garching , Germany — [2]Department of Polymer Science and Engineering, University of Massachusetts Amherst, MA 01003 , USA — [3]Lawrence Berkeley National Laboratory, Advanced Light Source Berkeley , CA 94720 , USA — [4]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching , Germany

The nanomorphology can strongly influence the physical properties of thin films. For example, polymer:fullerene mixtures used in the application for organic photovoltaics vary significantly in performance depending on the inner film morphology. Tracking the actual crystallization and aggregation processes on length scales ranging from sub-nanometers to several tens of nanometers reveals how the different growth processes compete with each other leading to the final film morphology.[1] We can track solvent removal, fullerene aggregation and polymer crystallization with time for different exerimental conditions using grazing incidence x-ray scattering revealing fundamental mechanisms of thin film formation. This information correlated with device performance helps to derive design principles for large scale, industrial thin film fabrication.

[1] Pröller et al, Adv. Energy Mater. DOI:10.1002/aenm.201501580

DY 40.3 Wed 16:45 H42

Following the crystallization in PEDOT:PSS films during printing — Claudia M. Palumbiny[1], Feng Liu[2], Thomas P. Russell[2,3], Alexander Hexemer[4], Cheng Wang[4], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Materials Science Division, LBNL, Berkeley, USA — [3]Department of Polymer Science and Engineering, UMass, Amherst, USA — [4]Advanced Light Source, LBNL, Berkeley, USA

PEDOT:PSS is one of the most promising electrode materials beyond ITO. Printed films of PEDOT:PSS are compared with ethylene glycol (EG)-doped PEDOT:PSS films and films that are treated with EG after printing and annealing, so-called EG-post-treatment. In-situ GIWAXS is used to determine the structure of the molecules in the crystallites during the printing. During film formation, the dependence of different processing conditions on the resulting interchain coupling (characterized by the pi-pi stacking distance), molecular orientation, and crystallite size are determined as a function of film composition. Thus, understanding the film evolution during the printing process allows for directed modification of solutions and printed films for enhanced organic electronic device performance.

15 min. break

DY 40.4 Wed 17:15 H42

Towards a multiscale study of aggregation of PCPDTBT in presence of a solvent — •Nancy C. Forero-Martinez[1], Tristan Bereau[1], Bjoern Baumeier[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Mathematics and Computer Science and Institute for Complex Molecular Systems, Eindhoven University of Technology,The Netherlands

Conjugated donor-acceptor polymers are excellent candidates as donor materials for organic photo-voltaic devices due to their charge transport properties. In particular, the microstructure of the low-bandgap PCPDTBT polymer is considered to be affected by the change in morphology of side chains and/or by the processing solvents. The performance of PCPDTBT-optimised solar cells is thus intrinsically linked to the initial preparation of the system: out-of-equilibrium conditions influence the equilibrium system. In this work, we perform multiscale simulations to monitor how the initial presence of solvents drives the formation of PCPDTBT aggregates. We propose as a first step a simplified model of the polymer system that takes into account only CPDT monomers, since their crystalline structure is known experimentally. An atomistic description of the potential energy and the corresponding coarse grained representation are used to study the structure and dynamics of CPDT monomers in solution. We intend to characterise the interactions between polymer and solvent to identify the mechanism promoting aggregation.

DY 40.5 Wed 17:30 H42

Revealing Structure Formation in conjugated polymers such as PCPDTBT by Optical Spectroscopy — •Anna Köhler[1], Christina Scharsich[1], Florian Fischer[2], Kevin Wilma[3], Fabian Panzer[1], Richard Hildner[3], and Sabine Ludwigs[2] — [1]Experimental Physics II, University of Bayreuth, Bayreuth, Germany — [2]IPOC-Functional Polymers, University of Stuttgart, Stuttgart , Germany — [3]Experimental Physics IV, University of Bayreuth, Bayreuth, Germany

There is increasing evidence that the performance of conjugated polymers in organic solar cells is strongly affected by the presence of small crystallites or aggregates. However, short-range order is difficult to detect using structural techniques. Here, we show that optical spectroscopy can be employed to reveal the presence of short-range ordered structured as well as their formation mechanism. We present a comprehensive study of the optical properties as a function of temperature for PCPDTBT in solution and in thin films with two distinct morphologies.[1] Using absorption and photoluminescence spectroscopy as well as Franck-Condon analyses, we show that PCPDTBT in solution undergoes a phase transition (critical temperature: 300 K) from a disordered to a truly aggregated state upon cooling. Comparison is made to the formation of aggregtes in P3HT.[2] The saturation value of aggregates in solution is reached in PCPDTBT thin films at any temperature. In addition, we demonstrate that a low percentage of thermally activated excimer states is present in the films at temperatures above 200 K.

DY 40.6 Wed 17:45 H42

Comparing molecules and solids across structural and al-

chemical space — •Sandip De — Laboratory of Computational Science and Modelling, Institute of Materials, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Evaluating the (dis)similarity of crystalline, disordered and molecular compounds is a critical step in the development of algorithms to classify structures, search chemical space for better compounds and materials, and drive the next generation of machine-learning algorithms for predicting the stability and properties of atomic systems. In recent years several strategies have been designed [1-3] to compare atomic coordination environments. In particular, the Smooth Overlap of Atomic Positions has emerged as a natural framework to obtain translation, rotation and permutation-invariant descriptors of atomic environments, driven by the design of various classes of machine-learned inter-atomic potentials. Here we will present few examples showcasing how one can construct a Sketchmap[4-6] representation of databases of both molecular and bulk structures, using (dis)similarity definitions based on such local descriptors that can treat alchemical and structural complexity within a unified framework.

[1] A. P. Bart ok, et al, Phys. Rev. B88, 054104(2013) [2] Ali Sadeghi et al, J. Chem. Phys. 139, 184118 (2013) [3] Sandip De et al, Phys. Rev. Lett. 112, 083401(2014) [4] G. A. Tribello et al,Proc. Acad. Natl. Sci. U.S.A. 109 5196 (2012) [5] M. Ceriotti et al, Proc. Acad. Natl. Sci. U.S.A. 108 13023 (2011) [6] M. Ceriotti et al, J. Chem. Theory Comput. 9 1521 (2013)

DY 40.7 Wed 18:00 H42

Area confined nucleation and position control by vapor deposition — •Oleg Buller[1], Hong Wang[2], Wenchong Wang[2], Lifeng Chi[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, WWU, Münster — [2]Physikalisches Institut and Center for Nanotechnology, WWU, Münster

Experimentally it is possible that after vapor deposition of organic molecules on surfaces, prepatterned with a regular gold grid, in basically each cell a single nucleus is formed (defects less than 2%) exactly in the center of each grid. This enormous nucleation and position control can be reproduced for different organic molecules. Via combination of kinetic Monte Carlo simulations and analytical calculations a theoretical explanation for this high quality is provided. In this way it is possible to understand, e.g. that the size of the grid and the external flux simultaneously have to be varied in order to stay in the regime of perfect nucleation and position control. A direct comparison between the experimental and theoretical results is presented.

DY 40.8 Wed 18:15 H42

Coverage dependent nucleation of PTCDI-C_8 studied by AFM and *in situ* real time XRR and GISAXS — •Anton Zykov[1], Sebastian Bommel[2], Christopher Wolf[1], Linus Pithan[1], Christopher Weber[1], Paul Beyer[1], Gonzalo Santoro[3], Stephan V. Roth[2], and Stefan Kowarik[1] — [1]Inst. f. Physik, Humboldt Universität Berlin — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg — [3]Inst. de Ciencia y Tecnología de Polímeros, CSIC, Madrid

Assembly of molecular building blocks into functional nanomaterials is of great importance for devices however it is difficult to follow molecular scale morphology during growth. Here we show that modern synchrotron small angle X-ray scattering (GISAXS) and X-ray reflectivity (XRR) agree with post growth AFM measurements of roughness and island densities of PTCDI-C_8 on silicon oxide, but additionally offer *in situ* and real time capability. We observe interesting differences in the growth of the 1^{st} and 2^{nd} monolayer (ML) such as different molecular adsorption probabilities and a transition of the island shapes. From the scaling of saturation island densities with substrate temperature and growth rate we evaluate ML dependent nucleation energies and critical nucleus sizes. We discuss our results in the framework of nucleation theories and find that 2^{nd} ML nucleation does not proceed in the often applied diffusion limited aggregation regime. This work shows that X-ray techniques are similarly suited for continuously monitoring multilayer growth and unravel intricate details about sub-monolayer growth.

DY 41: Quantum Chaos

Time: Wednesday 15:00–17:45 Location: H48

Invited Talk DY 41.1 Wed 15:00 H48

Visualizing quantum chaos in four dimensions — •Arnd Bäcker — TU Dresden, Institut für Theoretische Physik and Center for Dynamics, Dresden — MPI für Physik komplexer Systeme, Dresden

As the simplest example of higher-dimensional systems with a mixed phase space we consider 4D maps. The global organization of regular tori is visualized using 3D phase-space slices [1, 3]. Representing regular and chaotic eigenstates in the 3D phase-space slice allows for comparing with classical structures to investigate the semiclassical eigenfunction hypothesis.

Such 4D maps can also be interpreted as two coupled 2D systems. If these two subsystems are strongly chaotic, we demonstrate that spectral statistics show a universal transition towards random matrix fluctuations for increasing interaction strength [2]. Moreover, entanglement in eigenstates, as measured by the von-Neumann entropy, shows a universal transition to nearly maximal entanglement.

[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. C. L. Srivastava, S. Tomsovic, A. Lakshminarayan, R. Ketzmerick, and A. Bäcker, *Universal scaling of spectral fluctuation transitions for interacting chaotic systems*, arXiv:1509.02329, Phys. Rev. Lett. in press.
[3] For videos of 3D phase space slices see:
`http://www.comp-phys.tu-dresden.de/supp/`

DY 41.2 Wed 15:30 H48

Interplay between chaos and indistinguishability in multiparticle scattering — •Juan-Diego Urbina[1], Jack Kuipers[1], Klaus Richter[1], Quirin Hummel[1], and Sho Matsumoto[2] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Graduate School of Science and Engineering, Kagoshima University, 1-21-35, Korimoto, Kagoshima, Japan

In this presentation we generalize the Hong-Ou-Mandel effect to the mesoscopic regime of complex scattering and to macroscopically occupied incoming wavepackets. This is achieved by a complete enumeration of all processes in terms of interfering many-body paths that allow us to study universal effects due to the interplay between instability of the single-particle classical motion and quantum indistinguishability.

We show how, in the limit of large particle number, one finds a mesoscopic version of the bosonic birthday paradox responsible for a sharp quantum-classical transition. Furthermore, under a scaling that defines the classical-quantum boundary we predict a macroscopic, experimentally accessible Hong-Ou-Mandel profile.

Our results are obtained by a combination of Random Matrix Theory and semiclassical methods, and can be extended to the quantum optics domain, and point towards a mesoscopic implementation of the boson sampling problem of current interest as a possible first realization of a quantum simulator for a certified hard problem.

DY 41.3 Wed 15:45 H48

Chaotic transport in resonance channels in 4D maps — •Franziska Onken[1,2], Steffen Lange[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

The dynamics of Hamiltonian systems (e.g., planetary motion, electron dynamics in nano-structures, chemical reactions) can be understood by studying the corresponding symplectic Poincaré maps. A central new feature in higher-dimensional systems is the transport in resonance channels. While such channels are usually investigated in frequency space, we visualize the relevant invariant objects in phase space revealing a highly non-trivial geometry. It is governed by families of elliptic and hyperbolic 1D-tori together with their stable and unstable manifolds. This provides a visualization of a turnstile in higher dimensions which allows for the escape from the channel.

DY 41.4 Wed 16:00 H48

Resonance-assisted tunneling in deformed optical microdisk

cavities — •Julius Kullig and Jan Wiersig — ITP, Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany

In generic systems tunneling not only occurs at energy barriers but also between classically disjoint regions in phase space. Nonlinear resonance chains which arise generically from system perturbations drastically enhance the tunneling effect which is then called resonance-assisted tunneling (RAT). While RAT is well studied for kicked Hamiltonian systems and experimentally observed in microwave billiards its application to optical cavities is less investigated. But here a recent experiment by [Kwak et al., Sci. Rep. 2015] suggests a particular relevance. In our talk we use perturbative methods for RAT to predict quality factors and optical mode structures of deformed microdisk cavities.

DY 41.5 Wed 16:15 H48

Three-dimensional description of optical microcavities — •Jakob Kreismann and Martina Hentschel — TU Ilmenau, Ilmenau, Deutschland

Microcavity lasers made of deformed dielectric disk resonators such as the Limaçon-shaped cavity have attracted a lot of interest because they show directional light emission. Both ray optics and wave simulations for two-dimensional model systems confirm the support of whispering gallery-like modes with high quality factors while possessing directional light emission. In reality, however, these microcavities are three-dimensional objects with finite heights. Therefore we perform numerical simulations of the full three-dimensional system and investigate the influence of the cavity height on the resonance energies, their quality factors and far-field profiles. We discuss analogies of the structure between the two-dimensional and three-dimensional modes, and find a dependence on the ratio of the cavity height to the wavelength that can be quantified in terms of the effective refractive index model. The analysis of the three-dimensional far-field profiles reveals directional emission in azimuthal direction (i.e. in the plane of the resonator) as known from the two-dimensional case, and furthermore directional emission inclined to that plane as a truly three-dimensional effect. We use this new effect for a possible technical application, and design a sensor that can detect particles in the environment based on changes in the emission direction.

15 min. break

DY 41.6 Wed 16:45 H48

Triangular microlasers in the ray picture — •Pia Stockschläder and Martina Hentschel — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We apply ray-optical methods to dielectric optical microcavities in the shape of triangles made of low refractive index material. Geometrical optics is extended by the inclusion of intensity amplification along the optical path to achieve a better description of active, lasing cavities. Far-field emission patterns of triangular cavities obtained in this way agree well with experimental results. We find ray trajectories that maximize the intensity inside the cavity to determine the far-field emission characteristics. As these maximum intensity orbits need not to be periodic we suggest that they provide a more general explanation for emission patterns of microlasers than single periodic orbits. We present results for triangles of different symmetry classes.

DY 41.7 Wed 17:00 H48

Phase-space localization of chaotic resonance states — •Konstantin Clauss[1], Martin Körber[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

In open quantum systems with escape a fundamental question concerns the phase-space localization of resonance states. For fully chaotic systems the resonance states are supported on a fractal set of classically trapped orbits. We investigate the possibility of quantum ergodicity, i.e. equidistribution of resonance states with respect to suitable classical densities on this fractal set. We observe remarkable deviations from naturally expected fractal densities on large scales and study their origin.

DY 41.8 Wed 17:15 H48

Experiments on microwave graphs with anti-unitary symmetry squaring to minus one — •Aimaiti Rehemanjiang[1], Markus Allgaier[2,1], Christopher Joyner[5], Sebastian Müller[3], Martin Sieber[3], Hans-Jürgen Stöckmann[1], and Ulrich Kuhl[4,1] — [1]Quantum chaos group, Fachbereich Physik der Philipps-Universität, Marburg, Germany — [2]Integrated Quantum Optics, Applied Physics, Universität Paderborn, Paderborn, Germany — [3]School of Mathematics, University of Bristol, Bristol, UK — [4]Laboratoire de Physique de la Matière Condensée, CNRS UMR 7336, Université Nice Sophia Antipolis, Nice, France — [5]School of Mathematical Sciences, Queen Mary University of London, London, UK

Following an idea by Joyner et al. [1] a microwave graph with antiunitary symmetry squaring to -1 has been realized. The Kramers doublets expected for such systems have been clearly identified and could be lifted by a perturbation which breaks this antiunitary symmetry. The found spectral level spacings distribution of these Kramers doublets is in agreement with the predictions from the Gaussian symplectic ensemble, expected for chaotic systems with such an antiunitary symmetry.

[1] C. Joyner, S. Müller, M. Sieber, EPL, 107 (2014) 50004

DY 41.9 Wed 17:30 H48

A new type of *PT*-symmetric random matrix ensembles — •Steve Mudute-Ndumbe, Eva-Maria Graefe, and Matthew Taylor — Imperial College London, London, United Kingdom

In this talk I will introduce two new random matrix ensembles which can potentially be used to model non-Hermitian PT-symmetric quantum systems, an area of quantum mechanics which has attracted a considerable amount of attention recently. The new ensembles consist of matrices which are Hermitian with respect to the split-complex and split-quaternionic number systems. The eigenvalues of these matrices are either real or come in complex conjugate pairs. I will present some analytical and numerical results on their spectral statistics, focusing in particular on the spectral fluctuations, in the 2×2 and general $N \times N$ matrix size cases.

DY 42: Focus: Multiscale Simulations for Soft Matter: The Challenge of Dynamics (joint session CPP/DY, organized by CPP)

Organizers: Tristian Bereau , Joseph F. Rudzinski, Kurt Kremer (all MPI Polymerforschung, Mainz)

Multiscale simulations have gained increasing interest in soft matter, due to their ability to better reach the many underlying length and timescales spanning these systems. While significant development of coarsegraining methodologies which aim to accurately describe static equilibrium properties has led to a variety of successful applications, obtaining an accurate description of dynamics remains challenging. This focus session aims at bringing together researchers making various contributions to improving the description of dynamics in coarsegrained models, whether providing a theoretical background, improving parametrization protocols, or studying the limits of existing models.

Time: Wednesday 15:00–18:15 Location: H51

DY 42.1 Wed 15:00 H51

Reactive molecular dynamics simulations of NaOH solutions — •Matti Hellström and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

Sodium hydroxide (NaOH) is soluble in water up to very high concentrations and has many applications in chemical industry. Still, sur-

prisingly little is known about the structural and dynamical properties of its aqueous solutions. Using a high-dimensional neural network potential for NaOH(aq) based on dispersion corrected density-functional theory calculations, we have performed large-scale molecular dynamics simulations with close to ab initio quality. First results on many different phenomena like ligand exchange, ion clustering and proton transfer as well as their dependence on concentration are presented and discussed.

DY 42.2 Wed 15:15 H51

Benchmark of a Reparametrized OPLS Force Field for Chlorinated Hydrocarbons Using Molecular Dynamics Simulations — •Zhu Liu, Jakob Timmermann, Karsten Reuter, and Christoph Scheurer — Theoretical Chemistry, Technische Universität München

The dielectric permittivity sensitively reflects the unique microscopic characteristics of a material [1]. To our knowledge no flexible non-polarizable force field for chlorinated hydrocarbons reliably reproduces this important physical property. We address this situation by reparametrizing an OPLS-AA (Optimized Parameters for Liquid Simulations, All-Atom) force field [2] to optimize the description of dynamic and dielectric properties. Specifically, we refitted the torsional potential energy profile and the atomic partial charges for several molecules from this class to match quantum chemical data. We find the new parametrization to yield a range of physical properties (especially the dielectric constant, isothermal compressibility, and thermal expansion coefficient) in excellent agreement with experimental data for a range of chlorinated hydrocarbon solvents, in addition to getting the surface tension and heat capacity at least as well as the original OPLS-AA model.

[1] C.J.F. Böttcher, Theory of Electric Polarization, Vol. I: Dielectrics in Static Fields, Elsevier B.V., Amsterdam (1973).
[2] W.L. Jorgensen *et al.*, Proc. Natl. Acad. Sci. **102**, 6665 (2005).

DY 42.3 Wed 15:30 H51

Thermodynamics of polymer nematics: particle-based simulations versus mean-field calculations — •Cristina Greco, Kurt Kremer, and Kostas Daoulas — Max Planck Institute for Polymer Research, Mainz, Germany

Conjugated liquid crystalline (LC) polymers have emerged as promising materials for organic electronics. Predicting their large-scale morphology requires the implementation of mesoscale models. The statistical mechanics of such models is often addressed using mean-field (MF) approaches. These have been very successful in polymer physics and are attractive because of their computational efficiency and straightforward description of thermodynamic properties. For LC polymers, however, deviations between MF predictions and experimental results have been reported, e.g. for the molecular weight dependence of the nematic-isotropic transition. The question then arises: are the discrepancies due to the MF approximation or do they reveal fundamental limitations of the model, e.g. transferability?

To address this issue, we consider a model representing polymer nematics as worm-like chains interacting through soft anisotropic potentials and investigate its phase behaviour by (i) MF calculations based on partial enumeration of conformations, (ii) Monte Carlo simulations. In the latter, accurate free energies are obtained via a special thermodynamic integration scheme which avoids thermodynamic singularities. By comparing the results of the two methods, we can evaluate the effect of fluctuations and local correlations on the macroscopic behaviour.

DY 42.4 Wed 15:45 H51

Comparing atomistic and coarse-grained simulations of P3HT — •Jonathan Gross, Momchil Ivanov, and Wolfhard Janke — ITP Uni Leipzig

Poly(3-hexylthiophene) (P3HT) is a key material used in organic photovoltaics (OPVs). In this study we assess the validity of two coarse-grained models of P3HT. We compare coarse-grained Monte Carlo simulations to fully atomistic molecular dynamics simulations. Structural properties of single polymer chains of short to medium lengths are compared between the three representations.

Invited Talk DY 42.5 Wed 16:00 H51

A coarse-grained model for DNA: dynamics of self-assembling biological systems and nanostructures. — •Ard Louis — Theoretical Physics, University of Oford

DNA is a particularly promising candidate for large-scale self-assembly because the specific binding of DNA bases can be accurately designed to build dynamic structures on the nanoscale with atomic precision. Inside the cell, DNA not only stores information in a digital code, but controls its readout by subtle modulation of its dynamic properties.

To study processes on these time and length-scales we employ oxDNA[1], a nucleotide level coarse-grained model that can model dynamical DNA structures with thousands of nucleotides. We are able to accurately reproduce the dynamics of exchange reactions, a key component of dynamic DNA nanotechnology, and also make detailed predictions for the hybridization dynamics of DNA duplexes. Larger structures such as a DNA nanobot can also be studied. For the dynamics of large-scale addressable assemblies, we develop a new multi-scale technique. As is the case for many other coarse-grained systems, correctly interpreting dynamical results is subtle[2].

[1] http://dna.phyiscs.ox.ac.uk [2] J.T. Padding and A.A. Louis, Phys, E 74, 031402 (2006)

15 min. break

DY 42.6 Wed 16:45 H51

Cycle representatives for the coarse-graining of systems driven into a non-equilibrium steady state — •Fabian Knoch and Thomas Speck — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7-9, 55128 Mainz, Germany

A major current challenge in statistical mechanics poses the systematic construction of coarse-grained Markov State Models [1] that are dynamically consistent, and, moreover, might be used for systems driven out of thermal equilibrium. Here we present a novel prescription that extends the Markov state modeling approach to driven systems violating detailed-balance [2]. In more detail, we decompose a given Markov State Model in cycles and introduce the concept of cycle representatives, which stand for many cycles that share similar properties. The coarse-graining involves the renormalization of transition rates that preserves the entropy production of the original Markov State Model. We illustrate our new methodology by an intuitive example: A particle trapped in a 2-dimensional double well potential and driven by a non-conservative force.

[1] Prinz, J.-H., Wu, H., Sarich, M., Keller, B., Senne, M., Held, M., Chodera, J. D., Schütte, C. and Noe, F. Markov models of molecular kinetics: Generation and validation. JCP 134(17), 2011
[2] Knoch, F. and Speck, T. Cycle representatives for the coarse-graining of systems driven into a non-equilibrium steady state. New Journal of Physics 17(11), 2015

DY 42.7 Wed 17:00 H51

Improving the kinetics from molecular simulations using biased Markov state models — •Joseph Rudzinski, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Molecular simulations can provide microscopic insight into the physical and chemical driving forces of complex molecular processes. Despite continued advancement of simulation methodology, model errors may lead to inconsistencies between simulated and experimentally-measured observables. This work presents a robust and systematic framework for reweighting the ensemble of dynamical paths sampled in a molecular simulation in order to ensure consistency with a set of given kinetic observables. The method employs the well-developed Markov state modeling framework in order to efficiently treat simulated dynamical paths. We demonstrate that, for two distinct coarse-grained peptide models, biasing the Markov state model to reproduce a small number of reference kinetic constraints significantly improves the dynamical properties of the model, while simultaneously refining the static equilibrium properties.

Invited Talk DY 42.8 Wed 17:15 H51

Principle of Maximum Caliber and its application in biology — •Kingshuk Ghosh — University of Denver

We will describe the principle of Maximum Caliber (MaxCal), a variational approach to model dynamical fluctuations. MaxCal is similar to the Maximum Entropy principle but applied in the trajectory space, natural language in describing several biological systems ranging from macromolecular dynamics to networks. We will briefly describe the general formalism and show the equivalence between MaxCal and Markov processes. Next we will present application of MaxCal to model stochastic dynamics in biological systems, in particular genetic networks. These applications will highlight the role of MaxCal in

describing complex systems with cooperativity, non-linearty and feedback in a coarse-grained manner and yet provide us with quantitative tools to analyze data and gain valuable insights.

Invited Talk DY 42.9 Wed 17:45 H51

Coarse-graining of conservative and non-conservative interactions in molecular liquids — •Nico van der Vegt — Technische Universität Darmstadt, Darmstadt, Germany

In my talk, I will discuss two central challenges in multiscale simulations of soft matter: How can we improve the transferability of bottom-up coarse grained models? How can we improve the coarse-grained model's dynamical properties? Both questions are important, in particular when transport and nonequilibrium processes are studied. I will present a bottom-up coarse-graining procedure for constructing conservative and non-conservative (dissipative and stochastic) interactions for Dissipative Particle Dynamics (DPD) models of molecular liquids. This procedure is based on the Conditional Reversible Work (CRW) method.[1] I will address the chemical and state-point transferability of conservative potentials for coarse-grained molecular liquids in bulk and at interfaces,[2,3] and discuss challenges that remain in modelling dynamical properties of molecular liquids with CRW-DPD models.[4]

References: (1) E. Brini, V. Marcon, N. F. A. van der Vegt, PCCP 13, 10468-10474 (2011). (2) E. Brini, N. F. A. van der Vegt, J. Chem. Phys. 137, 154113 (2012). (3) V. R. Ardham, G. Deichmann, N. F. A. van der Vegt, F. Leroy, J. Chem. Phys. 143, 243135 (2015) (4) G. Deichmann, V. Marcon, N. F. A. van der Vegt, J. Chem. Phys. 141, 224109 (2014)

DY 43: Statistical Physics in Biological Systems III (joint DY/BP)

Time: Wednesday 15:30–16:15 Location: H46

DY 43.1 Wed 15:30 H46

Bursting noise in gene regulation networks: exact and numerical results for stationary distributions and first passage times — •Yen Ting Lin[1], Charles Doering[2], and Tobias Galla[1] — [1]The University of Manchester, Manchester, UK — [2]University of Michigan, Ann Arbor, USA

Understanding how effects of noise propagate from one level of modelling to another is key in a number of applications in physiological or biological systems. Including short-lived mRNA populations in models of gene regulation networks introduces bursting noise, and understanding the effects of this in higher-level models is an open task. In this talk, I will present a coarse-graining method to construct mesoscopic models for such type of dynamical systems, which fully accounts for the bursting noise. We systematically compare different levels of modeling, ranging from individual-molecule-based models including mRNA populations, over protein-only individual-based models to mesoscopic models such as diffusion-type models and our proposed model. We show that the proposed mesoscopic model outperforms conventional diffusion-type models. In a one-dimensional autoregulated network, we present closed-form analytic solutions for both the stationary distribution of protein expression as well as first-passage times of the dynamical system. We present numerical solutions for higher-dimensional gene regulation networks, in which case we also carry out analysis in the weak-noise limit. References: arXiv:1508.02945, arXiv:1508.00608 (*J. R. Soc. Interface* in press)

DY 43.2 Wed 15:45 H46

Population dynamics in switching environments — •Peter Hufton, Yen Ting Lin, Tobias Galla, and Alan McKane — School of Physics and Astronomy, The University of Manchester, Manchester, UK

In gene regulatory networks, the binary state of a single gene can have drastic effects on the dynamics of a population of proteins. Similarly, switches between environmental states are important in bacterial populations and in models of epidemic spread. The mathematical treatment of problems of this type—populations in switching environments—is an open challenge. We present a systematic approach to computing stationary states of these problems. We identify two sources of randomness: the stochasticity from environmental switches, and the intrinsic noise from fluctuations in the population. By extending the linear-noise approximation and utilising a piecewise-deterministic Markov process, we develop a method which incorporates both these effects.

DY 43.3 Wed 16:00 H46

Geometry Dependence of the Diffusion Coefficient in Molecular Dynamics Simulations with Periodic Boundary Conditions — •Martin Vögele and Gerhard Hummer — Max-Planck-Institut für Biophysik, Frankfurt am Main

We investigate the dependence of the diffusion coefficient on the box geometry and its application to lipid membrane simulations.

For this purpose, we compare predictions from a simple analytic correction based on hydrodynamic arguments to molecular dynamics simulations of liquid argon. Increasing the box size in two dimensions, we find a logarithmic dependence on the system size. Increasing the box size in only one dimension, we find a linear dependence. In both cases, diffusion is anisotropic. Additionally, we observe an upper limit for the diffusion coefficient in the limit of infinite systems.

We also test the effect of box geometry on the diffusion in lipid membranes, which are usually simulated in very flat periodic boxes. There we find the predicted logarithmic increase with growing edge lengths.

DY 44: Critical Phenomena and Phase Transitions

Time: Wednesday 15:30–17:15 Location: H47

DY 44.1 Wed 15:30 H47

Finite-size scaling of free-energy barrier in droplet formation and nucleation-like processes — •Johannes Zierenberg, Philipp Schierz, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Germany

We study the nucleation free-energy barrier of the droplet formation process upon a temperature change. Employing generalized-ensemble methods allows us to directly access estimates of the free-energy barrier from energy probability distributions. Phenomenological arguments reveal that in this scenario the free-energy barrier scales with $N^{1/2}$, confirmed by an extensive finite-size scaling analysis. The same scaling is supposed to remain true for other nucleation-like processes such as polymer aggregation.

DY 44.2 Wed 15:45 H47

Multifractal finite-size scaling at the Anderson transition in the unitary symmetry class — •Jakob Lindinger, Andreas Buchleitner, and Alberto Rodriguez — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg

We carry out a full characterization of the Anderson transition in the unitary symmetry class. We apply multifractal finite-size scaling [A. Rodriguez, L. J. Vasquez, K. Slevin, R. A. Römer, Phys. Rev. B 84, 134209 (2011)] to the 3-D Anderson model subjected to a homogeneous magnetic field, and estimate the critical parameters as well as the multifractal exponents with high precision using wavefunction data of systems up to $L^3 = 120^3$, obtaining the critical exponent $\nu = 1.460(1.452, 1.468)$. We examine the scaling of the probability density function of wavefunction intensities and explore the possibility of finding a fingerprint of the transition in the correlation function of the phase of the complex wavefunctions.

DY 44.3 Wed 16:00 H47

Analytical continuation of perturbation series in the context

of phase transitions — •Sören Sanders — Institut für Physik, Carl von Ossietzky Universität - D-26111 Oldenburg, Germany

Critical phenomena occuring at continuous phase transitions render a (low-order) perturbative description invalid; to obtain knowledge beyond the phase transition an analytical continuation is required. A recently proposed scheme to obtain nonperturbative physics from low-order perturbation theory utilizing hypergeometric functions [1] is applied in this context [2] and shown to vastly outperform well-established methods such as Shanks transformation and Padé approximation.

[1] H. Mera, T. G. Pedersen, and B. K. Nikolić, Phys. Rev. Lett. **115** (2015) 143001. [2] S. Sanders, C. Heinisch and M. Holthaus, EPL, **11** (2015) 20002.

DY 44.4 Wed 16:15 H47

Driven Markovian Quantum Criticality — •Jamir Marino[1] and Sebastian Diehl[2] — [1]Institut für Theoretische Physik Universität zu Köln — [2]Institut für Theoretische Physik Universität zu Köln

We identify a new universality class in one-dimensional driven open quantum systems with a dark state. Salient features are the persistence of both the microscopic non-equilibrium conditions as well as the quantum coherence of dynamics close to criticality. This provides a non-equilibrium analogue of quantum criticality, and is sharply distinct from more generic driven systems, where both effective thermalization as well as asymptotic decoherence ensue, paralleling classical dynamical criticality. We quantify universality by computing the full set of independent critical exponents within a functional renormalization group approach.

DY 44.5 Wed 16:30 H47

Condensation of methane in Metal Organic Frameworks (MOFs): Interfaces between dilute coexisting phases — •Mojtaba Eshraghi, Nicolas Höft, and Jürgen Horbach — Universitätstraße 1, 40225-Düsseldorf, Germany

Metal-Organic Frameworks (MOFs) are nanoporous crystalline materials where metal oxide complexes are connected to each other by organic linkers[1]. Grandcanonical Monte Carlo simulations in conjunction with advanced sampling methods are used to study the condensation of CH_4 in the MOF systems of IRMOF-1 and IRMOF-8. Two different types of condensation transitions are found, each of them ending in a critical point[2]: (i) a fluid-fluid transition at higher densities (the analog of the liquid-gas transition in the bulk) and (ii) a phase transition at low densities on the surface of the MOF structure. For the latter transition, interfaces between coexisting phases are analyzed in terms of the critical scaling of the interfacial free energy and capillary wave fluctuations.

References

1. H. Li, M. Eddaoudi, M. O'Keeffe, and O. M. Yaghi, *Nature* **402**, 276 (1999).
2. N. Höft and J. Horbach, *J. Am. Chem. Soc.* **137**, 10199-10204 (2015).

DY 44.6 Wed 16:45 H47

Planar order in the 3D plaquette gonihedric Ising model — Marco Mueller[1], Desmond A. Johnston[2], and •Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, D-04009 Leipzig, Germany — [2]Department of Mathematics and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Riccarton, Edinburgh, EH14 4AS, Scotland

We conduct a careful multicanonical simulation of the isotropic 3D plaquette ("gonihedric") Ising model and confirm that a planar, "fukinuke" type order characterises the low-temperature phase of the model. From consideration of the anisotropic limit of the model we define a class of order parameters which can distinguish the low- and high-temperature phases in both the anisotropic and isotropic cases. We also show that the order parameter like behaviour of the standard magnetic susceptibility χ_m observed in previous Metropolis simulations was an artefact of the algorithm failing to explore the phase space of the macroscopically degenerate low-temperature phase.

D.A. Johnston, M. Mueller, and W. Janke, Mod. Phys. Lett. B **29** (2015) 1550109;
M. Mueller, W. Janke, and D.A. Johnston, Nucl. Phys. B **894** (2015) 1;
W. Janke, M. Mueller, and D.A. Johnston, J. Phys.: Conf. Ser. **640** (2015) 012002.

DY 44.7 Wed 17:00 H47

Phase Transitions of Disordered Traveling Salesperson Problems solved with Linear Programming and Cutting Planes — •Hendrik Schawe and Alexander K. Hartmann — Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, Oldenburg (Germany)

The Traveling Salesperson problem asks for the shortest cyclic tour visiting a set of cities given their pairwise distances and belongs to the NP-hard complexity class, which means that typical instances are not solveable in polynomial-time (if P $\neq$ NP holds), i.e. it is *hard*. Though that does not mean, that there are not subsets of the problem which are typically *easy* to solve. To examine a transitions from an easy to a hard phase, we study an ensemble of random configurations of cities in an Euclidean plane, characterized by a parameter σ, which governs the strength of the randomness. The instances are treated using a linear programming approach with selected cutting planes. We observe several phase transitions from easy to hard phases, depending on the types of cutting planes used. These transition are related to physical properties of the shortest tours and analyzed using finite-size scaling techniques.

DY 45: Brownian Motion and Transport

Time: Wednesday 16:30–17:45 Location: H46

DY 45.1 Wed 16:30 H46

Velocity and displacement statistics under nonlinear friction showing bounded particle speed — •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Often, models on the stochastic motion of colloidal particles in a surrounding fluid assume linear "viscous" friction. This case can be solved analytically for free Brownian motion of non-interacting particles.

A prominent example of nonlinear friction is given by "dry" friction of the Coulomb type. In this case, the friction always shows the same magnitude as soon as the particle is in motion. Stochastic models using this type of friction were broadly analyzed over the past few years using different technical tools.

In the present contribution, we introduce a different type of nonlinear friction. It increases linearly with the velocity at low particle speed; it increases more than linearly at higher speeds; finally, it diverges at a certain maximum particle speed. Both, velocity and displacement statistics, are evaluated under stochastic motion in one dimension using the Fokker-Planck approach. For a specific value of the maximum particle speed, significant analytical progress can be made, revealing a formal connection to the Schrödinger equation for an infinite square-well potential. The mean-squared displacement is found to still increase linearly in time, while higher-order moments signal non-Gaussian displacement statistics. Using elements from quantum-mechanical perturbation theory, the influence of an additional drift force is included. Our description should apply for the stochastic motion in shear-thickening environments, possibly starch suspensions.

DY 45.2 Wed 16:45 H46

Friction dynamics of colloidal crystal layers in shear flow — •Sascha Gerloff and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Friction at the nanoscale is characterized by complex non-equilibrium dynamics, whose understanding is relevant for various different systems. An important example is the frictional dynamics of two atomically flat crystalline surfaces in contact, which currently attract strong attention from both, the theoretical and experimental point of view. Here we present results from overdamped Brownian dynamic simulations to investigate the non-equilibrium dynamics of confined colloidal suspensions in shear flow. We focus on slit-pore confinement where the

colloids form colloidal crystal layers. We first revisit the shear-induced dynamics of a one-component bilayer system, displaying a pronounced de-pinning transition related to shear induced melting. Using a one-particle model we estimate the critical shear rate for this transition. As a second step we investigate the frictional dynamics of layers with different crystalline structure. To this end, we introduce an additional layer of small colloids to the system and stabilize it via a constant force. For this system, the dynamics at small shear rates is dominated by a local transport mechanism related to density excitations. Investigating the properties and dynamics of these density excitations is key to understand the overall dynamics of the layer. For small shear rates, we find the relative velocity of the layer to be proportional to the number and velocity of the density excitations.

DY 45.3 Wed 17:00 H46

Quantum-state diffusion approach to the dissipative dynamics of a 1-d double-well system — •Chiara Liverani[1], Michael Finnis[1,2], and Eva-Maria Graefe[3] — [1]Department of Physics, Imperial College London — [2]Department of Materials, Imperial College London — [3]Department of Mathematics, Imperial College London

The generalisation of classical transition rate theory to quantum mechanics is a long-standing problem. A common approach is to interpret Feynman's isomorphism between a quantum-mechanical particle and a periodic ensemble of harmonically interacting classical particles in a dynamical sense, leading for example to the so-called ring-polymer molecular dynamics (RPMD) method.

Here we investigate a toy model to shed further light on the connection between this type of semiclassical description for the open quantum dynamics and the results based on the quantum master equation. We study the time evolution of a particle in a double-well potential governed by a Lindblad equation, as a quantum analogue of a classical Langevin equation. We use the quantum state diffusion approach, where the evolution of the density operator is modelled by an ensemble average over stochastic Schrödinger equations. We investigate the effects of quantum-mechanical tunnelling and coherence in comparison to the classical dynamics and to that yielded by the RPMD method.

DY 45.4 Wed 17:15 H46

Large deviations in Taylor dispersion — •Marcel Kahlen[1], Andreas Engel[1], and Christian Van den Broeck[2] — [1]Institut für Physik, C. v. Ossietzky Universität, 26111 Oldenburg, Germany — [2]Faculty of Sciences, Hasselt University, B-3590 Diepenbeek, Belgium

Taylor dispersion plays an important role in our daily life. Addressing the dispersion of particles in shear flow, it is important for problems reaching from environmental pollution to the construction of water pipes.

A useful approach to analyze Taylor dispersion is to discretize the flow into N layers with different advection velocities. In this way it has been shown, that for sufficiently large time the distribution of particles is to leading order Gaussian. The theory of large deviations goes beyond this Gaussian approximation by quantifying the probability of exponentially rare realizations of particle distributions. The Gaussian result can be regained by a Taylor expansion of the large deviation function. Since the dispersion of particles is directly related to the sojourn times of the particles in the respective layers, the large deviation properties of the particle separations may be deduced from the large deviation behaviour of the empirical density.

In the talk, we apply the theory of large deviations to particle dispersion in an N-layer model. For $N = 2$ we check our results against the exact analytic solution that exists for this case. Results for $N > 2$ are compared to extensive numerical simulations. For $N \to \infty$, we show that our approach is in agreement with the Donsker-Varadhan result for the empirical density.

DY 45.5 Wed 17:30 H46

Brownian Nanoparticle Racetracks — •Stefan Fringes, Michael J. Skaug, and Armin W. Knoll — IBM Research - Zurich, Rüschlikon, Switzerland

Inspired by the transport principle of molecular motors in cells, artificial Brownian motors have been studied theoretically and experimentally to achieve directed motion and sorting of particles in a fluidic environment. Ingredients of such Brownian motors are a spatially asymmetric potential landscape and unbiased external inputs driving the system out of equilibrium. In our implementation we exploit the interaction potential of charged 60 nm gold-nanospheres to like charged confining surfaces in a nanofluidic slit. We shape the asymmetric potential by patterning a 3D ratchet topography in one of the two confining surfaces using thermal scanning probe lithography. The system is driven out of equilibrium by applying a zero-mean AC-electric field. We observe a net drift of several microns per second along a direction dictated by the ratchet geometry. All relevant physical quantities can be measured *in-situ* enabling a parameter free comparison to theory. Our concept works on highly scaled ratchet tracks having a track width of $< 500\,\mathrm{nm}$ and a curvature down to $1\,\mu\mathrm{m}$ radius. We demonstrate the directed motion of nanoparticles in a complex racetrack and on demand transport along orthogonal racetrack directions.

DY 46: Poster: Wetting, Nano- and Microfluidics

Time: Wednesday 18:15–21:00 Location: Poster B2

DY 46.1 Wed 18:15 Poster B2

Theoretical study of slip effects on a dewetting drop — •Tak Shing Chan[1], Joshua D. McGraw[1,2], Thomas Salez[3], and Martin Brinkmann[1] — [1]Experimental Physics, Saarland University, D-66041, Saarbrücken, Germany — [2]Département de Physique, Ecole Normale Supérieure / PSL Research University, CNRS, 24 rue Lhomond, 75005 Paris, France — [3]PCT Lab, UMR Gulliver 7083, ESPCI ParisTech, PSL Research University, 75005 Paris, France

A recent experimental study on the dewetting of polymer microdroplets have shown that slip plays a dominating role on the shape evolution and the motion of the contact line (Under review). Particularly, a transient bump is observed for relatively small slip lengths, while a bump is avoided for larger values. In this theoretical study, we investigate the dewetting of a drop in a wider regime of parameter space. Using the boundary element method, we solve for the axisymmetric Stokes flow with i) the Navier-slip boundary condition at the solid/liquid boundary, and ii) a time-independent microscopic contact angle at the contact line position. We compute the profile evolution for different slip lengths and equilibrium contact angles. We find that when decreasing the slip length, the characteristic size of the bump first increases, and then decreases. More interestingly, the size of the bump even reaches zero, meaning no bump is observed, if the slip length is small enough. This remarkable result may indicate a crossover to the quasi-static regime when the slip length is very small.

DY 46.2 Wed 18:15 Poster B2

Inertial migration of elastic capsules in Poiseuille flow — •Christian Schaaf, Kevin Irmer, Christopher Prohm, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin

Deformable particles such as capsules, vesicles, and red blood cells assemble at fixed equilibrium positions in a microfluidic channel. This behavior can be used to separate particles with different cell properties. For example, softer cells travel closer to the center than stiffer ones.

Using the lattice-Boltzmann method, we study the dynamics of single deformable particles in a microfluidic channel for intermediate Reynolds numbers.

We show that particles move to different equilibrium position depending on their size and deformability. For Reynolds numbers below 100, their equilibrium positions collapse onto a single master curve depending only on the Laplace number. The steady state of the particles is determined by the lift force profiles, which we determine for different channel aspect ratios.

DY 46.3 Wed 18:15 Poster B2

Pairs of rigid particles in inertial microfluidics — •Felix Rühle, Christopher Prohm, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

We investigate rigid spherical particles in rectangular microchannels under the influence of Poiseuille flow at intermediate Reynolds num-

bers. It is well known that a single particle shows inertial focussing in this regime [1]. Furthermore, for rectangular channels with sufficiently large aspect ratio only two lateral equilibrium positions exist.

In this contribution we present first results on the behaviour of a particle pair in such a channel thus increasing the complexity of the one-particle system that has already been thoroughly examined [2]. An in-depth understanding of the multi-particle interactions will provide insights into the properties and dynamics of particle chains as well as the formation of so-called microfluidic crystals [3].

The particle pair is placed in the channel with variable axial distance and lateral positions. Inertial migration in the cross section of the channel is quantified by the lift force profile. We determine how it changes due to the presence of a neighboring particle. This helps us to explain the observed passing trajectories, where particles overtake each other, swapping trajectories, and damped oscillations. The latter involve both axial and lateral motion and occur when particles are on opposite sides of the channel centerline.

[1] G. Segré and A. Silberberg, *Nature* **189**, 209 (1961).
[2] C. Prohm and H. Stark, *Lab Chip* **14**, 2115 (2014).
[3] W. Lee et al., *PNAS* **107**, 22413 (2010).

DY 46.4 Wed 18:15 Poster B2

Super Liquid Repellency — •Frank Schellenberger, Jing Xie, Noemí Encinas, Maxime Paven, Doris Vollmer, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

The Pandora box of surfaces able to repell liquids is still a hot research topic. These surfaces are able to remove dust (self-cleaning) and can even hinder the growth of microorganism colonies.

Over the past years we have created superhydrophobic coatings (water repellent) where water droplets sit on microscopic pockets of air, which are trapped beneath the liquid drops. We even designed superamphiphobic coatings (i.e. water and oil repellent). One of these types are the so called slippery surfaces, where after infusing a rough/porous structure with a lubricant a deposited drop will slip by tilting the surface by a few degrees. This pressure-stable omniphobicity opens exciting applications for anti-biofouling, anti-icing or anti-frost performances. However, the mechanism how a drop moves on slippery surfaces is still unclear.

In this case, we used Laser Scanning Confocal Microscopy (LSCM) to observe the contact angles and evaluate the dynamics of droplet motion on the microscale.

DY 46.5 Wed 18:15 Poster B2

Silica stabilized Pickering-emulsions for hydroformylation — •Judith Witte[1], Dmitrij Stehl[1], Regine von Klitzing[1], Tobias Pogrzeba[1], Marcel Schmidt[1], Reinhard Schomäker[1], Lena Hohl[2], Matthias Kraume[2], Tina Skale[3], and Anja Drews[3] — [1]TU-Berlin, Straße des 17. Juni 124, 10623 Berlin — [2]TU-Berlin, Frauenhoferstr. 33-36, 10587 Berlin — [3]HTW Berlin, Wilhelminenhofstr. 75 A, 12459 Berlin

Pickering-emulsions (PEs) are particle stabilized emulsions. PEs can be used for catalytic reactions, for example for the hydroformylation of long chained olefins in a water in oil (w/o-) emulsion. In this study, the water droplets (water phase) which are surrounded by SiO2-nanoparticles as stabilizer, contain [HRh(CO)(TPPTS)3] as homogeneous catalyst. The particle-stabilized water droplets are emulsified in 1-Dodecene (oil phase). After the hydroformylation, the water droplets with the expensive catalyst can be easily separated from the product by membrane filtration and used again for the next reactions. This is a huge advantage in comparison to surfactant stabilized emulsions, which often break during filtration processes. Preliminary experiments showed that an increase in the amount of SiO2-nanoparticles leads to an increase of the product yield (Tridecanal) and decreases the droplet size from 0.02 to 0.005 mm. An addition of surfactant (Triton X-100) at low concentrations (<cmc) increases the product yield as well.

DY 46.6 Wed 18:15 Poster B2

Contact Line Dynamics and Hydrodynamic Boundary Conditions in Stepped Liquid Films — •Marco Rivetti[1], Thomas Salez[2], Michael Benzaquen[2], Elie Raphaël[2], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany — [2]UMR Gulliver, CNRS and ESPCI ParisTech, PSL University, Paris, France

For flows on the micro- and nanoscale, the physics of the contact line as well as the hydrodynamic boundary condition at a solid surface play a crucial role. In past few years much has been learned about both phenomena from flows that are driven by capillary forces. We here discuss some recent results involving thin liquid films which exhibit slip or no-slip boundary conditions. In the absence of slip, the relaxation of a liquid nanostripe on a smooth, hydrophilic substrate has evidenced the occurrence of, both, stationary and receding contact line regimes [1]. Self-similarity of the liquid profiles in the stationary regime has been proved, and a universal transition between the two regimes has emerged by rescaling with regard to the viscosity, surface tension and film thickness. In the second part we discuss the relaxation of initially perturbed liquid surfaces [2], i.e. stepped liquid films in the absence of contact lines. We find strong evidence that this relaxation process is also sensitive to the slip boundary condition at the solid/liquid interface. Thin film models comprising slip enable a quantification of the slip length of viscous liquids of various molecular properties. [1] Rivetti et al., Soft Matter 11 (2015) [2] McGraw et al., Phys. Rev. Lett. 109, 128303 (2012)

DY 46.7 Wed 18:15 Poster B2

Fluid invasion in porous media: front morphology, residual saturation, and the Cieplak-Robbins-transition — •Stephan Herminghaus[1], Ralf Seemann[2], Kamaljit Singh[2], Hagen Scholl[2], Marco Di Michiel[3], and Mario Scheel[3] — [1]MPI für Dynamik und Selbstorganisation, Göttingen — [2]Fakultät für Physik, Universität des Saarlandes, Saarbrücken — [3]ESRF, Grenoble

The fluid front morphologies emerging during fluid invasion into random piles of spherical beads are investigated in real time by X-ray micro-tomography and analyzed theoretically. Depending on the wettability of the invaded medium, we observe two distinct displacement regimes exhibiting strongly different liquid front morphologies. These regimes are separated by a pronounced transition, at which the residual saturation of the defending liquid (RSD) changes abruptly by one order of magnitude. We show that the critical contact angle at which this transition takes place can be quantitatively predicted on the basis of a quasi-static consideration of the wetting geometry of the progressing front. Furthermore, we find that the RSD agrees, within experimental scattering, quantitatively with our predictions from analytical theory, without invoking any fitting parameter.

DY 46.8 Wed 18:15 Poster B2

Particle Confinement by Marangoni Convection in Microchannels — •Michael Orlishausen, Lorenz Butzhammer, and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Universitätsstr. 30 95447 Bayreuth

We have investigated the flow of unary and binary liquids near a liquid-gas interface in a mirochannel device due to Marangoni Convection caused by a gradient in temperature and concentration (in the case of the binary liquids). By using latex microparticles of 1*m diameter we were able to visualize the resulting currents through optical microscopy. Depending on the position of the meniscus in the microchannel and other factors, one or two convection rolls appear. Surprisingly, however, the particles are confined to certain streamlines and regions in the microchannel and characteristic depletion zones form around them. In order to explain the origin of this observation we have performed finite elements simulations to the flow in the microchannel and identified the outermost streamline containing particles as being connected to the minimum distance to the meniscus one of those particles can take up. Additionally, we have investigated the influence of diffusion on particles in such a flow by means of Langevin simulations. The counter-intuitive result is an enhanced particle confinement caused by particle diffusion between different streamlines.

DY 46.9 Wed 18:15 Poster B2

Onset of motion of a sliding droplet — Simeon Völkel and •Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

We investigate experimentally the onset of motion of a water drop on an inclined plane with contact angle hysteresis. The onset of motion is triggered either through increasing the volume of the drop with an inkjet printer head or through tilting the plane with a stepper motor. Based on an analysis of both top view and side view images, we explore the evolution of the drop shape with time in the vicinity of the depinning transition and discuss how different ways to trigger the motion influence the bifurcation scenario of the transition. Finally, we analyze the eccentricity of the drop as a function of bond number that measures the ratio of gravitational forces to surface tension forces and compare our results with numerical simulations.

DY 46.10 Wed 18:15 Poster B2

Mechanical properties of highly porous super liquid-repellent surfaces — •Maxime Paven, Regina Fuchs, Doris Vollmer, Michael Kappl, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The poor mechanical properties of highly porous materials restrict their utilization for a wide range of applications such as light weighted, insulating or super liquid-repellent coatings. Especially, the design principles of super liquid-repellent surfaces aim at maximizing roughness at the nano or micrometer scale, making them inherently mechanically weak. To find a balance between repellency and stability investigation of the surfaces*s mechanical properties is essential. Here, we use atomic force microscopy, colloidal probe, nanoindentation, and pencil scratching to investigate the mechanical properties of super liquid-repellent surfaces prepared by soot templating. We varied the reaction paramteres, i.e. the thickness of the template-stabilizing silica shell and the sintering temperature to investigate their influence on the wetting and mechanical properties. Sintering at 1000 °C increased the effective elastic modulus of the surface by more than an order of magnitude. Sintering at 1150 °C led to a smoothening of the porous silica network and the effective elastic modulus increased by up to five orders of magnitude. At the same time, however, for droplets of n-hexadecane the roll-off angle increased and the receding contact angle decreased. This emphasizes the delicate balance of stability and repellency for super liquid-repellent surfaces.

DY 46.11 Wed 18:15 Poster B2

Geometry induced asymmetric contact angles — •Bang-Yan Liu — National Taiwan University, Department of Chemical Engineering, 10617 Taipei, Taiwan — Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany

Triangle post decorated surfaces were studied in this research. Triangular posts were arranged in square lattice and made from PDMS. Asymmetric contact angles were observed, both advancing and receding contact angle in triangle base direction were higher than that in the tip direction. Structures with various triangle sizes and post heights were examined and the three-phase contact line motion was analyzed to study this phenomenon. As water spreading, a strong pinning always happened on the outermost edges of triangular post structure related to droplet center, and with the increase of structure edge presence in three-phase contact line, advancing contact angle raised dramatically. The geometry difference of triangle tip and base resulted in different edge presence of three-phase contact line and caused contact angle asymmetry. However, when the structure height grew, advancing contact angle of both directions increased, and the asymmetry was reduced. On the other hand, de-wetting showed different behavior. Three-phase contact line pinned on the inner edge of structure and one-by-one depinning behavior was observed. Receding contact angle happened when the retreating three-phase contact line depinned from the very last structures to another row of structures. By designing and tuning structure geometry, an easy-produced asymmetry surface can be obtained.

DY 46.12 Wed 18:15 Poster B2

Wetting Characteristics in Bidisperse Sphere Packings — •Robabeh Moosavi[1], Julie Murison[2], Martin Brinkmann[1,3], and Matthias Schröter[1] — [1]Max-Planck Institute of Dynamics and Self-Organization, Göttingen, Germany — [2]Clariant Produkte GmbH, Competence Center Interface and Formulation Technology, Frankfurt, Germany — [3]Universität des Saarlandes, Saarbrücken, Germany

We report experiments on liquid two-phase flow in bidisperse sphere packings consisting of small and large beads which are either oil wetting or water wetting. Aim of our work is to understand the parameters determining the average wettability of these samples and their residual oil saturation after the packing was invaded by water. The former is studied by measuring the capillary pressure saturation curves [1], the latter by imaging the samples with X-ray tomography. We find that mixed wet samples show a smaller dissipation during a complete drainage/imbibition cycle than when the sample is composed of beads of one type of wetting behavior.

[1] Murison et al., *Phys. Rev. Appl.* **2014**, 2, 034002

DY 46.13 Wed 18:15 Poster B2

Wettability controls immiscible fluid displacement through local interfacial instabilities — Micheal Jung[1], Martin Brinkmann[1,2], Marta Sanchez de La Lama[2], Thomas Hiller[2], Stephan Herminghaus[2], and •Ralf Seemann[1] — [1]Experimental Physics, Saarland University, Saarbrücken — [2]Max Planck Institute for Dynamics and Self-Organisation

Slow immiscible fluid displacement is studied in a transparent quasi two-dimensional Hele-Shaw cell with cylindrical posts for different wetting conditions of the invading fluid. Employing various combinations of fluids and cell materials allows to cover a range of advancing contact angles θ_a of the invading fluid between 46° and 180° in our experiments. In parallel, we performed numerical simulations of the displacement process employing a particle-based method that accounts for wall wettability in the same arrangements of cylindrical posts as in experiments. A cross-over between capillary fingering at high values of $\theta_a \gtrsim 120°$ and stable interfacial displacement at $\theta_a \lesssim 80°$ is observed in experiments and simulations, and quantified through the front length and the final saturation of the displaced fluid. Analysis of the local displacement processes in experiments and simulations demonstrate that the evolution of the front shape is governed by the local advancing modes for quasi-static interfacial displacement as proposed by Cieplak and Robbins [Phys. Rev. Lett. **60** (1988)]. A comparison of the relative frequency of certain advancing modes reveals a cross-over between cooperative interfacial instabilities for good wetting conditions and non-cooperative instabilities for poor wetting conditions.

DY 46.14 Wed 18:15 Poster B2

Wetting properties of n-alkane nanostructures — •Diego Diaz[1], Tomas Corrales[2], Maria Retamal[1,3], Marcelo Cisternas[1], Patrick Huber[4], and Ulrich Volkmann[1] — [1]Centro de Investigación en Nanotecnología y Materiales Avanzados, CIEN-UC, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Instituto de Alta Investigación, Universidad de Tarapacá, Arica, Chile — [3]Facultad de Química, Pontificia Universidad Católica de Chile, Santiago, Chile — [4]Materials Physics, Hamburg U. of Technology, D-21073 Hamburg, Germany

Recently, we have shown that it is possible to modify the surface coverage and morphology of an n-alkane molecular layer over silicon by controlling the withdrawal velocity of the substrate from solution (T.P. Corrales et al., ACS Nano 8, 9954-9963, 2014). As a follow-up work, we study here the wetting properties of silicon surfaces coated with molecular layers of n-alkane as a function of the surface coverage and morphology, using a drop shape analysis procedure. We have found from our measurements that both the coverage and morphology of the underlying nanostructures affects the contact angle of the surface. In particular, stripe-like structures present lower contact angles than dendritic structures that have roughly the same coverage and thickness. All films consist of a single n-alkane molecular layer with a height of around 5 nm. Furthermore, we find differences in the contact angles measured parallel and perpendicular to the withdrawal direction of the substrate from solution.

DY 47: Scientometric Maps and Dynamic Models of Science and Scientific Collaboration Networks (SYSM)

Time: Thursday 9:30–12:15 Location: H1

Invited Talk DY 47.1 Thu 9:30 H1

Science Forecasts: Measuring, Predicting, and Communicating Scientific Developments — •Katy Börner — Indiana University

In a knowledge-based economy, science and technology are omnipresent and their importance is undisputed. Equally evident is the need to allocate resources, both monetary and human, in an effective way to foster innovation. In the preceding decades, data mining, metrics, and indicators have been embraced to gain insights into the structure and evolution of science; but there have been no significant efforts into mathematical, statistical, and computational models that can predict future developments in science, technology, and innovation (STI).

While it may not be possible to predict the nature, essence, or the precise extent of impact of the next scientific or technological innovation, it is often possible to predict the circumstances leading to it, i.e., where it is most likely to happen and under which conditions. See Scharnhorst, Börner, and Besselaar, eds. 2012. Models of Science Dynamics: Encounters Between Complexity Theory and Information Science. Springer Verlag for an overview of major model types.

This talk reviews and demonstrates the power of computational models for simulating and predicting possible STI developments and futures. In addition, it showcases novel means to broadcast moderated STI forecasts to make them accessible and understandable for a general audience.

Invited Talk DY 47.2 Thu 10:00 H1

Mapping science with variable-order Markov dynamics reveal overlapping fields and multidisciplinary journals — •Martin Rosvall — Umeå University, Sweden

To better understand the parallel human endeavor of science, we need good maps that both simplify and highlight the flows of ideas and underlying research organization. However, current maps of science cannot effectively identify the multilevel and overlapping fields of science with multidisciplinary journals. For example, whereas maps based on citations between journals in first-order Markov models can only assign each journal to a single field, maps based on multi-step citation chains in higher-order Markov models become computationally infeasible already for moderate-sized systems. To overcome these problems, we introduce a method that uses model selection to find the appropriate variable-order Markov model. We also present interactive maps of science that highlights the assignments of multidisciplinary journals and how ideas flow through those journals.

Invited Talk DY 47.3 Thu 10:30 H1

Network algorithms for reputation and quality in scholarly data — •Matúš Medo, Manuel Mariani, and Yi-Cheng Zhang — University of Fribourg, Fribourg, Switzerland

The ever-increasing quantity and complexity of scientific production have made it difficult for researchers to keep track of advances in their own fields. This, together with growing popularity of online scientific communities, calls for the development of effective information filtering tools. Network theory is an important driving aspect for such algorithms. We will first discuss the case of an online scientific community where users and papers form a bipartite network which can be effectively used to evaluate the reputation of users and fitness of papers. We show that when the input data is extended to a multilayer network including users, papers and authors, the resulting performance improves on multiple levels. In particular, top papers have higher citation count and top authors have higher h-index than top papers and top authors chosen by other algorithms. We will then move to stress the role of time in scholarly data. Most research metrics either ignore time (such as the h index) or consider it in an ad-hoc fashion (such as the m quotient). On the example of PageRank which has been used in the past to assess the quality of papers, we show that a demonstrably better ranking of papers can be obtained by considering time in a principled way.

15 min. break

Invited Talk DY 47.4 Thu 11:15 H1

Modeling scientific networks in social media — •Cassidy Sugimoto — School of Informatics and Computing, Indiana University Bloomington, USA

This talk will examine the role of social media in constructing new or reinforcing old epistemic communities. In particular, we will analyze the interconnectivity of scientists on social media platforms according to their disciplinary affiliation and the degree to which these networks reinforce or contrast with models constructed through collaboration and citation relations. We will analyze the role of gender and other socio-demographic characteristics where possible.

Invited Talk DY 47.5 Thu 11:45 H1

Modeling scientific collaboration across multiple scales: from individuals to Europe — •Alexander Petersen — IMT Lucca Institute for Advanced Studies, Lucca, Italy

Quantitative measures are becoming increasingly prevalent at all scales of scientific evaluation, largely due to the advent of large comprehensive publication databases that allow for detailed studies of ideas, people, and institutions, and the vast networks connecting them. As such, there is plenty of room to apply methods from complex systems to address policy-oriented issues relevant to the entire science system. In the first half, I will discuss micro-scale patterns of collaboration from a researcher's local 'ego' perspective, showing that scientific collaboration is characterized by a high turnover rate juxtaposed with frequent 'life partners'. I will show that these extremely strong collaborations have a significant positive impact on productivity and citations – the apostle effect – representing the measurable advantage of 'super' social ties. In the second half, I will discuss macro-scale collaboration patterns concerning the evolution the European Research Area (ERA), a cross-border labor, funding, and mobility scheme aimed at fostering innovation and growth within Europe. However, despite decades of integration policies, recent analyses have shown there to be little cross-border integration in the EU above global trends – i.e. Europe remains a collection of national innovation systems. I will show that high-skilled mobility – i.e. brain drain, largely from East to West following the 2004/2007 EU enlargement – can explain why the cross-border integration of R&D within the ERA is lagging.

Right after the symposium, participants are invited to enjoy a guided tour of the Places and Spaces: Mapping Science exhibition (http://scimaps.org) on display in the foyer of the university library.

DY 48: Wetting, Nano- and Microfluidics I (joint session CPP/DY)

Time: Thursday 9:30–12:45 Location: H42

Invited Talk DY 48.1 Thu 9:30 H42

Provoking liquids to dewet and to slide: About concave drops and hungry droplets — •Karin Jacobs — Experimental Physics, Saarland University, D-66041 Saarbrücken

Usually, liquids exhibit a 'no-slip' boundary condition to a solid substrate, i.e. the atoms or molecules of a liquid that are the closest to the solid substrate are at rest. However, a polystyrene film that moves over hydrophobized (by a self-assembled monolayer of silanes) Si wafers can be provoked to slide, i.e. there is a non-zero interfacial velocity of the fluid in contact with the solid, and friction occurs [1,2]. This implies variations in the energy dissipation mechanisms in these systems and leads to a strikingly different behaviour of fluids in different geometric situations [3-5]: With slip, the dewetting of flat films is faster on solid surfaces (A), Rayleigh-Plateau-type instabilities exhibit an increased dynamics (B) and droplets that were prepared in a non-equilibrium situation can reach equilibrium via a stadium where their topology is concave (C). Yet, why does a liquid slide? Possible explanations including recent findings by scattering methods will be reviewed. Moreover, if more liquids were sliding, would that change things in our everyday life?

[1] O. Bäumchen et al., PRL 113 (2014) 014501; [2] J. D. McGraw et al., Colloid and Interface Science 210 (2014) 13; [3] S. Haefner et al., Nature Comm. 6 (2015) 7409; [4] S. Haefner, O. Bäumchen, K. Jacobs, Soft Matter 11 (2015) 6921; [5] J. McGraw et al., (submitted)

DY 48.2 Thu 10:00 H42

Soft Levelling: Capillary Relaxation of Thin Liquid Films on Elastic Substrates — •Marco Rivetti[1], Thomas Salez[2], Christine Linne[1], Maxence Arutkin[2], Elie Raphaël[2], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany — [2]UMR Gulliver, CNRS and ESPCI ParisTech, PSL University, Paris, France

A thin liquid film with non-zero curvature at its free surface spontaneously relaxes towards a flat configuration. The flow of this liquid film is driven by Laplace pressure gradients and it is resisted by viscosity. In the last few years the dynamics of this system has been studied experimentally, numerically and analytically. Inspired by recent pro-

gresses on the wetting behaviour of liquid droplets on soft substrates, we here consider the relaxation of a thin viscous film supported by an elastic foundation. We present experiments involving thin polystyrene films on polydimethylsiloxane substrates, where the dynamics of the liquid-air interface is monitored using an atomic force microscope. In this system, Laplace pressure gradients not only drive the flow but they also induce elastic deformations on the substrate. These deformations affect the flow and the shape of the liquid-air interface itself, giving rise to an original example of elasto-capillary interaction that is not mediated by the presence of a contact line. We show that the width of the profile scales with the time to the power 1/6, rather than 1/4 which we consistently observed on rigid substrates. A theoretical model that describes the coupled evolution of the elastic-liquid and liquid-air interfaces is also presented.

DY 48.3 Thu 10:15 H42

Rayleigh-Plateau Instability and Capillary Droplet Propulsion on a Fiber — •Sabrina Haefner[1,2], Michael Benzaquen[3], Oliver Bäumchen[2,4], Thomas Salez[3], Robert Peters[2], Joshua McGraw[1], Elie Raphaël[3], Kari Dalnoki-Veress[2,3], and Karin Jacobs[1] — [1]Saarland University, Dept. of Experimental Physics, D-66041 Saarbrücken, Germany — [2]McMaster University, Dept. of Physics & Astronomy, Hamilton, ON, Canada — [3]PCT Lab, UMR CNRS 7083 Gulliver, ESPCI ParisTech, PSL Research University, Paris, France — [4]Max-Planck Institute for Dynamics & Self-Organization (MPIDS), 37077 Göttingen, Germany

The Rayleigh-Plateau instability (RPI) of a liquid column underlies a variety of hydrodynamic phenomena. Compared to the classical case of a free liquid column, the description of a liquid layer on a fiber requires the consideration of the solid/liquid interface in addition to the free surface. We revisit the RPI of a liquid layer on a solid fiber by varying the hydrodynamic boundary condition at the fiber/liquid interface from no-slip to slip. We find that the growth rate depends on the system geometry and the boundary condition, which is in agreement with theory [1]. In the late stages of liquid column breakup on slip-fibers, a three-phase contact line can be formed on one side of the droplet. The resulting capillary imbalance leads to droplet propulsion, which is studied as a function of temperature and molecular weight [2].

[1] S. Haefner et al., Nat. Commun., 6 (2015), 7409.
[2] S. Haefner et al., Soft Matter, 11, (2015), 6921.

DY 48.4 Thu 10:30 H42

Rayleigh-Plateau instability of slipping viscous filaments in v-shaped grooves — •Martin Brinkmann[1,3], Tak Shing Chan[1], Ralf Seemann[1], Krishna Khare[2], and Stephan Herminghaus[3] — [1]Experimental Physics, Saarland University, Saarbrücken — [2]Indian Institute of Technology Kanpur — [3]Max Planck Institute for Dynamics and Self-Organisation, Göttingen

Since the seminal works of Rayleigh and Plateau on the break-up of free-standing liquid jets, a large number of studies have addressed the instability of cylindrical interfaces in various experimental settings. The most unstable wavelength λ of a viscous liquid filament wetting the bottom of a v-shaped groove is mainly governed by the slope angle ψ, the contact angle θ of the interface on the solid, and the initial width w of the filament. A linear stability analysis using the method of boundary elements reveals that the characteristic timescale of the decay is affected not only by viscosity, interfacial tension, and geometry. Slip has a substantial effect on the wavelength λ of the fastest growing mode whenever the transverse dimension w of the filaments is comparable or smaller than the Navier slip-length b. In this limit $b/w \to \infty$ we find $\lambda/w \to \infty$ while the timescale τ saturates to a finite lower bound, similar to the case of a free-standing viscous liquid cylinder. In the opposite limit $b/w \to 0$ the corresponding timescale τ of the decay increases only logarithmically with b/w while λ tends to $\sqrt{2}$ times the neutrally stable wavelength λ^*. A linear stability analysis based on long wavelength approximations of the flows agree with the numerical results only for 'flat' filaments $0 < \theta - \psi \ll 1$ with $\lambda^* \gg w$.

DY 48.5 Thu 10:45 H42

Waves at viscoelastic surfaces — •Julian Kappler and Roland R. Netz — Institut für Theoretische Physik, Freie Universität Berlin, 14195 Berlin, Germany

Waves on water, whose properties depend on gravity and surface tension, are a well-known phenomenon. If there is a surfactant that reacts viscoelastically under compression, like e.g. a biomembrane on water, also another type of surface wave, called longitudinal capillary wave, can exist. On the other hand, on viscoelastic solids there exist Rayleigh waves. These are surface waves which, on a large scale, can be excited by earthquakes, or, on a small scale, can be excited on materials to measure their mechanical properties non-destructively.

We present a unified treatment of all the above waves: We consider a viscoelastic medium covered by a viscoelastic interface and derive a general equation characterizing localized waves at the interface. We show how the aforementioned waves can be derived from this general equation, identify a new surface wave, and discuss how all these waves are interrelated.

Reference: J. Kappler, R. R. Netz. Multiple surface wave solutions on linear viscoelastic media. EPL, 112(1):19002, 2015.

15 min. break

DY 48.6 Thu 11:15 H42

Non-equilibrium interfacial tension during relaxation — •Markus Bier — Max Planck Institute Int. Sys. and University of Stuttgart, Germany

The concept of a non-equilibrium interfacial tension, defined via the work required to deform the system such that the interfacial area is changed while the volume is conserved, is discussed in the context of the relaxation of an initial perturbation of a colloidal fluid towards the equilibrium state. It is shown that the non-equilibrium interfacial tension is not necessarily positive, that negative non-equilibrium interfacial tensions are consistent with strictly positive equilibrium interfacial tensions and that the sign of the interfacial tension can influence the morphology of density perturbations during relaxation.

References:
[1] M. Bier and D. Arnold, Phys. Rev. E **88**, 062307 (2013).
[2] M. Bier, Phys. Rev. E **92**, 042128 (2015).

DY 48.7 Thu 11:30 H42

Hydrodynamic cavitation in Stokes flow of anisotropic fluids — •Tillmann Stieger[1], Hakam Agha[2], Martin Schoen[1], Marco G. Mazza[2], and Anupam Sengupta[3] — [1]TU Berlin — [2]MPIDS Göttingen — [3]Massachusetts Institute of Technology

Cavitation is ubiquitous in fluid dynamics, and has significant effects on a wide range of industrial and biomedical applications. Investigations in anisotropic fluids are scarce, and till date, no systematic attempt has been made to study them. Here we report flow-induced cavitation in an anisotropic fluid, studied by combining microfluidic experiments and nonequilibrium molecular dynamics (MD) simulations. Cavitation domains nucleate due to sudden drop in pressure upon flow past a micron-sized obstacle in microchannels, which over time, progressively grows in volume after attaching at the downstream obstacle surface. The inception and growth of cavitation domain ensue in Stokes flow regime. Using MD simulations we study the physical principles governing the cavitation phenomena in nematic liquid crystals (LC), and identify a critical value of Reynolds number Re_{cr} for the cavitation inception that scales inversely with the characteristic order parameter of the LC. Strikingly, the critical Re_{cr} can be as low as $\sim 50\%$ of the cavitation threshold in isotropic fluids. Corresponding results for the LC in the isotropic phase and for a Lennard–Jones fluid reveal that the drop in Re_{cr} is a consequence of the long range ordering in anisotropic fluids. The findings suggest that long range ordering, and its tunability, can be potentially applied as a novel control parameter to modulate cavitation inception in anisotropic fluids.

DY 48.8 Thu 11:45 H42

Sliding Drops - stationary states and large-scale dynamics — •Sebastian Engelnkemper, Markus Wilczek, Svetlana Gurevich, and Uwe Thiele — Institut für Theoretische Physik, Westfälische Wilhelms Universität Münster, Corrensstr. 2, 48149 Münster

The long-wave evolution equation for a liquid film (or Thin-Film-Equation) describes structures including drops and ridges. Including a lateral driving force (e.g., inclined substrate) all structures begin to move and change their shapes. Experiments show this and, in addition, a further instability where large drops emit small satellite drops [1]. Implementing the Thin-Film-Equation in the continuation-toolbox PDE2PATH [2], we analyze the primary bifurcations from a flat film in the case without driving using the mean film height as bifurcation parameter. Then, with lateral driving forces we track sliding drops in dependence of either drop volume or substrate inclination. We analyze the shape changes and compare them to previous 1d results [3].

Finally, we focus on the bifurcation that is responsible for the satellite drops and relate the results of continuation to direct numerical simulations for single drops and ensembles of many drops. [1] T. Podgorski, J.-M. Flesselles, L. Limat, Phys. Rev. Lett. 87, 036102 (2001); [2] H. Uecker, D. Wetzel, J.D.M. Rademacher, arXiv:1208.3112v2 (2012); [3] U. Thiele et al., Phys. Rev. E, 64, 061601 (2001).

DY 48.9 Thu 12:00 H42

Autophobing drops, fuelled by oil/water interfacial chemistry — Bijoyendra Bera, •Michael Duits, Dirk van den Ende, Martien Cohen Stuart, and Frieder Mugele — University of Twente, Enschede, The Netherlands

We report a hitherto not observed wetting phenomenon, namely the retraction of a drop after deposition on a solid substrate, caused by an interfacial reaction between cations in the aqueous drop and fatty acids in the ambient oil. We investigate how this process depends on the concentrations of the reactants, the chain lengths of fatty acid and alkane solvent, and the solid substrate material. We demonstrate with contact angle and AFM measurements that deposition of amphiphilic molecules on the solid takes place only after assembly at the oil-water interface. Deposition of material by the moving contact line leads to an increasingly hydrophobic local substrate and a concomitant increase in contact angle, which we call autophobing. This phenomenon is observed both on mica and on silica substrates, for several fatty acids and alkane solvents. The time-dependent contact angle can be described with a theoretical model in which the adsorption reaction at the oil-water interface is rate-limiting, and transfer to the solid is determined by a mass flux balance (similar to a Langmuir Blodgett transfer). The ensuing time-dependent oil-water and solid-oil interfacial tensions then produce the evolution of the contact angle.

DY 48.10 Thu 12:15 H42

Compact nanosensors probe microdroplets — •Julian Schütt[1], Felix Zörgiebel[1,2], Bergoi Ibarlucea[1,2], Sebastian Pregl[1,2], Daijiro Nozaki[1], Walter Weber[2,3], Thomas Mikolajick[2,3,4], Larysa Baraban[1,2], and Gianaurelio Cuniberti[1,2] — [1]Max Bergmann Center of Biomaterials and Institute for Materials Science, Dresden University of Technology, Budapesterstrasse 27, 01069 Dresden, Germany — [2]Center for Advancing Electronics Dresden, 01062 Dresden, Germany — [3]Namlab GmbH, Nöthnitzerstraße 64, 01187 Dresden, Germany — [4]Institute for Semiconductors and Microsystems, TU Dresden, 01062 Dresden

Smart combination of nanosensors and droplets based reactors represents a powerful tool for monitoring and high throughput analysis of the kinetics of biological and chemical reactions, staying miniaturized, highly sensitive and optically label-free. Here we present a first demonstration of droplets microfluidics with the compact silicon nanowire field effect transistor (SiNW FET) on a single chip for in flow electrical detection of aqueous reactor-drops. Apart from detection events, we chemically probe the content of numerous droplets in a row as independent events (up to ten thousands), and resolve the pH values and ionic strength of the solution, resulted in a change of a source-drain current through the nanowires. Optic-less and noninvasive measurements of these parameters in aqueous droplets have a great impact on the area of biodetection and bioanalytics as a high throughput screening tool for pathogens, drug assays, and evaluation of the enzymatic activities.

DY 48.11 Thu 12:30 H42

Stability of emulsions against coalescence and transport: Influence of surfactants — •Birte Riechers[1,2], Philipp Gruner[2], Florine Maes[1,2], and Jean-Christophe Baret[1,2] — [1]CNRS, Univ. Bordeaux, CRPP, UPR 8641, Pessac, France — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Monodisperse aqueous droplets within emulsions become evermore attractive for use as separate microreactors in pharmaceutical and biotechnological applications [Theberge *et al.*, Angewandte 2010]. These applications need constant experimental conditions inside the droplets. To date stabilization against coalescence is mainly obtained using surfactants. Surfactants also affect the solubility of solutes inside the continuous oil phase, thereby restricting their use [Gruner *et al.*, Curr. Opin. Colloid Interface Sci. 2015]. Microfluidic tools provide insight into the mechanisms of interfacial stabilization:
Here we perform a complete analysis of the adsorption kinetics of a surfactant typically used in droplet-based microfluidic applications. We combine pH measurements at the micronscale and coalescence experiments in droplet-based microfluidics with bulk measurements to show that the kinetics of the transport of molecules across interfaces directly relates to those of interfacial stabilisation. Combining all information, we derive a simple model of adsorption in the kinetic-limited regime and show that two interfaces are only stabilized against coalescence for surfactant concentrations which are close to or above the critical micellar concentration.

DY 49: Pattern Formation (joint session DY/BP)

Time: Thursday 9:30–13:00 Location: H46

Invited Talk DY 49.1 Thu 9:30 H46

Patterns formation through elastic instabilities, from thin sheets to twisted ribbons — •Pascal Damman — Université de Mons, Mons, Belgium

Hydrodynamics instabilities, such as Bénard-Marangoni convection, Rayleigh-Plateau, Rayleigh-Taylor and many others, are well known to produce beautiful patterns. Capillary, viscous and/or inertial forces conspire to generate very regular morphologies. In this seminar, we will see that elasticity can also produce complex structures, either regular or fully random, provided that slender objects are used. These objects are usually classified as rods, shells or sheets.

In the "classical picture", thin sheets constrained by external forces minimize the elastic energy through focalization of deformation in singularities. We will see that, due to geometric constraints, these origami structures cannot always be obtained. In the second part, the formation of very regular wrinkles in sheets "glued" on a soft foundation will be discussed. At the threshold, these wrinkles reflect the competition between various forces. For large deformations, however, the morphology is surprisingly determined by the nature of the foundation. Fold localization or period-doubling bifurcations are indeed observed for liquid or solid substrate, respectively. Finally, the effect of specific geometrical constraints produced by twisting thin ribbon of elastic materials will be discussed.

Finally, these various studies also highlight the effort of this growing interdisciplinary researcher community to the emergence of a global picture of elastic instability.

DY 49.2 Thu 10:00 H46

Shear driven instabilities in hard–core anisotropic colloids: Pressure tensor dynamics — •Henning Reinken, Rodrigo Lugo-Frias, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Systems of hard anisotropic particles display interesting flow induced behavior that modifies their internal structure and rheological properties [1, 2]. In soft matter theory, using the well known Doi–Hess approach, these systems have been studied in the bulk [3] and close to the boundaries [4].
Within this framework, we study how the pressure tensor is influenced by the average orientation of the particles coupled to the velocity field. To do so, we start from an isotropic or nematic equilibrium configuration and apply simple shear flow (Couette geometry) observing the emergence of instabilities (shear banding) in both scenarios. A novel finding is the appearance of coexisting stationary and oscillatory dynamics within the bands. We also discuss the resulting stress-strain relations.

[1] S. M. Fielding, Soft Matter, **3**, 1262-1279 (2007).
[2] J. K. G. Dhont, M. P. Lettinga, *et al.*, Faraday Discuss, **123**, 157-172 (2003).
[3] D. Strehober, H. Engel and S. H. L. Klapp, Phys. Rev. E **88**, 012505 (2013).
[4] S. Heidenreich, P. Ilg, and S. Hess, Phys. Rev. E **75**, 066302 (2007).

DY 49.3 Thu 10:15 H46

Towards a more thorough understanding of dislocation

contributions in shape-memory alloys — •Heike Emmerich[1] and Julia Kundin[2] — [1]Universität Bayreuth, Lehrstuhl Material- und Prozesssimulation, Universitätsstraße 30, D-95447 Bayreuth — [2]Universität Bayreuth, Lehrstuhl Material- und Prozesssimulation, Universitätsstraße 30, D-95447 Bayreuth

The scientific interest in solid state cooling technologies has been renewed and increased since the discovery of of new materials with giant ferrocaloric effects - and with it the interest in understanding the hysteresis effects associated with the rise of crystal defect evolution as a result of plastic deformations at diverse time scales more thoroughly. In this contribution we show how phase-field modeling including elastic and plastic contributions tight to incoherent martensitic phase transitions can contribute to shade light into this scenario. Additionally we elucidate from a fundamental point of view how the associated enthalpic contributions can be reconciled and validated with atomistic concepts.

DY 49.4 Thu 10:30 H46

Pattern orientation in finite domains without boundaries — •Lisa Rapp, Fabian Bergmann, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

We investigate the orientation of nonlinear stripe patterns in finite domains. Motivated by recent experiments, we introduce a control parameter drop from supercritical inside a domain to subcritical outside without boundary conditions at the domain border. As a result, stripes align perpendicular to shallow control parameter drops. For steeper drops, non-adiabatic effects lead to a surprising orientational transition to parallel stripes with respect to the borders. We demonstrate this effect in terms of the Brusselator model and generic amplitude equations. Preprint available at arXiv:1512.05576 [cond-mat.soft]

DY 49.5 Thu 10:45 H46

Reflection and orientation of nonlinear traveling waves in finite domains without boundaries — •Fabian Bergmann, Lisa Rapp, and Walter Zimmermann — Theoretische Physik, Universitaet Bayreuth, Bayreuth, Germany

We investigate the reflection and orientation of nonlinear traveling waves in finite domains. In a finite domain (part of large system) the control parameter is assumed to be supercritical inside the domain and to drop to subcritical values outside. In 2d systems we find that a control parameter drop orients the propagation of traveling waves parallel to the domain boundaries. In quasi 1d systems steep control parameter variations at the ends of a finite domain cause reflections of traveling waves. Steep drops may also lead to complex spatio-temporal scenarios inside the finite domain. This study is motivated by recent experiments [1], where traveling waves in finite stripes have been investigated. Our analysis is compared with a recent work on stationary stripe patterns in finite domains without boundary conditions for the dynamical fields [2].

[1] J. Schweizer, M. Loose, M. Bonny, K. Kruse, I. Moench, P. Schwille, Proc. Natl. Acad. Sci. (USA)109, 15283 (2012)

[2] L. Rapp, F. Bergmann, W. Zimmermann, arXiv:1512.05576 (2015)

15 min. break

DY 49.6 Thu 11:15 H46

Self-assembly in colloidal systems with tunable particle interactions — •Hauke Carstensen, Vassilios Kapaklis, and Max Wolff — Dept of Physics & Astronomy, Box 516, SE-751 20 Uppsala, Sweden

We present a system that allows tunable magnetic self-assembly of microbeads. Two types of beads, magnetic and non-magnetic ones, are dispersed in a ferrofluid (FF), which alters their effective magnetic behaviour. By changing the FF concentration, the interactions between the beads can be tuned. The particles are confined in two dimensions. Depending on the interaction and the particle composition, lattices like square or hexagonal are assembled. Additionally, in less dense conditions metastable structures like branching chains are observed. The samples are analysed by transmission optical microscopy and images are taken in a scanning mode. Sets of images can be stitched together to create large scale maps of each sample. The particle positions are extracted by image analysis. Phases are detected via characteristic angles and lattice constants. A phase diagram is created by combining the observed phases with the particle interactions and the sample compositions. This can be applied to the fundamental understanding of colloidal crystal formation and chain formation in magnetorheological fluids.

DY 49.7 Thu 11:30 H46

Subcritical chaos and localized convection in the asymptotic suction boundary layer over a heated plate — •Stefan Zammert[1] and Bruno Eckhardt[1,2] — [1]Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]J.M. Burgerscentrum, Delft University of Technology, 2628 CD Delft, The Netherlands

The asymptotic suction boundary layer over a heated plate, a parallel and open flow, can be considered as a model for the properties of thermal boundary layers. A stability analysis of the base state shows that the flow undergoes a subcritical instability with increasing Rayleigh number. This instability creates spatially periodic convection patterns. We will show how bifurcations of these secondary solutions create a chaotic attractor in the subcritical regime which is turned into a chaotic saddle by a crisis bifurcation. Long-wavelength instabilities of the secondary solutions create various stationary convection solutions which are localized in one or two directions parallel to the plate. These localized structures also exist in subcritical regime and can potentially be used to study plume dynamics in thermal boundary layers.

DY 49.8 Thu 11:45 H46

Spontaneous autocatalysis in a primordial broth — •Sabrina Scherer[1], Eva Wollrab[2], Varun Giri[1], and Albrecht Ott[1] — [1]Biologische Experimentalphysik, Universität des Saarlandes — [2]Laboratory of Microbial Morphogenesis and Growth, Institut Pasteur

Driven non-linearities lead to pattern formation. Here we study the dynamics of a complex chemical system, driven by electric discharge that forms from a gas mixture of methane and ammonia in the presence of water. Using real-time mass spectrometry, we observe the generation of a primordial broth composed of thousands of different molecules in a mass range from 50 to 1000 Dalton. The temporal development of the primordial broth reveals the spontaneous emergence and disappearance of oligomeric surfactants. Strong non-linearities are required for these aperiodic chemical oscillations. The phenomenon is robust against different gas compositions and concentrations, temperatures and many details of the experimental set-up. We analyze the chemical composition of the solution by different methods like (high-resolution) mass spectrometry, NMR and gas-chromatography to find high-reactive molecules and possible catalysts. We find that oxidation and doping with small amounts of an active broth can trigger the production of the oligomers. We suggest that surface active molecules lead to phase transfer catalysis in the oil/water mixture and self-organize to a spontaneously emerging autocatalytic network.

DY 49.9 Thu 12:00 H46

A Protein Flux-based Mechanism for Midcell Sensing in Bacteria — •Silke Bergeler[1], Dominik Schumacher[2], Lotte Søgaard-Andersen[2], and Erwin Frey[1] — [1]ASC for Theoretical Physics, Ludwig-Maximilians-Universität, München, Germany — [2]Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

Precise positioning of the cell division site is crucial for the correct separation of the genetic material into the two daughter cells. In myxobacteria a cluster of Pom proteins (PomX, PomY, PomZ) is formed on the chromosome that performs a biased random walk to midcell and positively regulates cell division. To investigate how the Pom cluster, consisting of PomX and PomY, moves to midcell, we introduce a mathematical model in which PomZ dimers can attach to, diffuse on the nucleoid and can hydrolyze ATP and subsequently detach from the nucleoid primarily at the cluster. It is known that this type of particle dynamics leads to different fluxes of PomZ into the cluster from both sides along the long cell axis, if the cluster is at an off-center position, but it is not known how the force to move the cluster is generated. We model the PomZ dimers as springs, based on the observation that the bacterial chromosome and several proteins have elastic properties. As springs the PomZ dimers can exert a force on the PomXY cluster. Our model explains mid-plane localization of the Pom cluster. It predicts a decrease in the efficiency to find midcell for a large number of PomZ dimers in the cell and small ATP-hydrolysis rates of the ATPase PomZ, which is in agreement with our experimental findings. In summary, our study provides new mechanistic insights into intracellular positioning.

DY 49.10 Thu 12:15 H46

Cyclosis-mediated transfer of reactive oxygen species and its relation to the formation of pH bands in Chara alga cells — •Alexey Eremin[1], Ralf Stannarius[1], Anna Komarova[2], and Alexander Bulychev[2] — [1]Institute of Experimental Physics, Otto von Guericke University Magdeburg — [2]Faculty of Biology, Lomonosov Moscow State University, 119992 Moscow, Russia

In internodal cells of characean algae, cyclosis participates in formation of light-dependent patterns of surface pH and photosynthetic activity. Hydrogen peroxide, being a signalling molecule and a stress factor, is known to accumulate under excessive irradiance. In our study, we explore the spatio-temporal dynamics of pH-band formation on the surfaces of internodal Chara corallina cells and study the kinetics of H2O2 production in chloroplasts and its release into the cytoplasm under local illumination. We demonstrate that in cells exhibiting active streaming, H2O2 first accumulates in the illuminated region and then enters into the streaming cytoplasm. The results suggest that H2O2 released from chloroplasts is transported along the cell with the cytoplasmic flow. It is proposed that the shift of cytoplasmic redox poise and light-induced elevation of cytoplasmic pH facilitate the opening of H+/OH-permeable channels in the plasma membrane.

DY 49.11 Thu 12:30 H46

Improvement of unpinning and termination of spiral waves by reducing excitability — •Jiraporn Luengviriya[1], Malee Sutthiopad[2], Metinee Phantu[2], Porramain Porjai[2], Jarin Kanchanawarin[2], Stefan C. Müller[3], and Chaiya Luengviriya[2] — [1]Department of Industrial Physics and Medical Instrumentation, King Mongkut's University of Technology North Bangkok, Thailand — [2]Department of Physics, Kasetsart University, 50 Phaholyothin Road, Jatujak, Bangkok 10900, Thailand — [3]Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Spiral waves are common found in excitable systems. Such waves may drift and eventually annihilate at the boundary. However, they can be stabilized when pinned to obstacles. Spiral waves of electrical excitations in cardiac systems connect to some arrhythmias so that they should be eliminated. We present an investigation of the release of pinned spiral waves from unexcitable obstacles and the termination of free spiral waves at the boundary in a reaction-diffusion system. An advective field is applied as the external forcing. For a given obstacle size, the critical value of advection to release as well as that to terminate the spiral waves decrease when the excitability of the system is reduced. Therefore, this study shows that decreasing the excitability can facilitate elimination of spiral waves, either in the presence of obstacles or not.

DY 49.12 Thu 12:45 H46

Coexistence of stable branched patterns in anisotropic inhomogeneous systems — Badr Kaoui[1,2], Achim Guckenberger[1], Alexei Krekhov[1,3], Falko Ziebert[1,4], and •Walter Zimmermann[1] — [1]Theoretische Physik, Universitaet Bayreuth, Bayreuth, Germany — [2]Biomechanics and Bioengineering, Universite de Technlogie de Compiegne, Compiegne, France — [3]Max-Planck-Institute for Dynamics and Self-Organization, Goettingen, Germany — [4]Physikalisches Institut, Albert-Ludwigs-Universitaet Freiburg, Freiburg, Germany

A new class of pattern forming systems is identified and investigated: anisotropic systems that are spatially inhomogeneous along the direction perpendicular to the preferred one. By studying the generic amplitude equation and a model equation, we show that branched stripe patterns emerge, which for a given parameter set are stable within a band of different wavenumbers and different numbers of branching points (defects). Moreover, the branched patterns and unbranched ones (defect-free stripes) coexist over a finite parameter range. We propose two systems where this generic scenario can be found experimentally, surface wrinkling on elastic substrates and electroconvection in nematic liquid crystals, and relate them to the findings from the amplitude equation.

B. Kaoui, A. Guckenberger, A. Krekhov, F. Ziebert, W. Zimmermann, New J. Phys. 17, 103015 (2015); B. A. Glatz, M. Tebbe, B. Kaoui, R. Aichele, C. Kuttner, A. E. Schedl, H.-W. Schmidt, W. Zimmermann, A. Fery, Soft Matter 11, 3332 (2015)

DY 50: Glasses

Time: Thursday 9:30–13:00 Location: H48

Invited Talk DY 50.1 Thu 9:30 H48

A new look at atomic tunneling systems in glasses containing isotopes with nuclear quadrupol moments — •Andreas Reiser — Kirchhoff Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg, Germany

The physical properties of disordered materials at low temperatures are governed by atomic or molecular tunneling systems. The standard tunneling model explains many properties such as thermal conductivity and heat capacity well. In dynamic experiments for example dielectric susceptibility measurements or polarization echo experiments clear deviations from the standard tunneling model are observed. In particular, the strong influence of nuclear moments inherent in tunneling atoms was proven experimentally recently. We will discuss the mechanism that leads to the interplay of nuclear moments and atomic tunneling systems and will show that at ultra low temperatures a new type of relaxation process enabled by nuclear moments is present. Contrary to previous assumptions this process governs the energy relaxation of the tunneling systems in the limit of lowest temperatures rather than the one phonon process.

DY 50.2 Thu 10:00 H48

Theoretical investigation of mechanism and statistical properties of a model two-dimension silica glass. — •Projesh Kumar Roy[1] and Andreas Heuer[2] — [1]Graduate school of chemistry, Institute of physical chemistry , Correnstrasse 28/30, D-48149, Muenster — [2]Institute of physical chemistry , Correnstrasse 28/30, D-48149, Muenster

The discovery of 2D silica glass [1] [2] has offered a realistic description of random network theory of silica glass structure; debated for over 80 years[3]. This extremely thin material consists of two layers of silica and exhibits 2D properties in all phases. In the glass phase, the silica network shows a log-normal ring distribution with a typical microstructure or triplet distribution. For simulations two different models based on a Soft - core Yukawa potential[4] and a Stillinger Weber type multi-body potential, have been employed with a binary mixture of silicon and oxygen type particles. After energy minimization, the defect free structures were identified and their ring statistics were compared with the experiment. Going beyond the experiment, the observations can be related to the underlying local energies. Furthermore, two major mechanisms turn out to be responsible for creating various random networks. On this basis a new Monte-Carlo algorithm is proposed for generating random networks of defect free 2D silica.

[1] Heyde M., Shaikhutdinov S., Freund H.-J., Chem. Phys. Lett. 550, 1 (2012). [2] Huang P. Y. et al, Nano Lett. 12, 1081 (2012). [3] Zachariasen W.H., J. Am. Chem. Soc. 54, 3841 (1932). [4] Mendez-Maldonado G.A., et al., J. Chem. Phys. 137, 054711 (2012).

DY 50.3 Thu 10:15 H48

Relevance of Nuclear Quadrupoles to the Low Temperature Dielectric Properties of Glasses — •Annina Luck, Benedikt Frey, Wiebke Scholz, Guido Homann, Anne Zeissner, Nils Hauff, Philipp Wesp, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The standard tunneling model based on two level systems describes many properties of solids at low temperatures. Over the years the measurements of dielectric and acoustic properties have, however, shown significant deviations from predictions made by this model. Despite enormous efforts these deviations are yet unexplained.

One aspect which is missing in the prediction of low frequency dielectric properties by the tunneling model is the relevance of nuclear spins, which has been proven to be important in dielectric polarization echo experiments at 1 GHz. Despite of this, modelling the consequences of this effect on the low frequency dielectric and acoustic susceptibility has proven difficult.

In order to experimentally investigate the role of nuclear quadrupoles

in the dielectric susceptibility we have investigated multiple glass samples containing elements with different quadrupole moments in a wide frequency range spanning from Hz to GHz.
We have found clear indications for a novel nuclear spin driven two level system relaxation process at very low temperatures.

DY 50.4 Thu 10:30 H48

Glass transition and stable glass formation of carbon tetrachloride — •Yeong Zen Chua[1], Michael Tylinski[2], Mark D. Ediger[2], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Rostock 18051 Germany — [2]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706 USA

There have been attempts to find correlations between the ability to form stable glasses and general characteristic of the materials. It was argued that asymmetric molecules, which allow anisotropic packing on the surface during deposition, are a prerequisite for stable glass formation. This leads to the question whether symmetric molecules can form stable glasses. Carbon tetrachloride (CCl_4) is an ideal molecule to verify this hypothesis, since the molecule is pseudo spherical with no orientation. On the other side, the formation of stable glasses is thought to be mediated by a highly mobile surface layer. So it might be expected that CCl_4, as a small and simple organic molecule, has enhanced mobile surface layer and thus increases its ability to form stable glasses. These conflicting factors lead to our investigation of CCl_4 glasses produced by physical vapor deposition with *insitu* AC chip nanocalorimetry. Kinetically stable glasses have been observed to form at substrate temperature around 0.8 T_g, consistent with previous work on stable glass formers. The isothermal transformation of the as-deposited glasses into supercooled liquid state gave further evidence to support the stable glass formation, thus disproving molecular asymmetry as a prerequisite. The glass transition temperature is determined as T_g = (78±2) K, which is different from previously reported values.

DY 50.5 Thu 10:45 H48

Influence of MCM-41 on the dynamical and phase behaviors of aqueous mixtures — •Matthias Sattig and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

The dynamics of aqueous mixtures in bulk and confinement is a topic of great interest. Two model systems, which exhibit rather different behavior upon varring water concentration are propylene glycol- and propylene glycol monomethyl ether-mixtures. This was attributed to the different ability of both alcohols to form hydrogen bonds in neat systems and in aqueous mixtures. The formation of H-bond networks can be altered by geometrical confinement, whose surface interacts with the guest molecules and provides spatially restriction. Here we provide temperature dependent deuteron-NMR data of heavy water in mixture with PG, PGME or di-PGME confined in mesoporous MCM-41 in a broad dynamic range. We examin the rotational autocorrelation using stimulated echo experiments and spin-lattice-relaxation. The latter exhibits a typical minimum in its relaxation time T_1, below which several relaxation processes could be identified in the different mixtures, supporting the idea of a phase separation in confinement, that was proposed in QENS [1] and dielectric [2] investigations. We compare our results with the dynamics of water [3] and glycerol confined in the same material to discuss similarities and differences relating to the influence of confinement on the dynamics of neat and mixed systems.
[1] Swenson et al., JCP, 141, 214501, 2014 [2] Elamin et al., PCCP, 17, 12978, 2015 [3] Sattig et al., JCPL, 5, 174 - 178 , 2014

DY 50.6 Thu 11:00 H48

Spatio-temporal Correlations of Glass-forming Systems in Terms of Coupled Energy Landscapes — •Carsten Schroer[1,2] and Andreas Heuer[1,2] — [1]Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

The concept of the potential energy landscape is an effective tool for the physical description of supercooled liquids in the vicinity of the glass-transition. In this framework, typically small elementary systems are studied for which a strong correlation between its thermodynamic state and its dynamics can be found[1]. The transfer of these insights to macroscopic systems can be achieved by regarding the larger system as a superposition of elementary systems. The observed finite-size effects of the structural relaxation time contain important information about the coupling between these subsystems[2].

In this talk we discuss the impact of this coupling mechanism on the occurrence of spatio-temporal correlations, measured by four-point correlation functions. The results obtained by our model are compared with numerical data obtained by molecular dynamics simulations. We demonstrate that this model, based on the energy landscape of the small system plus the coupling, is sufficient to describe complex behavior of glass-formers.
[1] A. Heuer, *J. Phys.: Condens. Matter* **20**, 37 (2008).
[2] C. Rehwald and A. Heuer, *Phys. Rev. E* **86**, 051504 (2012).

DY 50.7 Thu 11:15 H48

Colloidal monodisperse hard ellipsoids — •Patrick Pfleiderer[1], Stefan Schütter[2], Nicolai Sänger[2], Matthias Klein[2], and Andreas Zumbusch[2] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Department of Chemistry, University of Konstanz, 78457 Konstanz, Germany

The hard sphere system has been generating hundreds of publications per year for the past decades. The focus of attention has recently been shifted towards anisotropic particles, as rotational degrees of freedom have been identified as key for progress in statistical mechanics models and engineering alike. One prominent puzzle is the violation of Stokes-Einstein(-Debye) relations near the glass transition.

The next obvious simple system besides spheres is the hard ellipsoid system. It lends itself to theoretical descriptions and simulations. While an experimental technique to prepare colloidal poly(methyl methacrylate) (PMMA) ellipsoids exists since the 1990s, little progress has been made towards an establishment anywhere near the 'fruit fly' hard spheres. This is due to the difficulties in endowing several desired properties simultaneously to the system: mass-density and refractive-index matching, hard-core interactions, long-term stability etc. We present the first 3D hard ellipsoid system which meets all these goals, fluorescently labeled with a unique core-shell structure [1], polydispersity as low as 3%, and study the interplay of rotational and translational degrees of freedom approaching the colloidal glass transition.
[1] M.K. Klein, N. Saenger, S. Schuetter, P. Pfleiderer, and A. Zumbusch, Langmuir 30, 12457 (2014).

15 min. break

DY 50.8 Thu 11:45 H48

Electron bombardment induced cation transport in an ion conducting glass — •Anneli Hein, Jan Wiemer, and Karl-Michael Weitzel — Fachbereich Chemie, Philipps-Universität Marburg

The bombardment induced ion transport (BIIT) technique has been developed for measuring ionic conductivities and activation energies for ion hopping. The original version is based on attaching a cation beam to the sample (cation-BIIT) inducing the transport of such cations towards a grounded backside electrode. In the current work the BIIT technique is extended to electron bombardment (e- - BIIT). Here a low energy electron beam has been attached to a mixed sodium and potassium conducting borosilicate glass mounted on a single grounded backside electrode. Attachment of the electrons to the surface induces cation transport towards this surface. In the first part of the experiment current-voltage curves have been measured. The specific conductivities as well as the activation energy for ion hopping derived agree with cation-BIIT data. In the second part of the experiment we have performed a long term electron bombardment of the glass sample at -25 eV. Ex situ - after the bombardment - the sample has been analyzed by time-of-flight secondary ion mass spectrometry (ToF-SIMS). The depth profiles obtained from the ToF-SIMS analysis clearly demonstrate that sodium has been neutralized at the front side of the glass sample due to the recombination of electrons with sodium ions. Reduction of the less noble potassium ions appears to be suppressed. The electrochemical implications of this observation will be discussed.

DY 50.9 Thu 12:00 H48

Residual stresses in glass forming systems — •Gaurav Prakash Shrivastav[1], Pinaki Chaudhuri[2], and Jürgen Horbach[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]The institute of Mathematical Sciences, Chennai, India

When a sheared glass is allowed to relax, stress does not decay to zero but tends towards a finite value. How the resulting residual stress is spatially distributed in the system is only poorly understood, especially in the case of a sheared system with shear bands. Also, the effect of different shear rates, with which the initial glass is deformed, and the effect of the amount of strain present in the initial deformed

glass on the residual stress distribution are open issues.

In the present work, we study, using molecular dynamics simulations, relaxation of stresses in a sheared model glass former. We first deform a binary glass forming Lennard-Jones mixture by shearing it with a constant strain rate. Then, we switch of the shear in different regimes of the stress-strain curve and allow the system to relax. We find that the amount of residual stress in the system depends on the initial strain before the shear cessation. By looking at the spatially resolved mean square displacement of particles, we find that the residual stress remains localized in regions where the shear band has been present before. We also find that the deformed glass has higher Poisson's ratio than the undeformed glass, consistent with previous observations.

References

[1] I Binkowski, G. P. Shrivastav, J. Horbach, S. V. Divinski, G. Wilde arXiv:1506.03031 (2015).

DY 50.10 Thu 12:15 H48

Nonlinear Microrheology of Supercooled Liquids in Terms of an Effective Temperature — •Carsten Schroer[1,2] and Andreas Heuer[1,2] — [1]Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Wilhelm-Klemm-Straße 10, 48149 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 this talk, we show that, for strong forces, the thermodynamic state and the local kinetics of the system is altered by the external force in a similar way as an increase of the (bath) temperatures. This behavior gives rise to the definition of an *effective temperature* that turns out to be characterized by a single force and temperature-independent parameter only, even for bath temperature below the computer glass transition. Combining these observations enables us to derive scaling relations for the nonlinear mobility and the diffusive properties of the tracer particle that are tested with our numerical data [3].

[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] C. F. E. Schroer, A. Heuer, *J. Chem. Phys.* (accepted) (2015).

DY 50.11 Thu 12:30 H48

Nonlinear Microrheology of Supercooled Liquids in Terms of an Effective Temperature — •Carsten Schroer[1,2] and Andreas Heuer[1,2] — [1]Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Wilhelm-Klemm-Straße 10, 48149 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.

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[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] C. F. E. Schroer, A. Heuer, *J. Chem. Phys.* (accepted) (2015).

DY 50.12 Thu 12:45 H48

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 very low temperature ($T = 0.01$) as well as above T_g. We also performed shear reversal simulations.

In previous work on unsheared systems it was shown, that most of the physical properties of macroscopic systems are already encoded in small systems. We can show that finite size effects have only limited influence on major observables of the sheared system at $N = 130$.

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) and metabasins (MB) from the trajectories. The IS have zero strain and are therefore comparable to the unsheared system.

From the resulting statistical data we gain a microscopic understanding of macrorheological phenomena like the initial stress overshoot as well as shear thinning in the plastic flow regime from a potential energy landscape perspective.

DY 51: Delay and feedback Dynamics

Time: Thursday 10:00–11:15 Location: H47

DY 51.1 Thu 10:00 H47

Dynamical systems with time-varying delay: Dissipative and more dissipative systems — •David Müller, Andreas Otto, and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Dynamical systems with time-varying delay arise in many fields such as biology, chemistry, economy, engineering and physics.

We identify two different classes of systems with time-varying delay, whereby the the classification depends only on the characteristics of the delay. Systems with *conservative* delay can be transformed to systems with constant delay. Consequently, they exhibit the same type of dynamics. Systems with *dissipative* delay can not be transformed to systems with constant delay and the related dynamics differs from the dynamics of systems with constant delay. In typical models the delay is given by a parameter family. The systems show both types of delays and in general the delay type depends in a fractal manner on the delay parameters.

The difference in the dynamics of the delay classes becomes clear by the analysis of the evolution of small volumes on finite-dimensional subspaces of the infinite-dimensional state space of the delay system. For constant and conservative delays the system is dissipative. Hence, conservative time-varying delays "conserve" the well-known scaling behavior of the mean relaxation rate of the volume evolution corresponding to constant delays, which leads to the known logarithmic scaling of the Lyapunov spectrum. Dissipative delays lead to an additional contribution to the relaxation rate and change the scaling behavior.

DY 51.2 Thu 10:15 H47

Quantum coherent time-delayed feedback control of squeezing — •Manuel Kraft[1], Sven M. Hein[1], Judith Lehnert[2], Eckehard Schöll[2], Stephen Hughes[3], Alexander Carmele[1], and Andreas Knorr[1] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Dynamik und Kontrolle, Hardenbergstr. 36, 10623 Berlin, Germany — [3]Department of Physics, Engineering Physics and Astronomy, Queen's University, Kingston, Ontario, Canada, K7L 3N6

Quantum coherent control schemes are measurement-free methods to control open quantum systems. In contrast to measurement-based schemes the control signals are fully quantum coherent and therefore do not introduce measurement induced noise into the system. We concentrate on the specific situation of a Pyragas-type control scheme where instantaneous and time-delayed signals are fed back directly into the quantum dynamics of the observable. In this talk we present how time-delayed quantum coherent self-feedback control [1, 2] can enhance the squeezing in the output fields of an externally pumped cavity containing a second order nonlinear crystal. This is of particu-

lar importance for phase and amplitude noise reduction.
[1] Carmele *et al.* Phys. Rev. Lett. **110**, 013601 (2013)
[2] Schulze *et al.* Phys. Rev. A **89**, 041801 (2014)

DY 51.3 Thu 10:30 H47

Harmonic Oscillator & PID: Precise and Fast Control of Microfluidic Transport — •Claus Fütterer — Biophysical Tools GmbH/Forschung, 04317 Leipzig, Germany

Microfluidic flow control presents a challenge as most methods rely on volume displacement (syringe pump, peristaltic pump). However, the application of pneumatic flow control simplified significantly the task and presents today the state-of-the-art (Fütterer et al., Injection and Flow Control in Microchannels, Lab Chip 4, 351, 2004).

By symmetrisation we could strongly improve the state-of-the-art. We describe the improvements, outline the mathematical model and present measurements. The new approach allows us to apply linear response theory to our control method, which permits total optimization only limited by causality and technical conditions as finite temperature, dead volume and medium properties. It turned out that the equations can be related to the inhomogeneous harmonic oscillator which alleviates the interpretation of the parameters and helps to understand the dynamics significantly. Stability and noise of the stationary as well as the simplest time dependent solutions are further topics of interest.

The presented model can be generalized to numerous other out-of-equilibrium systems involving control of transport of quantities obeying conservation laws.

DY 51.4 Thu 10:45 H47

The Hill-Floquet method for the analysis of periodic solutions in time-delay systems — •Andreas Otto and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

The Hill-Floquet method for the calculation of Floquet multipliers for periodic systems is introduced. The stability of an equilibrium can be analyzed via the characteristic equation. According to Floquet theory, the perturbations around a periodic solution can be decomposed into a periodic and an exponential part. The Fourier expansion of the periodic terms leads to an infinite dimensional characteristic equation, which is known as central equation in solid state physics, multi-frequency approach in engineering or Hill's infinite determinant method.

Based on this method a general transformation from the original finite dimensional periodic system to an infinite dimensional time-invariant system is presented, the so-called Hill-Floquet transformation. The transformation can be also used for the transformation of delay differential equations (DDEs) with periodic coefficients to time-invariant DDEs. As a result, a large variety of established methods for autonomous DDEs are made available for the analysis of periodic DDEs. In this talk, the Hill-Floquet method is combined with a Chebyshev collocation method for the numerical stability analysis of periodic solutions of nonlinear DDEs.

DY 51.5 Thu 11:00 H47

Semi-Analytic Treatment of Phase Noise in Oscillatory Systems under Time-Delayed Feedback Control — •Lina Jaurigue, Benjamin Lingnau, and Kathy Lüdge — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623Berlin, Germany

We study the effect of delayed coherent optical feedback on the phase noise in oscillatory systems. We derive a semi-analytical method [1] which gives further physical insight into the feedback dependence of the phase noise, and due to greatly reduced computation times allows for the investigation over greater parameter domains. We apply the method to passively-mode-locked semiconductor lasers to calculate the optical pulse timing jitter, showing an excellent agreement with numerical simulations as well as with experimental results. We derive an analytic expression for the timing jitter, which predicts a monotonic decrease in the timing jitter for resonant feedback of increasing delay lengths, scaling approximately as $1/\tau$ with increasing feedback delay time τ. This trend is not related to an increased stability of the system but to the increase in the history of the solutions, which results in the influence of the noise being reduced and the pulse positions being correlated over longer times.

[1] L. Jaurigue, A. Pimenov, D. Rachinskii, E. Schöll, K. Lüdge, and A. Vladimirov, Phys. Rev. A **92**, 053807 (2015)

DY 52: Extreme events

Time: Thursday 11:30–12:45 Location: H47

DY 52.1 Thu 11:30 H47

Branched Flow in Anisotropic Media — Henri Degueldre[1], Jakob Metzger[2], and •Ragnar Fleischmann[1] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation (MPIDS), 37077 Göttingen, Deutschland — [2]Rockefeller University, New York, NY 10065, USA

In many natural and technological systems, waves are weakly scattered by a complex medium that often is best described as random. Due to its internal structure, however, the randomness exhibits spatial correlations. If these correlations persist on scales longer or comparable to the wavelength, even tiny fluctuations in the medium will focus the waves into branches, leading to strong fluctuations in the wave intensity in a large variety of physical systems extending form the propagation of electrons in semiconductors to the focusing of tsunami waves. This phenomenon of *branched flow* generically leads to heavy tailed intensity distributions and extreme wave events. So far the theory of branched flows only described homogeneous, isotropic random media, however, many real systems show a pronounced anisotropy in their structure. For example, the geological processes that generate the ocean floor topography that scatters tsunami waves tend to be highly anisotropic. We present recent results on the theory of branched flows in anisotropic random media and especially show that the focusing has a strong, non-trivial angle dependence.

DY 52.2 Thu 11:45 H47

Study of large deviation probability for correlated Gaussian stochastic processes, motivated by a climate science issue — •Mozhdeh Massah and Holger Kantz — Max Planck Institute for Physics of Complex Systems, Dresden, Germany

As we have one and only one earth and no replicas, climate characteristics are usually computed as time averages from a single time series. For understanding climate variability, it is essential to understand how close a single time average will typically be to an ensemble average. To answer this question, we study large deviation probabilities (LDP) of stochastic processes and characterize them by their dependence on the time window. In contrast to iid variables for which there exists an analytic expression for the rate function, the correlated variables such as auto-regressive (short memory) and auto-regressive fractionally integrated moving average (long memory) processes, have not an analytic LDP. We study LDP for these processes, in order to see how correlation affects this probability in comparison to iid data. At last, we study the LDP for a series of standardized tree ring widths in Nevada (U.S) and compare it to the LDPs for stochastic processes that we have studied.

DY 52.3 Thu 12:00 H47

Event coincidence analysis for quantifying statistical interrelationships between event time series — Jonathan F. Donges[1,2], Carl-Friedrich Schleussner[1,3], Jonatan F. Siegmund[1,4], and •Reik V. Donner[1] — [1]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [2]Stockholm Resilience Centre, Stockholm, Sweden — [3]Climate Analytics, Berlin, Germany — [4]University of Potsdam, Germany

Despite its relevance and wide applicability for interdisciplinary research, the statistical analysis of interrelations between event time series has received relatively little attention in the literature so far. Here, we introduce the concept of event coincidence analysis (ECA) as a novel framework for quantifying the strength, directionality and time lag of statistical interrelationships between event series. ECA allows to formulate and test null hypotheses on the origin of the observed interrelationships including tests based on Poisson processes or, more generally, stochastic point processes with a prescribed inter-event time distribution. As an illustrative example, we apply ECA to country-level observational data on flood events and epidemic outbreaks, pro-

viding robust statistical evidence for corresponding relationships since the 1950s.

DY 52.4 Thu 12:15 H47

Capturing rogue waves by multi-point statistics — Ali Hadjihosseini[1], Matthias Waechter[1], Norbert Hoffmann[2], and •Joachim Peinke[1,3] — [1]ForWind - Center for Wind Energy Research, Institute of Physics, University of Oldenburg, 26111 Oldenburg, Germany — [2]Hamburg University of Technology, 21073 Hamburg, Germany — [3]Fraunhofer Institute for Wind Energy and Energy System Technology, 26129 Oldenburg, Germany

As an example for complex systems with extreme events we investigate ocean wave states exhibiting rogue waves. Mapping the complexity of multi-point data onto the statistics of hierarchically ordered height increments for different time scales, we can show that the wave data can be described by a stochastic cascade process with Markov properties, which is given by a Fokker-Planck equation. Conditional probabilities as well as the Fokker-Planck equation itself can be estimated directly from the available observational data. With this stochastic description surrogate data sets can in turn be generated allowing to work out statistical features of the complex sea state in general and extreme rogue wave events in particular. The results also open up new perspectives for forecasting the occurrence probability of extreme rogue wave events, and even for forecasting the occurrence of individual rogue waves based on precursory dynamics.

DY 52.5 Thu 12:30 H47

Harmful algal blooms as extreme events: Connectivity patterns in a coastal ecosystem — •Stephan Bialonski — Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany

Harmful algal blooms (HABs) are extreme events that can cause large-scale marine mortality incidents and affect human health and economy. Since HABs are observed to become more frequent and intense due to climate change, a better understanding of the mechanisms leading to their occurrence is highly desirable and may inform the development of mitigation and prevention strategies. We study the occurrence of HABs in the Southern California Bight, an area for which such events are well documented. Our cross-correlation analyses of HAB monitoring data and our Lagrangian particle simulations support the hypothesis that transport pathways, in addition to local environmental conditions, decisively influence the spatiotemporal sequence of occurrences of such extreme events in the study area. The observed connectivity patterns can be interpreted as a temporal directed network in which different regions (nodes) are temporarily connected via ocean flows (links). We speculate that deeper insights into the complex interaction between hydrodynamics and population dynamics will pave the way for methods with increased power to predict harmful algal blooms.

DY 53: Anomalous Diffusion in Complex Environments (joint session BP/CPP/DY)

Time: Thursday 15:00–17:45 Location: H15

Invited Talk DY 53.1 Thu 15:00 H15

Phenomenology of Collective Chemotaxis in Artificial and Living Active Matter — •Ramin Golestanian — University of Oxford

The non-equilibrium dynamics of active particles that send and receive chemical signals could lead to enhanced and/or anomalous diffusion, as well as spontaneous formation of interesting structures and patterns due to the long-range nature of the interactions. We examine theoretically the consequences of this interaction, and present some results that exemplify the type of emergent properties that could result from them, including: spontaneous formation of small stable clusters or "molecules" that can exhibit functionality that depends on geometry, collective chemotaxis in a solution of catalytically active colloids that could lead to cluster formation, aster condensation, and spontaneous oscillations, swarming - in the form of a comet - of light-induced thermally active colloids with negative Soret coefficient due to a shadowing interaction, and collective behaviour of a colony of cells that divide and interact chemotactically.

Invited Talk DY 53.2 Thu 15:30 H15

First-passage times of Markovian and non Markovian random walks in confinement — •raphael Voituriez — CNRS/ Université Pierre et Marie Curie, Paris, France

The first-passage time is a key quantity for evaluating the kinetics of various processes, and in particular chemical reactions involving "small" numbers of particles. A striking example is given by gene transcription, where specific proteins search for target sequences on DNA. I will present asymptotic results which enable the evaluation of the distribution of the first-passage time to a target site for a wide range of random processes in confined domains, and show how these results can be extended to non Markovian processes.

Invited Talk DY 53.3 Thu 16:00 H15

Cytoskeleton organization as an optimized, spatially inhomogeneous intermittent search strategy — •Heiko Rieger, Yannick Schröder, and Karsten Schwarz — Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

The efficiency of intracellular transport of cargo from specific source to target locations is strongly dependent upon molecular motor assisted motion along cytoskeleton filaments, microtubules and actin. Radial transport along microtubules and lateral transport along the filaments of the actin cortex underneath the cell membrane are characteristic for cells with a centrosome. Here we show that this specific filament organization for ballistic transport in conjunction with intermittent diffusion realizes a spatially inhomogeneous intermittent search strategy that is in general optimal for small thicknesses oft he actin cortex. We prove optimality in terms of mean first passage times for three different, frequently encountered intracellular transport tasks: 1) the narrow escape problem (e.g. transport of cargo to a synapse or other specific region of the cell membrane), 2) reaction kinetics enhancement (e.g. binding of two mobile reaction partners within the cell), 3) the reaction-escape problem (e.g. release of cargo at a synapse after intracellular vesicle pairing). Since homogeneous search strategies could only be realized by completely filling the search volume with randomly oriented cytoskeleton filaments, our results indicate that living cells realize optimal search strategies for various intracellular transport problems *economically* through a spatial cytoskeleton organization that involves only small amounts of randomly oriented actin filaments.

15 min break

Invited Talk DY 53.4 Thu 16:45 H15

Ergodicity violation and ageing in living biological cells — •Ralf Metzler — Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

In 1905 Einstein formulated the laws of diffusion, and in 1908 Perrin published his Nobel-prize winning studies determining Avogadro's number from diffusion measurements. With similar, more refined techniques the diffusion behaviour in complex systems such as the motion of tracer particles in living biological cells is nowadays measured with high precision. Often the diffusion turns out to deviate from Einstein's laws.

This talk will discuss the basic mechanisms leading to anomalous diffusion as well as point out the physical and biological consequences, for instance, in gene regulation or cargo transport in cells. In particular the unconventional behaviour of non-ergodic, ageing systems will be discussed. Concrete examples include the motion of submicron and nanoprobes in biological cells, uncrowded and crowded lipid membranes, as well as interacting many particle systems.

Invited Talk DY 53.5 Thu 17:15 H15

Anomalous diffusion within cells — Sarah Klein[1,2], •Cecile Appert-Rolland[1], and Ludger Santen[2] — [1]Laboratory of Theoretical Physics, CNRS, Univ. Paris-Sud, Bat 210, 91405 Orsay, France — [2]Fachrichtung Theoretische Physik, Univ. des Saarlandes D-66123 Saarbrücken, Germany

Within cells, various objects (vesicles, organelles,...) need to be transported. Some processive molecular motors get attached to these ob-

jects (or cargos) to form a complex that will have a stochastic motion along a network of microtubules. Intriguingly, there is some evidence that this motion results from a tug-of-war between teams of motors that pull in opposite directions.

A stochastic model for cargo-motors complex allows us to study the properties of the resulting motion along a single microtubule. We find some anomalous diffusion, both subdiffusive or superdiffusive depending on the timescale. Interestingly, such anomalous diffusion has indeed been observed experimentally. I will discuss the importance of fluctuations in the dynamics, and present some hypotheses why nature chose such a transport process to carry cargos through the crowded interior of cells.

[Klein, Appert-Rolland, Santen, EPL 107 (2014) 18004,
Eur. Phys. J. Special Topics 223 (2014) 3215,
EPL 111 (2015) 68005]

DY 54: Focus Session: Many-Body Interference and Quantum Statistical Physics (joint session DY/TT)

Fascinating experimental progress in controlling and monitoring quantum many-body systems has triggered broad activities to better understand quantum coherent many-body phenomena, in particular from the perspective of dynamics and many-particle interference in Fock space. In this focus session, both in experimental and theory talks, light is shed on many-particle interference phenomena, for bosonic and fermionic (massive) particles as well as for photons, and their implications for modern quantum statistical physics. [Organizers: Klaus Richter (Universität Regensburg) and Andreas Buchleitner (Universität Freiburg; Chairperson DPG-Section SAMOP)]

Time: Thursday 15:00–17:45 Location: H20

Invited Talk DY 54.1 Thu 15:00 H20

Between Localization and Ergodicity in Quantum Systems — •Boris Altshuler — Columbia University, New York

Strictly speaking the laws of the conventional Statistical Physics, in particular the Equipartition Postulate, apply only in the presence of a thermostat. For a long time this restriction did not look crucial for realistic systems. Recently there appeared two classes of quantum many-body systems with the coupling to the outside world that is (or is hoped to be) negligible: (1) cold quantum gases and (2) systems of qubits, which enjoy a continuous progress in their disentanglement from the environment. To describe such systems properly one should revisit the very foundations of the Statistical Mechanics. The first step in this direction was the development of the concept of Many-Body Localization (MBL) [1]: the states of a many-body system can be localized in the Hilbert space resembling the celebrated Anderson Localization of single particle states in a random potential. Moreover, one-particle localization of the eigenfunctions of the Anderson tight-binding model (on-site disorder) on regular random graphs (RRG) strongly resembles a generic MBL. MBL implies that the state of the system decoupled from the thermostat depends on the initial conditions: the time averaging does not result in equipartition distribution, the entropy never reaches its thermodynamic value i.e. the ergodicity is violated. Variations of e.g. temperature can delocalize many body states. However, the recovery of the equipartition is not likely to follow the delocalization immediately: numerical analysis of the RRG problem suggests that the extended states are multi-fractal at any finite disorder [2]. Moreover, regular (no disorder!) Josephson junction arrays (JJA) under the conditions that are feasible to implement and control experimentally demonstrate both MBL and non-ergodic behavior [3].

[1] D. Basko, I. Aleiner, and B. Altshuler, Ann. Phys. 321, 1126 (2006). [2] A. De Luca, B.L. Altshuler, V.E. Kravtsov, & A. Scardicchio, PRL 113, 046806, (2014) [3] M. Pino, B.L. Altshuler and L.B. Ioffe, arXiv:1501.03853, PNAS to be published.

Invited Talk DY 54.2 Thu 15:30 H20

Canonical description of short-range interacting few-body quantum systems — •Quirin Hummel, Benjamin Geiger, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

The theoretical study of quantum few-body systems poses a fundamental challenge since the absence of a large number of particles makes the usually simplifying description within the grand canonical formalism invalid. We analytically address the fundamental interplay between indistinguishability, interactions and many-body interference in bosonic and fermionic systems with strictly fixed total particle number; quantum statistics is treated exactly and interparticle forces are described non-perturbatively. We perform calculations for thermodynamic and spectral quantities by expanding the canonical partition function in terms of Ursell operators in the short-time approximation where the discreteness of many-body spectra is neglected. This approach is specially suitable for the few-body case as it generates thermodynamic and spectral properties in terms of a finite set of permutation and interaction events thus overcoming the inappropriate use of virial expansions.

For 1D systems with short-range interactions we present analytical expressions applicable to both integrable prototypical systems such as the Lieb-Liniger and Gaudin-Yang models as well as realistic non-integrable models with harmonic confinement.

Invited Talk DY 54.3 Thu 16:00 H20

One, Two, Three, Many: Manipulating Quantum Systems One Atom at a Time — •Selim Jochim — Physikalisches Institut, Universität Heidelberg, Germany

Experiments with ultracold gases have been extremely successful in studying many body systems, such as Bose Einstein condensates or fermionic superfluids. These are deep in the regime of statistical physics, where adding or removing an individual particle does not matter. For a few-body system this can be dramatically different. This is apparent for example in nuclear physics, where adding a single neutron to a magic nucleus dramatically changes its properties. In our work we deterministically prepare generic model systems containing up to ten ultracold fermionic atoms with tunable short range interaction. In our bottom-up approach, we have started the exploration of such few-body systems with a two-particle system that can be described with an analytic theory. Adding more particles one by one we enter a regime in which an exact theoretical description of the system is exceedingly difficult, until the particle number becomes large enough such that many-body theories provide an adequate approximation.

Our vision is to use our deterministically prepared tunable few-body systems as microscopic building blocks to assemble model systems that might help to gain insight into complex many-body systems.

15 min. break

Invited Talk DY 54.4 Thu 16:45 H20

Statistical Signatures of Many-Particle Interference — •Mattia Walschaers — Physikalisches Institut, Albert-Ludwigs-Universitat Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany — Instituut voor Theoretische Fysica, University of Leuven, Celestijnenlaan 200D, B-3001 Heverlee, Belgium

The complexity of a quantum system drastically increases with the number of its constituents, which gives rise to several difficulties, often associated with the interactions between particles. Nevertheless, already the indistinguishability of particles alone can lead to dynamical interference effects which go well beyond mere quantum statistics, even in the absence of interactions. Recently, these many-particle interferences became the centrepiece of the debate on boson sampling, connecting them to quantum simulation. As a core message, it was explicitly stressed that such interference patterns are computationally intractable. As a consequence, we are confronted with apparent difficulties for the certification of many-particle interferometers. However, from a complex systems perspective, the intractability of the determin-

istic behaviour of a physical system is common place, and motivates a statistical treatment. In this contribution, we present statistical signatures of different types of many-particle interference by studying correlation functions combined with techniques from random matrix theory [1]. We also show how these signatures are altered by varying the degree of indistinguishability of the particles.

[1] M. Walschaers, J. Kuipers, J.-D. Urbina, K. Mayer, M. C. Tichy, K. Richter, and A. Buchleitner, arXiv:1410.8547 (2014).

Invited Talk DY 54.5 Thu 17:15 H20

Boson sampling with integrated quantum photonics — •Fabio Sciarrino — Dipartimento Sapienza, Università di Roma, Roma, Italy

Boson sampling is a computational task strongly believed to be hard for classical computers, but efficiently solvable by orchestrated bosonic interference in a specialized quantum computer. Current experimental schemes, however, are still insufficient for a convincing demonstration of the advantage of quantum over classical computation. A new variation of this task, scattershot boson sampling, leads to an exponential increase in speed of the quantum device, using a larger number of photon sources based on parametric down-conversion. This is achieved by having multiple heralded single photons being sent, shot by shot, into different random input ports of the interferometer. We report the first scattershot boson sampling experiments, where six different photon-pair sources are coupled to integrated photonic circuits. We use recently proposed statistical tools to analyze our experimental data, providing strong evidence that our photonic quantum simulator works as expected. This approach represents an important leap toward a convincing experimental demonstration of the quantum computational supremacy.

DY 55: Polymer Dynamics and Rheology (joint session CPP/DY, organized by CPP)

Time: Thursday 15:00–18:30 Location: H40

DY 55.1 Thu 15:00 H40

Iso-flux tension propagation theory of driven polymer translocation through a nano-pore — •Jalal Sarabadani[1], Tapio Ala-Nissila[2], and Timo Ikonen[3] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Department of Applied Physics, Aalto University, Espoo, Finland — [3]VTT Technical Research Centre of Finland Ltd., Espoo, Finland

We investigate the dynamics of pore-driven polymer translocation mainly by using analytical model and also by molecular dynamics (MD) simulations [1]. By using the tension propagation theory within the constant flux approximation an explicit equation of motion for the tension front is derived. This equation leads us to a scaling relation for the average translocation time, τ, which captures the asymptotic result $\tau \sim N_0^{1+\nu}$. Here, N_0 is the chain length and ν is the Flory exponent. Moreover, we derive the leading correction-to-scaling term to τ which is a finite chain length correction term ($\sim N_0$) due to the effective pore friction. Then by incorporating the fluctuations in the initial configuration of the polymer into the model in addition to thermal noise, the model not only reproduces previously known results but also considerably improves the estimates of the monomer waiting time distribution and the time evolution of the translocation coordinate $s(t)$, showing excellent agreement with MD simulations. We also discuss the effect of a flickering pore and an oscillating external driving force on the translocation time using the new model [2]. [1] J. Sarabadani, T. Ikonen and T. Ala-Nissila, J. Chem. Phys. (141), 214907 (2014). [2] J. Sarabadani, T. Ikonen and T. Ala-Nissila, J. Chem. Phys. (143), 074905 (2015).

DY 55.2 Thu 15:15 H40

Polymer translocation through nanopores: An unbiased perspective on free energy landscapes and essential dynamics — Evangelos Tzaras, Florian Weik, Christian Holm, and •Jens Smiatek — Institut für Computerphysik, Universität Stuttgart, D-70569 Stuttgart, Germany

We studied the translocation of uncharged polymers through thin nanopores by coarse-grained Molecular Dynamics simulations in combination with a forward flux sampling approach. Our results for short and intermediate chain lengths reveal that the translocation behavior is mostly governed by the transition probabilities of single monomers. Specific configurational changes of the polymer or chain tension effects are minor important. We propose an analytic approach for the free energy landscapes which is in good agreement with the simulation results. The outcomes of an essential dynamics analysis verify that only a small number of eigenvectors is substantial for a reliable description of the polymer motion. A comparison with polymers in dilute bulk solution indicates the presence of quasi-equilibrium states which are important for the validity of the underlying free energy landscapes.

DY 55.3 Thu 15:30 H40

The Origin of Strong Slip Of Polymer Melts on Structured Surfaces: A Molecular Approach. — •Mischa Klos[1], Laurent Joly[2], Sebastian Backes[1], and Karin Jacobs[1] — [1]Saarland University, Dept. of Experimental Physics, D-66041 Saarbruecken — [2]Univ Lyon 1, Inst Lumiere Mat, 43 Blvd 11 Novembre 1918, F-69622 Villeurbanne

Flow dynamics at the solid/liquid interface gain more importance when it comes to small scales. In special systems, a liquid can reach a finite velocity at the boundary to the solid. Our experiments probe this phenomenon via the dewetting of thin polymer films on hydrophobic substrates [1]. As hydrophobic coatings we use thin amorphous polymers films or different types of ordered self-assembled silane monolayers on silicon substrates. On silane surfaces, polystyrene (PS) of low molecular weight exhibit slip lengths up to micrometers [2]. On AF1600, no significant slip is observed. Scattering studies indicate an interfacial layer at the interface depending on the structure of the substrate [3]. Simulations where able to refine the molecular idea of the used SAMs [4]. However, strong slip is reduced if PMMA or polyvinylpyridine (PVP) are used instead of PS. MD-Simulations of our systems allow detailed insights into the dynamics of the polymer melt. [1] O. Bäumchen, et.al., J. Phys. Condens. Matter 24 325102 (2012) [2] R. Fetzer, et. Al., Europhys Lett. 75 638 (2006) [3] P. Gutfreund, et. al., Phys. Rev. E 87 012306 (2013) [4] J.M. Castillo Sanchez, et.al., Langmuir 31, 2630 (2015)

DY 55.4 Thu 15:45 H40

Contact Kinetics in Fractal Macromolecules — •Maxim Dolgushev[1], Thomas Guérin[2], Alexander Blumen[1], Olivier Bénichou[3], and Raphaël Voituriez[3] — [1]Physikalisches Institut, Universität Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany — [2]Université de Bordeaux and CNRS, Laboratoire Ondes et Matière d'Aquitaine (LOMA), UMR 5798, 33400 Talence, France — [3]Laboratoire de Physique Théorique de la Matière Condensée, CNRS/UPMC, 4 Place Jussieu, 75005 Paris, France

We investigate the effect of the complex connectivity of macromolecules on the contact kinetics by focusing on the case of fractal macromolecules [1]. In our theoretical description, the non-Markovian feature of monomer motion, arising from the interactions with the other monomers, is captured by accounting for the non-equilibrium conformations of the macromolecule at the very instant of first contact. This analysis reveals a scaling relation for the Mean First Contact Time as a function of the equilibrium distance between the reactive monomers and of the spectral dimension of the macromolecule, which is independent on the microscopic details of the macromolecules. We show that the non-Markovian effects increase for the structures with higher degree of hyperbranching, for which the conformations at first contact are getting much more different from equilibrium looping conformations. Our theoretical predictions are in excellent agreement with numerical stochastic simulations.

[1] M. Dolgushev, T. Guérin, A. Blumen, O. Bénichou, and R. Voituriez, Phys. Rev. Lett. 115, 208301 (2015).

DY 55.5 Thu 16:00 H40

Branch Point Motion in Asymmetric Star Polymers Investigated by Molecular Dynamics Simulations — •Stefan Holler[1,2], Angel Moreno[2], Michaela Zamponi[1], and Dieter Richter[1] — [1]Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Centro de Fisica de Materiales, 20018 San Sebastian, Spain

Large-scale molecular dynamics simulations of three-arm asymmetric

star polymers have been performed to study the motion of the branch point and the so-called hopping parameter p^2 that characterizes the effective friction associated to the short side arm. The simulated star polymer systems consist of a large backbone (10 or 16 entanglements) and a central short unentangled side arm.

This work expands the investigation by Bacova et al. [1] in similar stars with entangled side arms. Surprisingly, the frictional contribution of the unentangled side arms on the motion of the linear backbone is much larger than assumed by theory. The value of p^2 can be calculated from the simulation data using general assumptions that hold true for all versions of hierarchical relaxation models. The most consistent description of the simulation results suggests that p^2 is not a constant but depends on architecture and molecular weight, and that hopping occurs in the bare, undilated tube.

[1] Bacova et al., Macromolecules 47 (2014) 3362

DY 55.6 Thu 16:15 H40

Disentanglement of Two Overlapping Polymer Chains: Contacts vs. Knots — •Diddo Diddens, Nam-Kyung Lee, Sergei Obukhov, Jörg Baschnagel, and Albert Johner — Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, 23 Rue du Loess, 67034 Strasbourg Cedex 2, France

The role of topological constraints is one of the remaining challenges in polymer physics. While it is evident that the non-crossability heavily affects the motion of long polymer chains in dense solutions and melts, these constraints are usually neglected in theoretical descriptions of the polymer dynamics in dilute solutions. However, the situation becomes less clear in the limit of long chains and/or rather dense polymer coils (e. g. close to the Θ-point), since even for a single chain, distinct segments are more likely to be intertwined or knotted.

To address this issue, we present a comprehensive study comprising MC and MD simulations as well as analytical calculations, and investigate the relevance of non-crossing constraints for two polymer chains brought into initial overlap. In particular, we join two long polymers by a labile bond, and focus on their separation directly after the cleavage of this bond. We demonstrate that the average time for this process strongly correlates with the number of monomeric contacts between the two strands. Moreover, in case of highly entangled or knotted starting configurations, the segregation time is several orders of magnitude larger than expected for a purely diffusive process, thus clearly highlighting the importance of topological constraints. Finally, we also give a brief account on the role of hydrodynamics.

15 min. break

DY 55.7 Thu 16:45 H40

Static and dynamic properties of polymer melts: equilibrium and non-equilibrium molecular dynamics studies — •Hsiao-Ping Hsu and Kurt Kremer — Max Planck Institute for Polymer Research

We present a detailed study of the static and dynamic behavior of semiflexible polymer chains in a melt starting from the previously obtained fully equilibrated high molecular weight polymer melts by a hierarchical strategy. For semiflexible chains in a melt, we see that results of the mean square internal distance, the probability distributions of the end-to-end distance, and the chain structure factor are all described very well by the theoretical predictions for ideal chains to some extent. We examine the motion of monomers in polymer melts by molecular dynamic (MD) simulations using the ESPResSo++ package. The scaling predictions of the mean square displacement of monomers based on the Rouse model, and the reptation theory are verified, and the related characteristic relaxation time scales are determined. We also check the topological structures of polymer chains through the primitive path analysis (PPA), and give the evidence that the entanglement length determined through PPA in the standard expression of the plateau modules is consistent with the value obtained from stresses using the Green-Kubo relation. Finally, the non-linear viscoelastic properties of deformed polymer melts after a step uniaxial elongation and the conformational changes of chains during the relaxation process are investigated through a non-equilibrium MD study. We acknowledge the cooperation of G. Zhang, T. Stuehn, and K. Ch. Daoulas.

DY 55.8 Thu 17:00 H40

Knots as Topological Order Parameter for Semiflexible Polymers — •Martin Marenz and Wolfhad Janke — Institut für theoretische Physik, Leipzig, Germany

We used a combination of the multicanonical Monte Carlo algorithm and the replica-exchange method to investigate the phase diagram of a semiflexible polymer in dependence of the polymer stiffness. We found a novel phase in the phase diagram which is best described by the knot type of the polymer conformation. Almost all conformations in these phases have the same knot type after applying a procedure which connects the termini of the polymer. Therefore, they are thermodynamically stable and considerable different from the knots found in the swollen and globular phase of flexible polymers. We also showed that a derivative of the Alexander polynomial is a well suited order parameter to distinguish the *knotted* phases. Moreover, the transitions into the knotted conformations exhibit a phase coexistence, but happen at an almost constant mean total energy, hence we observed no latent heat.

DY 55.9 Thu 17:15 H40

Packing Length Dependence of Chain Dynamics in Polymer Melts near the Unentangled-Entangled Crossover — •Herwin Jerome Unidad[1], Michaela Zamponi[1], Oxana Ivanova[1], Lutz Willner[2], Wim Pyckhout-Hintzen[2], Andreas Wischnewski[2], Dieter Richter[2], and Lewis J Fetters[3] — [1]JCNS, Outstation at MLZ, Forschungszentrum Juelich, Garching, Germany — [2]JCNS-1/ICS-1, Forschungszentrum Juelich, Juelich, Germany — [3]Department of Chemical and Biological Engineering, Cornell University, Ithaca, New York

Recently, we showed that the ratio between the critical molecular weight (Mc) and the entanglement molecular weight (Me) does not have the universal value of 2 for all polymer melts but rather shows a subtle dependence on the so-called packing length (p). All three parameters are important in describing the rheology and chain dynamics of polymer melts. With this, the packing length seems to be an important length scale for describing the non-universality of chain dynamics. To clarify this role, we performed neutron spin echo experiments on two polymer series with various molecular weights and different packing lengths. We obtained a good description of the measured intermediate scattering function using the Rouse model by suppressing long-wavelength internal modes. We then examine how this mode suppression could proceed as a function of both the chain length and the packing length. These findings are explained in the framework of earlier ideas on entanglement formation.

DY 55.10 Thu 17:30 H40

Disentanglement of polymers under shear — Maciej Kawecki[1], Philipp Gutfreund[2], Franz Adlmann[1], Stephane Longeville[3], Alain Lapp[3], Piotr Zolnieczuk[4], Peter Falus[2], and •Max Wolff[1] — [1]Department for Physics and Astronomy, Uppsala University, Sweden — [2]Institut Laue-Langevin, Grenoble, France — [3]Institut Leon Brillouin, Scala, France — [4]Oak Ridge National Laboratory, Oak Ridge, USA

Neutron Spin Echo spectroscopy provides unique insight into molecular and sub-molecular dynamics in soft matter. In polymer physics a stress plateau is observed for increasing shear rate, which might be explained by an entanglement-disentanglement transition and change the dynamics of the chains drastically. Neutron Spin Echo provides information about entanglement length and degree by probing the local dynamics of the polymer chains. Combining shear experiments and neutron spin echo is challenging since, first the beam polarisation has to be preserved during scattering and second, Doppler scattered neutrons may cause inelastic scattering. We demonstrate that a high beam polarisation can be preserved and present SANS data revealing shear-induced conformational changes in highly entangled polymers as well as Spin Echo measurements indicating an disentanglement transition under shear.

DY 55.11 Thu 17:45 H40

Extensional and shear rheology as a powerful tool for characterisation of physical networks in polymer nanocomposites — •Milan Kracalik — Johannes Kepler University Linz, Institute of Polymer Science, Altenberger Str. 69, 4040 Linz, Austria

Polymer nanocomposites are an interesting class of materials, in particular in the field of light weight construction. With increasing knowledge about proper processing protocol and resulting nanocomposite structure and property profile, respectively, it is possible to utilize polymer nanocomposites in many applications like automotive or aerospace industry. During material development procedure, rheological investigation possesses crucial information about material structure/performance already in the processing stage. Therefore, right compilation and interpretation of rheological measurements can sig-

nificantly speed up the developing procedure. In this contribution, selected polymer nanocomposites have been characterized by both extensional as well as shear rheology. Using novel evaluation of oscillatory shear flow data, it was possible to correlate data of shear rheometry with those of elongational rheometry and, consequently, to obtain complex rheological information about different physical networks of nanopartikel in polymer matrix.

DY 55.12 Thu 18:00 H40

Co-non-solvency of smart polymers: Physical concepts and computer simulations — •Debashish Mukherji and Kurt Kremer — Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Smart polymers are a modern class of soft materials that show drastic changes in their physical properties by a slight change in external stimuli. One such phenomenon is known as co-non-solvency. Co-non-solvency occurs when a polymer is added to a mixture of two (perfectly) miscible and competing good solvents. As a result, the same polymer collapses into a globule within intermediate mixing ratios. More interestingly, polymer collapses when the solvent quality remains good or even gets increasingly better by the addition of the better cosolvent [1]. This puzzling phenomenon, where the solvent quality is completely decoupled from the polymer conformation, is driven by strong local preferential adsorption of better cosolvent with the polymer [1,2]. Because a polymer collapses in good solvent, the depletion forces, that are responsible for poor solvent collapse, do not play any role in describing co-non-solvency [3]. Furthermore, it will be presented that this phenomenon can be understood within a universal (generic) concept. Therefore, a broad range of polymers is expected to exhibit co-non-solvency and the specific chemical details do not play any role in understanding these complex conformational behaviors [4].

[1] D. Mukherji and K. Kremer, Macromolecules (2013). [2] D. Mukherji, et al. Nat. Commun. (2014). [3] T. E. de Oliviera, et al., Soft Matter (2015). [4] D. Mukherji, et al, JCP (2015).

DY 55.13 Thu 18:15 H40

PNIPAM dynamics in water-methanol mixtures — •Konstantinos N. Raftopoulos[1], Konstantinos Kyriakos[1], Olaf Holderer[2], Oxana Ivanova[2], Michael Ohl[3], Peter Müller-Buschbaum[1], and Christine Papadakis[1] — [1]Physik-Department, Technische Universität München, Garching, Germany — [2]JCNS at Outstation MLZ, Garching, Germany — [3]JCNS at Outstation Oak Ridge, Tennessee, USA

In aqueous solutions, at low temperatures, the hydrophilic groups of Poly(N-isopropylacrylamide) form H-bonds with the water molecules and the polymer dissolves. Above the cloud point, the chain dehydrates and phase-separates. Although the polymer dissolves well in methanol too, the cloud point in water-methanol mixtures decreases considerably with respect to that in aqueous solutions. The phenomenon is termed cononsolvency. The physical mechanisms behind the process are still not clear and even less is known about the dynamics. Aiming to shed some light in this question, we followed the segmental dynamics of the polymer in water-methanol mixtures by neutron spin echo spectroscopy. The experiments were performed 2 and 5 K below the cloud points, in a temperature region where the solution is in θ-conditions. Methanol slows down the segmental dynamics of the polymer, but there is no evidence for a change of the mobility mechanism. The deceleration is more pronounced at higher polymer concentrations.

DY 56: Wetting, Nano- and Microfluidics II (joint session CPP/DY)

Time: Thursday 15:00–16:45 Location: H42

DY 56.1 Thu 15:00 H42

How water advances on superhydrophobic surfaces — •Frank Schellenberger, Noemí Encinas, Doris Vollmer, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

To a certain degree, it is possible to control the macroscopic wetting properties of a surface by its nano- and microstructure. In particular, super liquid-repellant-surfaces have received interest due to their many potential applications, such as anti-fouling for for example. Super liquid-repellency can be achieved by nano- and microstructuring a low energy surface in a way, that the structure can entrap air underneath the liquid. The common criteria for super liquid-repellency are a high apparent advancing contact angle and a low contact angle hysteresis.

For a better understanding of how a drop advances and recedes on such a structured surface, we imaged the motion of a water drop on a superhydrophobic array of micropillars by laser scanning confocal microscopy (LSCM). With LSCM, we imaged an advancing water front on a superhydrophobic surface at a resolution of 1 *m. The results give a qualitatively new picture of how water advances on the microscopic scale. We demonstrate that in contrast to traditional goniometer measurements, the advancing contact angle is close to 180° or even higher.

In contrast, the apparent receding contact angle is determined by the strength of pinning. We propose that the apparent receding contact angle should be used for characterizing super liquid-repellent surfaces.

DY 56.2 Thu 15:15 H42

Traction forces of water droplets on super-hydrophobic surfaces — •Martin Tress, Alexander Saal, Frank Schellenberger, and Noemí Encinas — Max Planck Institute for Polymer Research, Mainz

Surfaces with super-hydrophobic properties play an important role in both nature and science. Thereby, the artificial surfaces typically try to copy the characteristic features of their natural pendants. That is in general, a hydrophobic surface chemistry combined with a structured topography. To investigate the particular impact of these characteristics model surfaces with pillars of varying size, arrangement and surface coating have been employed [1]. While many studies used rigid pillars to maintain a well-defined topography, in the present work flexible pillars are focused. When imaged with a Laser Scanning Confocal Microscope, these flexible pillars act as cantilevers to detect traction forces of a drop resting on their top. By that, the distribution of the forces in parallel to the surface along the contact line is recorded. Especially the traction forces of the receding contact line of an evaporating drop will be illuminated.

[1] P. Papadopoulos et al. PNAS 9 (2013) 3254

DY 56.3 Thu 15:30 H42

Bioinspired Nanofur as Superhydrophobic Transparent Coatings and Translucent Films for Optical Applications — •Felix Vüllers, Maryna Kavalenka, Matthias Worgull, and Hendrik Hölscher — Institute of Microstructure Technology, Karlsruhe Institute of Technology, 76344 Karslruhe, Germany

A combination of high optical transmission with self-cleaning, water-repellency and anti-icing is of high interest for various optical applications and boosted interest to transparent superhydrophobic surfaces. We demonstrate a highly scalable hot-pulling method to produce flexible superhydrophobic thin nanofur films made from polycarbonate, which can be used both as a transparent coating and a translucent film. The surface of thin nanofur films is covered with densely packed high aspect ratio nano- and microhairs which are fabricated using heated sandblasted steel plates, making complex and expensive mold fabrication unnecessary. The films exhibit high water contact angles (>170°), low sliding angles (<4°) and self-cleaning abilities. Through index matching the thin nanofur coating's reflection in the visible regime is reduced to less than 4%. The translucent film's transmission is more than 85% with high forward scattering. Applied to OLEDs these optical properties lead to an efficiency increase of more than 10%. By combining these exceptional optical properties with the water-repellent and self-cleaning properties of the thin nanofur film, the films are beneficial for further optical devices. In addition plasma treatment changes the film wettability to underwater superoleophobic enabling the use of thin nanofur films as underwater oil-repelling coatings.

DY 56.4 Thu 15:45 H42

Dynamics of Drop Condensation on Lubricant-Impregnated Surfaces — •Tadashi Kajiya[1], Frank Schellenberger[1], Periklis Papadopoulos[2], Doris Vollmer[1], and Hans-Jürgen Butt[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]University of Ioannina, Dept. of Physics, 45110 Ioannina, Greece

We explored the dynamics of water drops condensing on a lubricant-impregnated surface, i.e., micropillar arrays infused with a ionic liquid. Growing drops were imaged in 3D using a laser scanning confocal microscope equipped with a temperature and humidity control. On a lubricant-impregnated hydrophobic micropillar array, different stages of condensation can be discriminated: - Nucleation on a lubricant surface. - Regular alignement between micropillars and formation of a three-phase contact line on a bottom of the substrate. - Deformation and bridging by coalescence, leading to a detachment of the drops from the bottom substrate to pillars*top faces. However, on a lubricant-impregnated hydrophilic micropillar array, the condensed water covers the micropillars by dewetting the lubricant. As a result, the surface loses its slippery property. Our results provide fundamental concepts how these solid/liquid hybrid surfaces can be applied for facile removal of condensed water.

DY 56.5 Thu 16:00 H42

Connecting and disconnecting nematic disclination lines in microfluidic channels — •Hakam Agha and Christian Bahr — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

The controlled creation of a disclination line in nematic liquid crystal (NLC) spanning along the microfluidic channel as a result of imposed anchoring conditions on the four confining channel walls has proven to be a novel and successful approach to guided transport of microfluidic cargo, with the disclination line serving as a soft rail [1]. In this study, we report on a method to connect and disconnect disclination lines using the interplay between anchoring, flow, and electric field. We design the anchoring conditions in a way that the formation of the disclination is suppressed in one or several short sections of the channel. The application of an external electric field across the channel and perpendicular to the NLC flow can overcome the imposed anchoring conditions and allows the disclination line to span across the forbidden regions, establishing a continuous disclination along the complete channel. Thus, the manipulation of the anchoring conditions combined with the effect of the electric field allows us to interrupt and to reestablish the transport of colloidal particles through the microchannel.

[1] A. Sengupta, C. Bahr, S. Herminghaus, Soft Matter, 2013, 9, 7251.

DY 56.6 Thu 16:15 H42

Lateral Adhesion Forces at Solid-Liquid Interfaces — •Nan Gao, Florian Geyer, Sanghyuk Wooh, Dominik Pilat, Doris Vollmer, Hans-Jürgen Butt, and Rüdiger Berger — Max Planck Institute for Polymer Research, Mainz, Germany

Using a laser deflection system we investigate lateral adhesion forces at solid-liquid interfaces. Our set-up consists of a laser, a deflectable capillary, and a position sensitive detector (PSD). Substrates of TiO2 nanopillars with various spacing distances between the nanopillars are used to regulate surface wettabilities. Drops of liquid resting on the nanopillar substrates have different lateral adhesion forces due to the surface wettabilities. In order to measure the forces at the solid-liquid interfaces, the drops are moved laterally against the substrates using the deflectable capillary. A laser beam incident on the capillary is reflected to the PSD, which instantly generates electric signals according to the lateral adhesion forces. With assistance of optical imaging, we have been able to resolve the drop motion synchronised to the force measurement. Our measurements have demonstrated that the instantaneous lateral adhesion forces at the solid-liquid interfaces are determined by the front and rear contact angles as well as the contact width. The values are in good agreement with theoretical predictions.

DY 56.7 Thu 16:30 H42

Light-driven delivery and release of materials using liquid marbles — •Maxime Paven[1], Hiroyuki Mayama[2], Takafumi Sekido[3], Hans-Jürgen Butt[1], Yoshinobu Nakamura[3,4,5], and Syuji Fujii[4] — [1]1Physics at Interfaces MaxPlanck Institute for Polymer Research Ackermannweg 10, D-55128 Mainz, Germany — [2]2Department of Chemistry, Asahikawa Medical University 2-1-1-1 Midorigaoka-Higashi, Asahikawa 078-8510, Japan — [3]3Division of Applied Chemistry, Graduate School of Engineering Osaka Institute of Technology 5-16-1 Omiya, Asahi-ku, Osaka, 535-8585, Japan. — [4]4Department of Applied Chemistry, Faculty of Engineering, Osaka Institute of Technology 5-16-1 Omiya, Asahi-ku, Osaka, 535-8585, Japan. — [5]5Nanomaterials Microdevices Research Center Osaka Institute of Technology 5-16-1 Omiya, Asahi-ku, Osaka 535-8585, Japan.

Remote control of the locomotion of small objects is a challenge in itself and may also allow for the stimuli control of entire systems. Here, we describe how encapsulated liquids, referred to as liquid marbles, can be moved on a water surface with a simple near-infrared (NIR) laser or sunlight. Using light rather than pH or temperature as an external stimulus allows for the control of the position, area, timing, direction and velocity of delivery. Our approach makes it possible to not only transport the materials encapsulated within the liquid marble but also to release them at a specific place and time, as controlled by external stimuli. Furthermore, we show that liquid marbles can work as light-driven towing engines to push or pull objects.

DY 57: Focus Session: Turbulence - From Pattern Formation to Stochastic Disorder

Turbulence is the natural state of motion for a fluid flow driven far from equilibrium. Beyond the laminar state, flows can show regular patterns superposed with mild turbulent fluctuations, like convection not too far from onset, or they can be vigorously turbulent in the fully developed turbulent regime. In some settings, regular large-scale patterns even coexist with strong turbulent fluctuations. This variety of states makes turbulence a paradigm of a complex system with a large number of strongly interacting degrees of freedom. With coherent structures on many scales interacting in a complex manner, fully developed turbulence falls in between purely random and pattern-forming systems. This unique combination makes it a challenging research field with connections to non-equilibrium statistical mechanics, pattern formation and stochastic processes. This focus session comprises contributions investigating the spectrum of flow states summarized above and shall review our current understanding of turbulence, its origin as well as its interplay with coherent large-scale patterns. (Organizers: Ronald du Puits, Joachim Peinke, Michael Wilczek)

Time: Thursday 15:00–18:45 Location: H46

Invited Talk DY 57.1 Thu 15:00 H46

The Transition to the Ultimate State in Turbulent Thermal Convection — •Eberhard Bodenschatz — Max Planck Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland

We report measurements of turbulent Rayleigh-Bénard convection in three cylindrical samples with the aspect ratios (diameter/height) $\Gamma = 1.00, 0.50$ and 0.33. All samples had the same diameter $D = 1.1$m, but different heights L. Compressed sulfur hexafluoride gas (SF_6) at pressures up to 19 bars was used as the fluid at the Göttingen Turbulence Facility (see www.EuHIT.org) The measurements were conducted over the Rayleigh-number range $10^{12} \lesssim Ra \lesssim 4 \times 10^{15}$ and for Prandtl numbers Pr near 0.8. In three independent measurements, namely global heat transport, local turbulent Reynolds number, and large scale circulation dynamics, we observed as a function of Rayleigh number a transition over a range of Ra from the classical regime to a regime that can be considered ultimate. Consequences thereof will be discussed and so will be the influence of rotation.

The work was conducted with Guenter Ahlers, Denis Funfschilling, Dennis van Gills, Xiaozhou He, Holger Nobach, and Stephan Weiss.

DY 57.2 Thu 15:30 H46

Percolation model for laminar-turbulent transition of a boundary layer: experimental insight by Particle Image Velocimetry — •Tom Wester, Dominik Traphahn, Pedro G. Lind, Gerd Gülker, and Joachim Peinke — Carl von Ossietzky University, Oldenburg, Germany

The boundary layer's transition from laminar to turbulent is a very complex process, which at present is not fully understood. In order to fully capture this complexity with a very limited number of characteristic stochastic properties, this experimental study aims at describing the phase transition by means of the directed percolation model.
In contrast to the majority of previous studies, the underlying data base is acquired experimentally by high-speed Particle Image Velocimetry. Thus, a boundary layer evolving on a flat plate can be captured in a highly resolved spatio-temporal manner. In this way, sufficient data is provided to determine critical probabilities and critical exponents which describe the transient area between laminar and turbulent boundary layer within the scope of directed percolation. First results from this approach will be presented and compared to theoretical expectations.

DY 57.3 Thu 15:45 H46

Boundary layers in turbulent Rayleigh-Bénard convection — •Ronald du Puits[1] and Christian E. Willert[2] — [1]Institute of Thermodynamics and Fluid Mechanics, Technische Universitaet Ilmenau, POB 100 565, 98684 Ilmenau, Germany — [2]Institute of Propulsion Technology, German Aerospace Center, 51170 Koeln, Germany

The heat transport throughout a fluid layer heated from below and cooled from above is mainly determined by two very thin flow regions adjacent to the hot bottom and the cold top wall. They are referred to as boundary layers. Following a hypothesis of Kraichnan [R. H. Kraichnan. Turbulent Thermal Convection at Arbitrary Prandtl Number. Phys. Fluids 5, 1374-1389 (1962)] it is widely believed nowadays that these boundary layers are of laminar type below a critical threshold in Rayleigh number and that they become turbulent above this limit. We show the results of highly resolved PIV measurements of the near-wall flow field in the large-scale convection facility Barrel of Ilmenau, an experiment which is seven meters in diameter and eight meters in height. Our measurements show that the dynamics of those boundary layers and the formation of coherent structures inside go far beyond a laminar shear layer of Prandtl-Blasius type although the Rayleigh number is considerably below the threshold predicted by Kraichnan.

DY 57.4 Thu 16:00 H46

Multi-PIV Measurements of an Adverse Pressure Gradient Turbulent Boundary Layer — •Christian Willert[1], Christian Kähler[2], Andreas Schröder[3], Julio Soria[4], Michel Stanislas[5], and Jean-Marc Foucaut[5] — [1]Institut für Antriebstechnik, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany — [2]Institut für Strömungsmechanik und Aerodynamik, Universität der Bundeswehr München — [3]Institut für Aerodynamik und Strömungstechnik, DLR, Göttingen, Germany — [4]Monash University, Melbourne, Australia — [5]Laboratoire de Mécanique de Lille, CNRS, Villeneuve d'Ascq, France

We report on a multi-national measurement campaign aimed at providing highly resolved flow field data of a turbulent boundary layer subjected to an adverse pressure gradient (APG). In the case of APGs the structure and dynamics of large scale turbulent flow structures along with their significance on the statistical properties of the flow is not well understood. Hence the fundamental aim was to resolve and characterise the large-scale coherent structures in an APG boundary layer flow. In addition to large-field-of-view PIV measurements using 16 sCMOS cameras along a 3.5m length, stereoscopic PIV measurements were performed at specific locations in order to also resolve the span-wise velocity statistics. Long-distance, high-speed micro-PIV measurements provided near wall statistics at selected locations including the time-resolved wall shear stress. The measurements were performed in the boundary layer wind tunnel of the Laboratoire de Mécanique de Lille (LML) and funded by EuHIT (www.euhit.org).

DY 57.5 Thu 16:15 H46

Microrheology of sphere-shaped and anisometric rod-shaped objects in 2D fluids — Christoph Klopp, •Alexey Eremin, and Ralf Stannarius — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

Flow phenomena in restricted geometries have been intensively studied in the last years with implications to different physical, chemical and biological systems. Those studies usually employ indirect measurements of the inclusion mobilities for the lack of a convenient 2D model system. On the other hand, smectic liquid crystals form freely-suspended fluid films of highly uniform structure and thickness, making them ideal systems for studies of hydrodynamics in two dimensions. We study the mobility of sphere-shaped and rod-shaped inclusions in freely-suspended liquid crystal films. We demonstrate that in thin films, the mobility is primary determined by the coupling of the fluid to the surrounding air, as predicted by the Saffman-Delbrück theory. The effect of particle anisometry appears when the size of the particle is comparable to or larger than the hydrodynamic size of the system (Saffman length).

The authors acknowledge the support by DFG (STA 425-28)

15 min. break

DY 57.6 Thu 16:45 H46

Characterizing multi-scale interaction in turbulence — •Cristian C Lalescu and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization

Turbulence is a true multi-scale phenomenon with a broad range of interacting spatial and temporal scales. It is well known that in a linear system, unique length scales are associated to well-defined time scales, through a dispersion relation. A naive application of the 1941 Kolmogorov theory also yields a simple characteristic time scale for each given length scale. In the case of real turbulence, however, interactions take place between structures with different characteristic sizes and life times, leading to a continuous spectrum of length scales associated to a time scale and vice versa.

In this work, we aim to characterize these turbulent multi-scale interactions quantitatively. To this end, we identify the time scales relevant for structures of a given size, both from an Eulerian and a Lagrangian perspective. By employing filtering techniques in space and time, we compare turbulent velocity fields containing length scales above a given cutoff-scale with time-filtered fields. Varying the filter widths and times yields a precise picture of the various interactions. In a second step, we generalize the analysis to the Lagrangian frame to study the impact of large- and small-scale fluctuations on turbulent particle transport.

DY 57.7 Thu 17:00 H46

Reproducibility of turbulent flows in wind tunnel experiments using different active grids — •Lars Kröger, Joachim Peinke, and Gerd Gülker — ForWind, Center for Wind Energy Research, University of Oldenburg, 26129 Oldenburg, Germany

As wind turbines are mainly working inside the turbulent atmospheric boundary layer, the performance of the turbine and resulting structural loads are strongly influenced by the dominating highly intermittent wind fields. Regarding the chaotic nature of turbulence, reproducible measurements in situ are quite difficult and wind tunnel experiments with reproducible and controllable turbulent inflow conditions are of increasing importance. Here we present an active grid with which customized turbulence can be generated in wind tunnel applications. Experiments have shown that it is already possible to replicate atmospheric like turbulence regarding specific statistical properties as intermittency, turbulence intensity or integral length. In this contribution results from hotwire measurements behind two active grids in two wind tunnels of different dimensions are presented. The aim is to determine which requirements are necessary to reproduce the same downstream turbulence behind the different grids as accurately as possible.

DY 57.8 Thu 17:15 H46

Lagrangian intermittency in an ensemble of Gaussian velocity time series with fluctuating time scales — •Laura Lukassen and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Goettingen

Turbulent velocity fluctuations exhibit intermittency in both, the Lagrangian and Eulerian frame. Here, we focus on the Lagrangian velocity increments whose probability density function shows a transition from a nearly Gaussian shape to highly non-Gaussian shapes for decreasing time lags. This inherent non-Gaussianity poses a challenge for statistical approaches suffering from the closure problem.

Our aim is to derive an analytically tractable model of turbulence which captures the characteristics of turbulence such as intermittency.

We discuss the properties of an ensemble of Gaussian velocity time series in which the characteristic time scales of the ensemble members are drawn from an underlying distribution of those scales. Such an ensemble naturally exhibits non-Gaussian statistics as has been demonstrated, e.g., in the context of multifractal modeling. In order to provide a more general approach, our model is based on the characteristic functional which captures the complete statistical information of the ensemble. As a result, non-trivial statistical information such as joint statistics of increments at various scales or joint statistics of acceleration and increments can be obtained. Based on that, we will discuss the potential of formulating novel closures in the framework of our approach.

DY 57.9 Thu 17:30 H46

Intermittent Inflow Generation in CFD — •Sebastian Ehrich[1], Bernhard Stoevesandt[2], and Joachim Peinke[1,2] — [1]University of Oldenburg, Institute of Physics, ForWind, Germany — [2]Fraunhofer IWES, Oldenburg, Germany

Complex and unsteady interactions between highly turbulent atmospheric inflow and the flow over wind energy converting systems (WECS) are of crucial importance with respect to the loads on the rotor blades. The disturbed inflow leads to a strong variation of the effective inflow angle over the entire rotor blade radius. Unsteady aerodynamic effects are the reason for phase shifts between excitation and resulting loads, but those effects have not been well described by models yet.

The content of this work is the implementation of a stochastic model based on continuous time random walks (CTRW) for wind fields in the CFD Opensource Code OpenFOAM as an inflow condition. The purpose of this project is the correct description and simulation of short scale fluctuations and extreme events described by longitudinal velocity increments. Those are interesting for load and fatigue calculations on wind turbines. Further, different simulation test cases are shown for proper analysis of turbulence characteristics of the model and the effect of filtering in LES compared to DNS simulations. Especially the decay of turbulence and the evolution of the increment probability density functions in space and time are considered.

DY 57.10 Thu 17:45 H46

Quantifying non-locality in fully developed incompressible turbulence — •Dimitar Vlaykov and Michael Wilczek — MPI for Dynamics and Self-Organisation, Goettingen, Germany

The complexity of turbulence flows is deeply rooted in the non-locality of the governing Navier-Stokes equations. The latter can be understood as the formal dependence of even the short-term evolution of a fluid element on the state of the entire system. In incompressible hydrodynamics, the Navier-Stokes equations encode this through the kinematic pressure gradient. The pressure is determined by a Poisson relation sourced by the difference between the squared rate-of-strain and the enstrophy. This links the non-local pressure to the small-scale topology of the flow.

In this presentation we aim at quantifying the nature and the range of the pressure contributions. In particular, we attempt to characterize the neighbourhood, which contains the governing part of the contributions, via a statistical analysis of a sequence of sub-domains of increasing size. Additionally, we consider the link between the small-scale structure topology and the destructive interference between vortices and strain sheets.

DY 57.11 Thu 18:00 H46

Large-scale structures in the temperature field in turbulent Rayleigh-Bénard convection — •Christian Resagk and Christian Kästner — TU Ilmenau, Ilmenau, Deutschland

Large-scale structures in temperature fields in turbulent convection is a less-studied phenomenon in large aspect ratio convection cells. Furthermore, the existence of superstructures in temperature fields is only known from direct numerical simulations and was not experimentally confirmed so far. Against this background we investigated large-scale circulation in water, applied to a Rayleigh-Bénard cell with large aspect ratio Γ=30 and Rayleigh numbers about Ra=10^4-10^6. We introduce temperature field measurements under the given conditions for the first time. Hence the major aim of this work was on the one hand checking the applicability of temperature field measurements and the accessible thermal resolution in turbulent flow by laser induced fluorescence (LIF) and thus the investigation of changing conditions from weak to strong turbulence, may yielding long term stabilization/oscillation of the convective flow. The Rayleigh number was controlled by adjusting the temperature gradient between hot bottom and cold top enclosure of the convection cell about ΔT=0-35 K. The convective flow of heat was monitored by particle imaging velocimetry (PIV) and compared with contact-less temperature field measurements by LIF, based on temperature induced fluorescence intensity variations of Rhodamin B added to the water. Both, PIV and LIF, were measured in 532 nm light sheet irradiation in the horizontal and vertical plane of the convective cell.

DY 57.12 Thu 18:15 H46

Cluster analysis of coherent structures in Rayleigh-Bénard convection — •Oliver Kamps — Center for Nonlinear Science, University of Münster

Turbulence is an ubiquitous physical phenomenon settled somewhere between randomness and order. On the one hand turbulent flows seem to be irregular and chaotic but on the other hand one can observe coherent structures, patterns or superstructures constituting the flow. The identification of these structures and their dynamics is crucial for the understanding of turbulent flows and therefore for applications in science and engineering.

In many cases the coherent structures live only for a certain time span followed by a rapid transition to another state like a different coherent structure. Such a transition can be regarded as an extreme event which is accompanied by strong distortions of observables like heat transport or mixing. In our approach we use clustering based methods [1] in order to identify these non-stationary states, estimate dynamical models for their time evolution and to anticipate extreme events. As example we apply our methods to Rayleigh-Bénard convection showing reversals.

[1] A. Hutt, M. Svensén, F. Kruggel and R. Friedrich, Phys. Rev. E **61** (2000)

DY 57.13 Thu 18:30 H46

Global flow modes in turbulent Rayleigh-Bénard convection — •Robert Kaiser and Ronald du Puits — Institute of Thermodynamics and Fluid Mechanics, Technische Universität Ilmenau, Postfach 10 05 65, Ilmenau 98694, Germany

The modes of the global flow structure inside a Rayleigh-Bénard convection cell are analysed by time resolved local wall heat flux data. The measurements were performed at the heating plate of the large scale convection facility, called the Barrel of Ilmenau, using infrared thermography. The experimental data reveals a fundamental change of the heat transport processes between an aspect ratio 1<G<3, where the large scale vortex splits into two smaller vortices. In 2007 du Puits et al. measured profiles of the velocity and temperature in the boundary layer below the cooling plate at various aspect ratios G in the Barrel of Ilmenau. Between 1.47<G<1.89, the maximum velocity falls down by 20%. Thus, the critical aspect ratio Gc of the change in the modes of the global flow structure was estimated by a linear interpolation at Gc=1.68. We re-evaluated this value by calculating the average life time of the one-vortex-state and the two-vortex-state between 1<G<3. The new Gc=1.65 states more precisely the change in the global flow structure in turbulent Rayleigh-Bénard convection.

DY 58: Networks: From Topology to Dynamics III (joint session DY/BP/SOE)

Time: Thursday 15:30–17:00 Location: H47

DY 58.1 Thu 15:30 H47

Complex Quantum Networks: From Universal Breakdown to Optimal Transport — •Oliver Mülken — Physikalisches Institut, Universität Freiburg, Freiburg, Deutschland

We study the transport efficiency of excitations on complex quantum networks with and without loops. For this we consider sequentially growing networks with different topologies of the sequential subgraphs. This can lead to a universal complete breakdown of transport for tree-like [1] or complete-graph-like [2] sequential subgraphs, while it leads to optimal transport for linear [1] or ring-like [2] sequential subgraphs. The transition to optimal transport for networks with loops can be triggered by systematically reducing the number of loops of complete-graph-like sequential subgraphs in a small-world procedure. These effects are explained on the basis of the spectral properties of the network's Hamiltonian. Our theoretical considerations are supported by numerical Monte-Carlo simulations for complex quantum networks with a scale-free size distribution of sequential subgraphs and a small-world-type transition to optimal transport in the case of loops.

[1] Phys. Rev. Lett. 115, 120602 (2015)
[2] arXiv:1511.00910

DY 58.2 Thu 15:45 H47

Resilience of complex networks — •Baruch Barzel — Bar-Ilan University, Ramat-Gan, Israel

Resilience, a system's ability to adjust its activity to retain its basic functionality under errors, failures and environmental changes, is a defining property of many complex systems. Despite widespread consequences on human health, economy and the environment, events leading to loss of resilience, from economic collapse to mass extinctions in ecological networks, are rarely predictable and often irreversible. These limitations are rooted in a theoretical gap: the current analytical framework of resilience is designed to treat low dimensional models of a few interacting components, and hence it is unsuitable for characterizing multidimensional systems consisting of a large number of components that interact through a complex network.In this talk we will bridge this theoretical gap by introducing a set of analytical tools to identify the natural control and state parameters of a multi-dimensional complex system. This analytical framework allows us to systematically separate the role of the system's dynamics and topology, collapsing the behavior of different networks onto a single universal resilience pattern. Our results unveil the network characteristics that can enhance or diminish resilience, offering avenues to prevent the collapse of environmental, infrastructural or socio-economic systems.

DY 58.3 Thu 16:00 H47

The totally asymmetric inclusion process (TASIP): how network topology determines condensation and transport properties — •Johannes Knebel, Markus F. Weber, Philipp Geiger, and Erwin Frey — Ludwigs-Maximilians-Universität, München, Deutschland

Transport phenomena are often modeled by the hopping of particles on regular lattices or networks. Such models describe, for example, the exclusive movement of molecular motors along microtubules: no two motors may occupy the same site. In our work, we study *inclusion processes* that are the bosonic analogues of the fermionic exclusion processes. In inclusion processes, many particles may occupy a single site and hopping rates depend linearly on the occupation of departure and arrival sites. Particles thus attract other particles to their own site. Condensation occurs when particles collectively cluster in one or in multiple sites, whereas the other sites become depleted.

We showed that inclusion processes on a network describe both the selection of strategies in evolutionary zero-sum games and the condensation of non-interacting bosons into multiple quantum states in driven-dissipative systems. The condensation is captured by the anti-symmetric Lotka-Volterra equation (ALVE), which constitutes a non-linearly coupled dynamical system. We derived an algebraic method to analyze the ALVE and to determine the condensates. Our approach allows for the design of networks that result in condensates with oscillating occupations, and yields insight into the interplay between network topology and transport properties.

DY 58.4 Thu 16:15 H47

Growing Boolean networks together with their attractors — Andrey Sakryukin and •Konstantin Klemm — School of Science and Technology, Nazarbayev University, Astana, Kazakhstan

We present a computational method for finding attractors of Boolean dynamics under asynchronous update. Starting from a single node or small network, it builds up the queried network by iterative node addition. The core idea is the mechanism for restricting Boolean dynamics to a subnetwork. Here a natural restriction rule is defined so that node addition never leads to shrinking of an attractor's state set. This facilitates tracking growth, merging and annihilation of attractors as the network itself is being built up.

Applications to Boolean models of biological regulation as well as metastable states of discrete energy landscapes, e.g. NK model, are discussed. At `http://goo.gl/eRzFoo` the implementation of the method and further material are available for download.

DY 58.5 Thu 16:30 H47

Synchronization of heterogeneous chemical relaxation oscillators — •Jan Frederik Totz[1], Julian Rode[1], Kenneth Showalter[2], and Harald Engel[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]West Virginia University, Morgantown, USA

Recently discovered synchronization patterns, such as chimera states and intertwined cluster synchronization in networks of identical nonlinear oscillators lead to the emergence of new theoretical concepts, most notably an extended master stability function for networks with permutation symmetries [1].

Optically coupled catalytic beads provide a versatile experimental tool to study the emergence of collective synchronization patterns with real oscillators under well-controlled laboratory conditions [2].

One important aspect is the impact of a broad oscillator frequency distribution. Instead of in-phase or cluster synchronization, experiments reveal phase wave synchronization through neighboring permutation symmetry clusters [3].

[1] Kuramoto, Battogtokh. Complex Syst. 4, 380 (2002); Pecora et al. Nat. Commun. 5, 4079 (2014) [2] Tinsley. Nat. Phys. 8, 662 (2012); Taylor et al. PCCP (2015) [3] Totz et al. PRE 92, 022819 (2015)

DY 58.6 Thu 16:45 H47

Biologically implementable attractors in Boolean network models of gene regulation — •David F. Klosik and Stefan Bornholdt — Institut für Theoretische Physik, Universität Bremen

Boolean networks have successfully been used as a modeling approach for gene regulatory networks. It is a well-known fact that in general the attractor landscape can change dramatically when moving from the original parallel deterministic update scheme applied in the first studies to asynchronous or otherwise noisy schemes believed to more plausibly represent the actual processes in the cell. However, the main dynamical features of many biological regulatory networks (e.g., the cell cycle network in yeast) can be captured in a parallel Boolean model, as well, in addition to its own stochastic biochemical implementation within the cell. This leads to the question of when Boolean networks are in fact biologically implementable, keeping certain transients or attractors. We here approach this question with an autonomous Boolean network model with underlying continuous dynamics, that has been proven useful in simulating biochemical stochasticity in regulatory networks[1].

[1] S. Braunewell and S. Bornholdt, Superstability of the yeast cell-cycle dynamics: Ensuring causality in the presence of biochemical stochasticity, J. Theor. Biol. 245 (2007) 638-643.

DY 59: Networks - From Topology to Dynamics IV (Joint Session BP/SOE/DY)

Joint session with SOE and DY organized by BP.

Time: Thursday 16:45–17:45 Location: H43

DY 59.1 Thu 16:45 H43

Fluctuations and transients in the actin cytoskeleton of chemotactic amoeba — •Jose Negrete JR[1,2], Alain Pumir[3], Hsing-Fang Hsu[2], Christian Westendorf[4], Marco Tarantola[2], Carsten Beta[2,5], and Eberhard Bodenschatz[2,6,7] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for Dynamics and Selforganization, Göttingen, Germany — [3]Ecole Normale Supérieure de Lyon, France — [4]University of Graz, Austria — [5]University of Potsdam, Germany — [6]University of Göttingen, Germany — [7]Cornell University, Ithaca, USA

Biological systems with their complex biochemical networks are known to be intrinsically noisy. Here we investigate the oscillatory dynamics in the actin cytoskeleton of chemotactic amoeboid cells. We show that the large phenotypic variability in the polymerization dynamics can be accurately captured by a generic nonlinear oscillator model in the presence of noise. The relative role of the noise is fully determined by a single dimensionless parameter, experimentally measurable, and whose distribution completely characterizes the possible cellular behavior. Also, we perturbed experimentally the oscillatory cytoskeletal dynamics by a short chemoattractant pulse and measured the spatio-temporal response of filamentous actin reporter, LimE, and depolymerization regulators Coronin1 and Aip1. After pulsing, we observed self oscillating cells to relax back to their oscillatory state after a noisy transient. Particularly long transients were observed for cells initially displaying highly correlated oscillations.

DY 59.2 Thu 17:00 H43

Distribution of pair-wise covariances in neuronal networks — •David Dahmen[1], Markus Diesmann[1,2,3], and Moritz Helias[1,3] — [1]Inst. of Neurosc. and Med. (INM-6) and Inst. for Advanced Simulation (IAS-6) and JARA BRAIN Inst. I, Jülich Research Centre, Germany — [2]Dept. of Psychiatry, Psychotherapy and Psychosomatics, Medical Faculty, RWTH Aachen University, Aachen, Germany — [3]Dept. of Physics, Faculty 1, RWTH Aachen University, Germany

Massively parallel recordings of spiking activity in cortical circuits show large variability of covariances across pairs of neurons [Ecker et al., Science (2010)]. In contrast to the low average, the wide distribution of covariances and its relation to the structural variability of connections between neurons is still elusive. Here, we derive the formal relation between the statistics of connections and the statistics of integral pairwise covariances in networks of Ornstein-Uhlenbeck processes that capture the fluctuations in leaky integrate-and-fire and binary networks [Grytskyy et al., Front. Comput. Neurosci. (2013)]. Spin-glass mean-field techniques [Sompolinsky and Zippelius, Phys. Rev. B (1982)] applied to a generating function representing the joint probability distribution of network activity [Chow and Buice, J. Math. Neurosci. (2015)] yield expressions that explain the divergence of mean covariances and their width when the coupling in the linear network approaches a critical value. Using these relations, distributions of correlations provide insights into the properties of the structure and the operational regime of the network. Partly supported by Helmholtz Association: VH-NG-1028 and SMHB; EU Grant 604102 (HBP).

DY 59.3 Thu 17:15 H43

Global stability reveals critical components in the structure of multi-scale neural networks — •Jannis Schuecker[1,4], Maximilian Schmidt[1,4], Sacha J. van Albada[1], Markus Diesmann[1,2,3], and Moritz Helias[1,3] — [1]Inst of Neurosci and Medicine (INM-6) and Inst for Advanced Simulation (IAS-6) and JARA BRAIN Institute I, Jülich Research Centre — [2]Department of Psychiatry, Psychotherapy and Psychosomatics, Medical Faculty, RWTH Aachen University — [3]Department of Physics, Faculty 1, RWTH Aachen University — [4]These authors contributed equally

One of the major challenges of neuroscience is the integration of the available experimental data into a coherent model of the brain. In this endeavor, the exploration of the inevitable uncertainties in anatomical data should be guided by physiological observations. To this end we devise a method based on a mean-field reduction of spiking network dynamics for shaping the phase space of large-scale network models according to fundamental activity constraints, prohibiting quiescence and requiring global stability. In particular, we apply this framework to a multi-area spiking model of macaque visual cortex and obtain plausible layer- and area-specific activity [Schuecker et al. 2015, arXiv:1509.03162] by controlling the location of the separatrix dividing the phase space into realistic low-activity and unrealistic high-activity states. The study systematically identifies modifications to the population-level connectivity within and between areas critical for the stability of the network. Partly supported by Helmholtz association: VH-NG-1028 and SMHB; EU Grant 604102 (HBP).

DY 59.4 Thu 17:30 H43

From Interactions to Topology: A Population Dynamics Approach to Network Formation — •Adrian Fessel and Hans-Günther Döbereiner — Institut für Biophysik, Universität Bremen, Deutschland

We present a mean-field model integrating interactions between populations of nodes to mimic the evolution of transportation networks. Changes in network topology are partitioned in basic events representing, e.g., fusion or growth of network fragments. Local dependencies are reflected by rate constants modifying the frequency of occurence of a given event.
The model presented shows promising results when compared to the percolating network of the slime-mold *Physarum polycephalum* [*Phys. Rev. Lett.* **109**, 078103 (2012)].

DY 60: Interfaces and Thin Films II (joint session CPP/DY, organized by CPP)

Time: Friday 9:30–12:00 Location: H51

DY 60.1 Fri 9:30 H51

Ring polymer chains in confined geometries: Massive field theory approach — •Zoryana Usatenko[1] and Joanna Halun[2] — [1]Institute of Physics, Cracow University of Technology — [2]Faculty of Physics, Mathematics and Computer Science, Cracow University of Technology

The investigation of a dilute solution of phantom ideal and real ring polymer chains with excluded volume interactions in a good solvent confined in a slit geometry of two parallel walls was performed. Taking into account the well known polymer - magnet analogy developed by de Gennes the calculations of the correspondent partition functions, depletion interaction potentials, depletion forces and the forces which exert phantom ideal ring polymer chain on the surfaces were performed in a fixed space dimensions d=3 for two repulsive walls, two inert walls and for the mixed case of one inert and one repulsive wall. Besides, for the case of ring polymer chain with EVI confined in a slit geometry of two parallel repulsive walls calculations were performed up to one-loop order. It was found that the confining of ring polymer chain to a slit geometry of two walls leads to the loss of configurational entropy and to arising of the repulsive force which exerts ring polymer chain on the surfaces. Increasing of the slit size leads to decreasing of the value of the exerted force on the surfaces at the same value of the end-to-end distance.

DY 60.2 Fri 9:45 H51

A theoretical approach to bis-urea molecules that form hydrogen-bonded supramolecular polymers in 2D — •Olga Guskova[1,2] and Jens-Uwe Sommer[1,2,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany — [3]Institute of Theoretical Physics, TU Dresden, Dres-

den, Germany

Supramolecular polymers, i.e. arrays of low-molecular-weight building blocks, usually held together by hydrogen bonding (HB) or other reversible noncovalent interactions. Bis-urea-based molecules with central bis-urea fragment exhibit the highest supramolecular polymerization ability, affording well-defined supramolecular fibers. In this talk, two major points concerning the arrangement and properties of HB bis-urea molecules on surfaces studied by QM/all-atom MD simulations will be addressed: (i) the ordering dynamics on graphite of two bis-urea molecules which differed only by a single cis-double bond in their side groups [1] and (ii) the electronic properties of isolated molecules, HB dimers and bis-urea tapes in adsorbed state on gold surface [2].

[1] R. Shokri, O. Guskova, A. Jamal, K. Jahanshahi, B. Isare, L. Bouteiller, L. Simon, J.-U. Sommer, G. Reiter, J. Phys. Chem. C 119 (39), 22596-22603 (2015).

[2] F. Vonau, R. Shokri, D. Aubel, L. Bouteiller, O. Guskova, J.-U. Sommer, G. Reiter, L. Simon, Nanoscale 6 (4), 8250-8256 (2014).

DY 60.3 Fri 10:00 H51

Towards large area atomically flat n-alkane layers: A real-time study of thermal annealing — •Linus Pithan[1], Eduard Meister[2], Chenyu Jin[3], Anton Zykov[1], Wolfgang Brütting[2], Hans Riegler[3], Andreas Opitz[1], and Stefan Kowarik[1] — [1]Inst. f. Physik, Humboldt Universität zu Berlin — [2]Inst. f. Physik, Universität Augsburg — [3]MPI für Kolloid- und Grenzflächenforschung, Potsdam

Highly anisotropic attachment energies of n-alkanes combined with low surface energies result in their unusual thin films growth and wetting behavior [1]. We analyze the thermal annealing behavior of n-tetratetracontane (TTC, $C_{44}H_{90}$) in detail with the aim to improve smoothness and to increase the lateral size of crystalline islands of polycrystalline TTC films on SiO, a material system also of interest from a device perspective [2]. We use *in situ* x-ray diffraction to find an optimum temperature leading to improved texture and crystallinity while avoiding an irreversible phase transition. Further, we employ real-time optical phase contrast microscopy with sub-nm height resolution [3] to track the diffusion of TTC across monomolecular step edges and show that the lateral island sizes increase by more than one order of magnitude from 0.5 μm to 10 μm. This desirable behavior of 2d-Ostwald ripening and the pronounced smoothing we observe is in stark contrast to many other organic molecular films where annealing leads to dewetting, roughening, and a pronounced 3d morphology.

[1] L. Pithan *et al.*, J. Chem. Phys. 143, 164707 (2015)
[2] M. Kraus *et al.*, J. Appl. Phys. 107, 094503 (2010)
[3] R. Köhler *et al.*, Appl. Phys. Lett. 89, 241906 (2006)

DY 60.4 Fri 10:15 H51

Photo-manipulation of the surface tension anisotropy at a liquid-crystal/ITO-glass interface — Hajnalka Nadasi, •Alexey Eremin, and Ralf Stannarius — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

We report direct measurements of the surface energy anisotropy (anchoring energy) at a glass-nematic liquid crystal interface containing a photo-active azo-dendrimeric surfactant. The photoisomerisation at the surface layer drives an anchoring transition from the homogeneous to the planar sate of the liquid crystal. The anchoring energy is measured using the Frederiksz transition as a function of the intensities of the UV and VIS light and is compared with a theoretical model. We also demonstrate optical manipulation of the nematic director field around microshperes and rods dispersed in the liquid crystal. In case of rod-shaped particles, the photo-driven change of the anchoring energy results in a reversible macroscopic rotation of the particles.

DY 60.5 Fri 10:30 H51

Kinetic Monte Carlo Simulations of Photo-Switchable Molecules Tethered to a Surface — •Raffaele Tavarone[1], Patrick Charbonneau[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Departments of Chemistry and Physics, Duke University, Durham, North Carolina 27708, USA

Photo-switchable molecules can undergo a light-induced *trans-cis* isomerization. They can be used to build functional monolayers with light-controlled macroscopic properties. A recent experiment [1] showed that, in a monolayer densely covered with photo-switchable molecules, the relaxation of the induced birefringence follows a glasslike power-law dynamics. Furthermore, the relaxation can be efficiently fastened by illumination of the sample with circularly polarized light.

We developed a molecular model for the monolayer in which the *trans* and *cis* isomers are modeled as straight and bent needles, respectively. The needles are allowed to overlap and the system dynamics is generated by a kinetic Monte Carlo algorithm. We demonstrate that the glasslike power-law dynamics can be traced back to spatio-temporal correlations in the local structure of the system, *i.e.*, to the formation of dynamical heterogeneities. Also, we find that the different degree of shape anisotropy of the two isomers has a significant effect on the system dynamics: the nearly isotropic *cis* isomers suppress the formation of extended dynamical domains. As a results, the relaxation is faster and follows a simple exponential decay.

[1] Fang, G. J., et al., Nature communications **4**, 1521 (2013).

15 min. break

DY 60.6 Fri 11:00 H51

Modulated structures in complex twist-bend nematic phases in bulk and thin-film geometry. — •Nerea Sebastian, Alexey Eremin, and Ralf Stannarius — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

Twist-bend nematic state (Ntb) has recently been discovered as a complex mesophase intermediate between the cholesteric and a uniform nematic phase. The molecules, being non-chiral, spontaneously form a helical twist-bend structure, where the director is inclined to the helical axis. The phase is believed to be driven by the inversion of the bend elastic constant K3. We report on an elastic behaviour in the vicinity of the nematic-Ntb transition and describe the transition between the Ntb and a modulated smectic phase which exhibits intricate labyrinthine structures of the layer dislocations in freely-suspended films. It also forms fluid cylindrical filaments with large slenderness ratios.

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Properties of a monomolecular water film flowing into a graphene-mica slit pore — •André Schilo, Nikolai Severin, Igor M. Sokolov, and Jürgen P. Rabe — Department of Physics, Humboldt-Universität zu Berlin, Germany

Nanoscopically confined water and water adsorbed at interfaces play an important role in e.g. biology, tribology or nanotechnology. Graphene has recently been demonstrated to replicate the substrate topography with a precision down to single macromolecules. Thus the flexible graphene cover provides the possibility of visualizing a water monolayer confined in a slit pore between graphene and mica. However, the phase of the confined water (solid or fluid) is still debated. Here we report high-resolution scanning force microscopy (SFM) imaging of water monolayers flowing into the slit pore. The initially dry pore gets filled upon raising the ambient humidity. We observed a layer of water wetting the sample in reproducible finger-shaped patterns with a step height of 2.8 Å. The flow kinetics are highly dependent on the rate of humidity change. Keeping the humidity constant at a value above the beginning of the wetting process and below the complete wetting, results in a nearly exponential saturation of the finger growth. A further increase of the humidity reactivates the growth of the fingers, eventually leading to a complete monolayer of water. From this we conclude that the confined water monolayer must be fluid.

DY 60.8 Fri 11:30 H51

A spectroscopic investigation of surface melting of ice — •M.Alejandra Sanchez, Mischa Bonn, and Ellen H.G Backus — Max Planck Polymer Research Institute,Mainz,Germany

In nature, ice is, amongst others, responsible for rock weathering, soil metamorphosis, thunderstorms and the ozone chemistry on stratospheric clouds. It has been generally accepted that from the bulk freezing point down to roughly 240 K, a quasi-liquid-layer is present on ice. However, the nature of this layer has been intensely debated. We study the nature of the interfacial water on well-defined single crystal ice surfaces. The surface sensitive technique sum frequency generation spectroscopy provides the vibrational spectrum of specifically the interfacial molecules. We find a sudden change in the spectrum around 255 K which is assigned to the phase transition from ice/air to ice/quasi-liquid/air. The experimental results are well reproduced by simulations that allow to relate the observed spectral changes to

information on the molecular scale.

DY 60.9 Fri 11:45 H51

Interfacial Melting in Ice/Nanocomposite Materials — •Hailong Li[1], Julian Mars[1,2], Henning Weiss[1], Thomas Buslaps[3], Wiebke Lohstroh[4], and Markus Mezger[1,2] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [3]ESRF-The European Synchrotron, Grenoble, France — [4]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany

The material properties of permafrost strongly depend on the molecular scale structure of the ice/solid interface. Early in 1859, Faraday proposed the existence of a quasi-liquid layer (qll) at ice surfaces. However, the understanding of the interfacial melting of ice and the structure of the qll is still under debate. Layered sheet silicates are ideal model systems to study the interfacial melting of ice in geologically relevant materials. Using x-ray diffraction, we determined the crystalline ice fraction in ice composites with high interface to volume ratio. From the anisotropy of the ice Bragg reflections in textured composite samples we extract the preferred orientation of ice crystals confined between the sheet silicates. Approaching the bulk melting point of ice, we observe a logarithmic growth law of the thickness of the qll. Quasielastic neutron scattering was employed to elucidate the mobility of the qll at hydrophilic and hydrophobic solid-ice interfaces.